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Dimensionality transformation of exciton state in quantum well with asymmetrical barriers

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Abstract. In the conditions of 2D–3D dimensionality transformation of one-particle states, the dependence of exciton binding energy E_{ex} on asymmerical well width h has been theoretically studied. It is shown that the contribution of one-particle continuous spectrum to exciton becomes considerable when the inverse exciton Bohr radius $1/a_B$ turns out to be comparable with the critical for 2D–3D transformation value of in-plane wave vector k_c. The lack of coincidence between electron and hole k_c values leads to the complicated shape of $E_{ex}(h)$ dependence, which has a minimum at intermediate values of h. The minimum value of E_{ex} appears to be less than 3D exciton binding energy.

In quantum wells with asymmetrical in height barriers and different effective masses in structure layers, the localized 2D states exist only within the limited range of in-plane wave vector k. The critical k_c value depends on the well width, barrier height ratio U_2/U_1 and the ratio of effective masses in the confining barriers. The k_c value can be quite small giving rise to some rather interesting effects [1]. One can control k_c value by the external electric and magnetic fields. The 2D–3D transformation of the exciton states in external electric field was experimentally observed in GaAs/AlGaAs quantum well structures [2]. As it was shown in [1], the drastic change of exciton binding energy occurs when the localized state in asymmetrical well still exists but the critical value of k_c becomes comparable to the inverse exciton Bohr radius $1/a_B$. In this case, the exciton state is constructed from the localized states of electron and hole as well as from the states of continuum.

In the conditions of dimensionality transformation the dispersion law becomes essensially non-parabolic for electron (hole) states. The wave functions depend on k, which doesn't allow one to describe exciton states within the usual variational approach [3].

In this paper, we present the method for description of exciton states in systems with complicated valence zone dispersion law [4] caused by heavy–light holes interaction [5]. In this method, the exciton wave function is represented as an expansion in terms of products of electron and hole wave functions with different in-plane motion momenta, taking into account the dependence of one-particle wave functions on k. The additional complication in our case is a necessity to consider the continuum states contribution to exciton state when $k > k_c$.

To simplify computational technique, we accept the following procedure: let us introduce the infinitely high barrier in the region of lower barrier U_2 of the structure on rather large distance L from the right edge of the well. In this case, the continuous spectrum is represented by a set of discrete states with very small distance between appropriate sub-bands. There is the change of wave function localization (from the well region $(0, h)$ to the region $(h, L + h)$) with the variation of wave vector k, instead of 2D–3D transformation. We have to achieve the convergence by varying the parameter L for adequate description

of continuous spectrum. Solving one-particle Schrödinger equations in described structure for different values of k, we obtain the energy spectrum $E_{c,v}^{n,m}(k)$ and the set of appropriate electron and hole wave functions.

Let us consider 1-S exciton state. We represent the exciton wave function as a following linear combination:

$$\Psi_{\text{ex}}(\mathbf{r}_e,\mathbf{r}_h) = \frac{1}{4\pi^2}\sum_{n_e,n_h}\int d\mathbf{k}_h\int d\mathbf{k}_e\, \Phi_{\mathbf{k}_e\mathbf{k}_h}^{n_e n_h}\exp(i(\mathbf{k}_e\rho_e - \mathbf{k}_h\rho_h))\psi_{n_e\mathbf{k}_e}(z_e)\psi_{n_h\mathbf{k}_h}^*(z_h),$$

