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A variational method for the description of the pressure-induced $\Gamma - X$ mixing in GaAs-based quantum wells

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Abstract

The mixing between Γ and X conduction band valleys in GaAs–$Ga_{1-x}Al_xAs$ quantum wells is investigated along the lines of a variational model. Trial wavefunctions are depending on a weighting variational parameter that accounts for the mixing by acting as a coefficient in the combination of both uncorrelated Γ and X states in the system. The dependencies of the calculated binding energy of a donor impurity and the correlated electron–hole photoluminescence peak energy upon hydrostatic pressure and quantum well width are presented.
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The study of the $\Gamma - X$ mixing phenomenon in GaAs-based systems has several antecedents in the last years [1,2]. Additionally, there have also been several works that investigate the effects of hydrostatic pressure on the optical and electronic properties in this kind of structures [3,4]. The influence of the $\Gamma - X$ mixing on the donor states in GaAs–AlAs quantum wells [3], as well as the dependence with the hydrostatic pressure of the electron–hole recombination peaks in the photoluminescence (PL) spectrum of single and double GaAs–$Ga_{1-x}Al_xAs$ quantum wells [4] can be mentioned as antecedents. The study of the combined action of the hydrostatic pressure and $\Gamma - X$ mixing on the donor impurity states in quantum wells based on GaAs has been recently reported [5]. In all these works, the model used to incorporate the $\Gamma - X$ mixing into the calculation has been the phenomenological one, put forward in Ref. [1]. The main purpose of this article is to present a variational scheme and, with its help, to obtain results for the PL properties associated to confined exciton states, as well as for the binding energy of a shallow-donor impurity in GaAs–$Ga_{1-x}Al_xAs$ quantum wells.

The uncorrelated states in the conduction band of the GaAs–$Ga_{1-x}Al_xAs$ structures for both the Γ and X minima [$F^{\Gamma}(z)$ and $F^{X}(z)$] are described by means of a two independent bands model. The corresponding 2×2

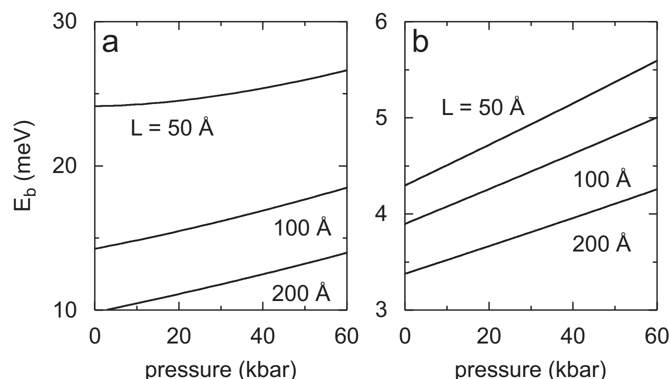

Fig. 1. Pressure dependence of the binding energy of a donor impurity in GaAs–$Ga_{0.7}Al_{0.3}As$ QWs. In (a) the binding energy is mainly described by the Γ-conduction band whereas in (b) by the X-conduction band.

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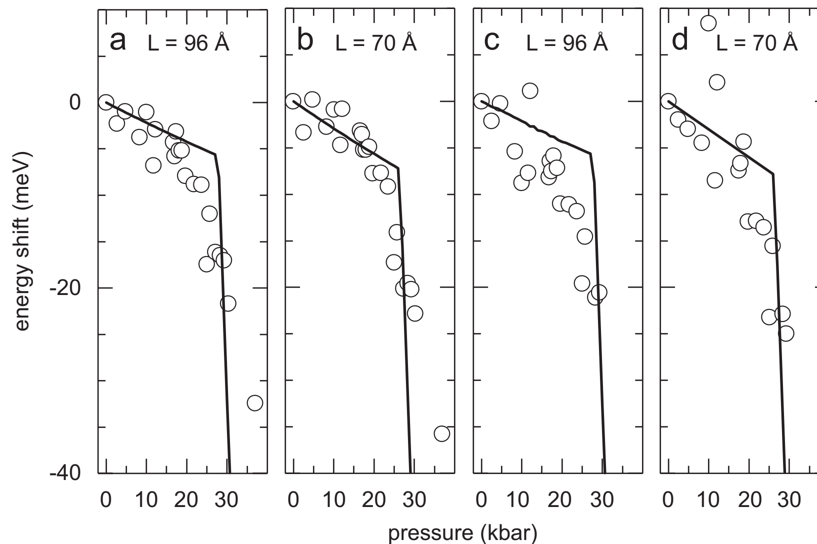

Fig. 2. Pressure dependent shift energy for the PL-peak transitions in GaAs–$Ga_{0.67}Al_{0.33}As$ QW. Results are for heavy-hole (a and b) and light-hole transitions (c and d). Solid lines are our theoretical findings. Open symbols are from Ref. [7].

matrix Hamiltonian **H** has the form $H_{\mu\nu} = h^{\nu}\delta_{\mu\nu}$ [3]. The variational calculation is proposed along the lines of the formalism put forward by Fox et al. [6]. It is accomplished via the introduction of the two trial wavefunctions $\Psi^1 = e^{-\lambda r}(\alpha F^{\Gamma} + \sqrt{1-\alpha^2}F^X)$ and $\Psi^2 = e^{-\lambda r}(-\sqrt{1-\alpha^2}F^{\Gamma} + \alpha F^X)$. Here, r is the electron impurity distance and λ and α are variational parameters.The variational evaluation implies finding the minimum of the quantity $\langle\Psi^i|H|\Psi^i\rangle$, $i = 1, 2$. The hydrostatic pressure effects are incorporated from the dependencies with pressure of the basic input parameters(see Ref. [5] and references therein). Similar procedure have been followed for the calculations of the exciton states but including the first hole uncorrelated functions [6].

In Fig. 1 we report our theoretical findings for the binding energy of a donor impurity in GaAs–$Ga_{0.7}Al_{0.3}As$ QWs as a function of the hydrostatic pressure for different values of the well width. We can observe that the impurity binding energy is enhanced with increasing pressure for electrons in both the Γ and X bands. This is mostly due to the decrease of the dielectric constant, which leads to an increasing of the electrostatic interaction.

Fig. 2 shows the pressure dependence on the shift energy for the PL-peak energy transitions in GaAs–$Ga_{0.67}Al_{0.33}As$ single QWs. It is shown that the $\Gamma - X$ conduction band mixing accounts for the experimentally detected behavior of the PL-peak energy for pressures over which the X band in the barrier region is below in energy to the corresponding Γ profile. The experiments clearly show two different regimes: the first one occurs in the low pressure range, with small pressure coefficient. It is associated with spatially direct excitonic transitions. The second one corresponds to the high pressure range, with larger values of the pressure coefficient. In this case the excitonic transitions involved are spatially indirect.

Summing up, the variational scheme proposed in this work provides a reliable and accurate way to study the influence of the conduction band mixing and the hydrostatic pressure on the properties of impurity and excitonic states in GaAs-based heterostructures. The results here presented show that a correct interpretation of the experimental results of Venkateswaran et al. [7] clearly requires the inclusion of the pressure effects on the X band.

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