(1)

where $\Phi_{\mathbf{k}_e\mathbf{k}_h}^{n_e n_h}$ are the Furier-expansion coefficients. It is convenient to use coordinates for center-of-mass motion $(\mathbf{Q},\mathbf{R})$ and relative motion $(\mathbf{k},\rho)$. By multiplying the Schrödinger equation by Ψ_{ex}^* and integrating over $\mathbf{R}$, ρ, z_e, z_h we obtain for the expansion coefficients the following set of coupled integral equations:

$$\left[E_c^{n_e}(\mathbf{k}+\mathbf{Q}/2) - E_v^{n_h}(\mathbf{k}-\mathbf{Q}/2)\right]\Phi_{\mathbf{k}\mathbf{Q}}^{n_e n_h} - C\sum_{n_e',n_h'}\int d\mathbf{k}'\Phi_{\mathbf{k}'\mathbf{Q}}^{n_e' n_h'}\int dz_e\int dz_h$$

$$\frac{\exp(-|\mathbf{k}-\mathbf{k}'||z_e-z_h|)}{|\mathbf{k}-\mathbf{k}'|}\psi_{n_e\mathbf{k}+\mathbf{Q}/2}^*(z_e)\psi_{n_e'\mathbf{k}'+\mathbf{Q}/2}(z_e)\psi_{n_h\mathbf{k}-\mathbf{Q}/2}(z_h)\psi_{n_h'\mathbf{k}'-\mathbf{Q}/2}^*(z_h),\quad(2)$$

where $C = e^2/2\pi\varepsilon$.

The calculations were performed in the assumption that $\mathbf{Q} = 0$ for optically active exciton [ ]. Let us make the values $\mathbf{k},z_e,z_h$ uniformly discrete in the considered regions and represent all the integrals in (2) as appropriate sums. Thus, we obtain a system of linear equations for $\Phi_{\mathbf{k}'}^{n_e' n_h'}$ instead of set of coupled integral equations. Avoiding the point of integrable singularity at $\mathbf{k} = \mathbf{k}'$, we solve the usual eigenvalue problem [ ].

The choice of integration interval for k is rather important in the method described. At the large h values in formation of 3D-exciton the quasi-continuous spectrum states that have equal degree of wave functions localization participate. The dispersion law is parabolic for every subband. One has to choose in (1) rather small integration interval over k ($\Delta k \sim 1/a_B$) and take into account a considerable number of subbands (variational approach) to achieve the convergence.

The situation is the same for the small h values, when the electron localized state is already vanished.

The situation is rather different for intermediate values of h when the binding energy corresponds to that of 2D-exciton. The parameter $1/a_B$ is so large that in a considerable range of h it can exceed the critical value k_c for dimensionality 2D–3D transformation of electron states. In this case the first subband states $E_c^1(\mathbf{k})$ provide the most considerable contribution to the expansion (1). In the conditions of 2D–3D transformation the appropriate wave functions can be considered as a full set of functions necessary for the exciton formation.

The calculations were made for the structure on the basis of GaAs/Al$_x$Ga$_{1-x}$As with aluminium concentration: $x = 0.4$ in the left barrier, $x = 0$ in the well, and $x = 0.06$ in the right barrier. The distance L necessary for continuum simulation was settled as 100 nm and was chosen from the condition of the convergence of results.

The described procedure allows one the consider exciton states in the whole range of structure parameters, i.e., in the bulk GaAs (with large h), bulk AlGaAs ($h = 0$), and the well widths corresponding to 2D–3D transformations of the hole ($h = 1.7$ nm) and electron ($h = 3.8$ nm) states.
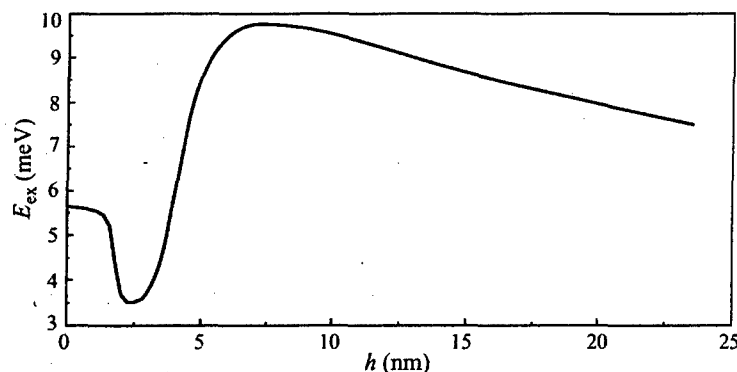
Fig. 1. The dependence of the exciton binding energy E_{ex} on the width h of asymmetrical well.

The dependence of exciton binding energy E_{ex} on the width h of asymmetrical well (obtained by the method described) is represented in Fig. 1. The dependence has a complicated shape with two extrema: minimum $E_{ex} = 3.5$ meV at $h_1 = 2.4$ nm and maximum $E_{ex} = 10$ meV at $h_2 = 7$ nm. The value E_{ex} obtained at $h = 0$ equals to 3D-exciton binding energy in bulk $Al_xGa_{1-x}As$ with aluminium concentration $x = 0.06$. This confirms the correctness of chosen computational technique.

As the well width h increases the conditions of 3D–2D transformation for the hole state are first met. The hole wave function localizes in the well region while the electron remains delocalized. This leads to the minimum of exciton binding energy at $h_1 = 2.4$ nm. It is essential that the minimum value E_{ex} appears to be less than the 3D-exciton binding energy in GaAs. The further increase in h leads to the electron 3D–2D transformation and, consequently, it's localization in the well. As a result, the oscillator strength of electron–hole transition rises, reaching maximum at $h = 7$ nm. The decrease in E_{ex} with the further growth of h is a due to the same reasons as in symmetric wells, i.e., a simultaneous decrease in the localization of electron and hole wave functions.

In Fig. 2 the inverse Bohr radius $1/a_B$ dependence on the well width h is shown (solid curve). The dashed curve represents the h dependence of the critical value of wave vector k_c where the 2D-3D transformation of electron state occurs. The curves intersect at $h = 5$ nm. From this moment the less h is (until the electron state vanishes) the more important role
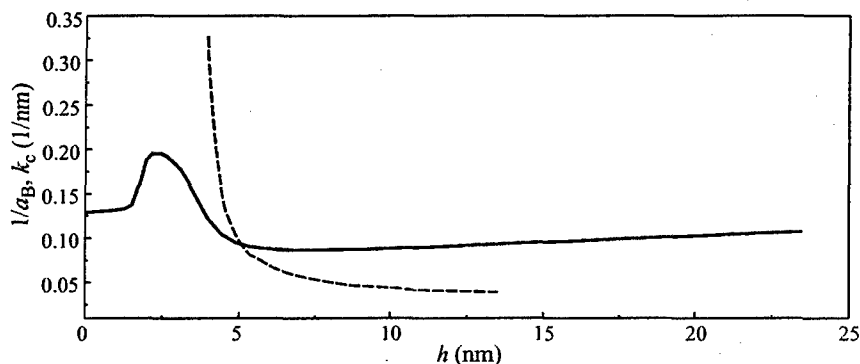

Fig. 2. Inverse Bohr radius $1/a_B$ dependence on the well width h (solid curve). Dashed curve is a similar dependence of the critical value k_c for 2D–3D electron states transformation.

in excition formation play the quasi-continuous states $E_c^1(\mathbf{k})$ $(k > k_c)$. For example, at $h = 4.1$ nm the integration interval in (1) $\Delta k \sim 1/a_B$ is approximately two times greater than k_c. As a result there are the equal contributions of electron localized and continuous spectrum states to exciton. When $h = 3.8$ nm the electron state is almost vanished $(1/a_B \gg k_c)$ and the exciton is formed by localized hole and electron continuum states.

To describe the exciton states the method of fractional dimension was proposed [ ]. In this method, the dimensionality is represented by value $\alpha = 2\sqrt{Ry^*/E_b} + 1$. Let us use this formula to estimate dimensionality in our case. At $h_0 = 5$ nm ($1/a_B$ and k_c crossing) the value $\alpha \sim 2.5$. The decrease of well width from h_0 to ~ 4 leads to α increase up to ~ 3. This illustrates essential influence of 2D–3D electron spectrum transformation on exciton dimensionality [ ].

Acknowledgements

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