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EXCITONS IN QUANTUM BOXES *

Garnett W. BRYANT

McDonnell Douglas Research Laboratories, St. Louis, MO 63166, USA

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Ultrasmall, quasi-zero-dimensional quantum box structures can now be made which exhibit complete quantum carrier confinement. We have calculated the exciton states in quantum boxes. Results are presented to illustrate the transition from complete to negligible confinement.

With the recent advances in the art of microfabrication, quasi-zero-dimensional quantum box nanostructures can be made which exhibit quantum carrier confinement in all three dimensions [1–4]. As a consequence, quantum box structures have generated much interest as a new class of artificially structured materials with interesting nonlinear optically properties [5] and atomic-like discrete states ideal for use in laser structures [6]. To develop a better understanding of quantum boxes and the effects of complete quantum confinement on their optoelectronic properties, we have performed extensive calculations of the exciton states in such structures.

Exciton states are studied by use of the multiparticle, effective-mass, Schrödinger equation for interacting electrons and holes in a quantum box. Microfabricated quantum boxes are constructed from narrow, two-dimensional quantum wells by processing the wells to confine the two-dimensional motion [1–4]. Typically, the width w of the two-dimensional well is an order of magnitude less than the length L of the side of the box (see fig. 1). As a simplification we model quantum boxes as two-dimensional rectangular boxes with $w=0$ and with infinite barriers. Use of a finite, narrow well width w weakens the Coulomb effect slightly but would not change the results qualitatively. The particle interaction is the Coulomb interaction screened by the background dielectric constant. Accurate exciton ground states are calculated by use of a variational approach. The exciton variational wave function is a product of the electron and hole single particle states ($n=1$) and a linear combination of Gaussian functions of the electron–hole separation. A configuration-interaction (CI) approach [7,8] has been used to calculate exciton excited

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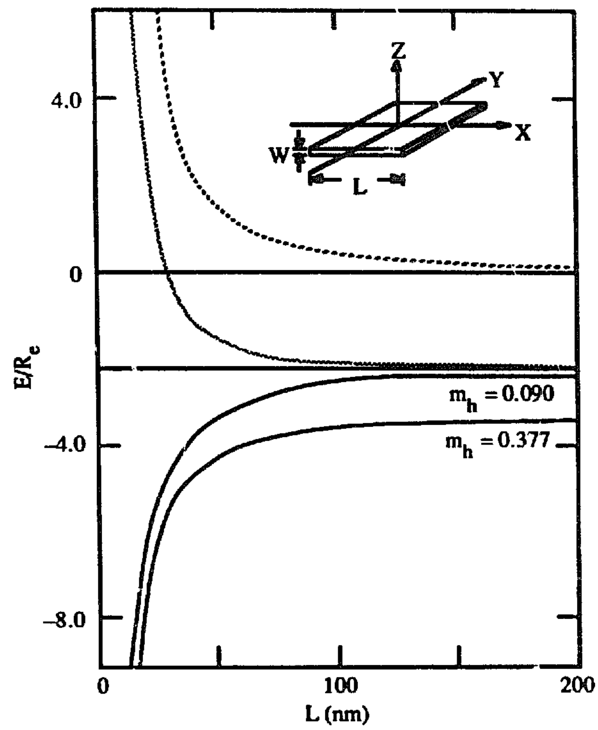

Fig. 1. Ground state energy of an exciton confined in a square box of width L. The solid (upper dashed) curve is the energy of an (non)interacting electron–hole ($m_h = 0.09$) pair. The lower dashed curves are the exciton binding energies for $m_h = 0.09$ and $m_h = 0.377$. The horizontal solid line gives the unconfined-exciton energy ($m_h = 0.09$). The inset shows the configuration of the box.

states. The multiparticle electron–hole wave functions are expanded in terms of Slater determinants constructed from the single-particle eigenstates.

Results are presented for excitons confined in square GaAs boxes with width L, dielectric constant $\varepsilon = 13.1$, electron effective mass (in units of the electron mass m_0) $m_e = 0.067$, and hole masses inside the box $m_h = 0.090$ and 0.377. Energies are scaled by the effective electron Rydberg $R_e = (\hbar^2/2m_0a_0^2)(m_e/\varepsilon^2) = 5.3$ meV.

In very large boxes the exciton ground-state energy (fig. 1) approaches the energy of the unconfined, two-dimensional exciton. However, the exciton energy is still shifted by five percent for boxes that are an order of magnitude wider ($L \approx 0.1$ μm) than the two-dimensional bulk-exciton radius R_{2D}(~ 0.01 μm). In contrast, the ground state energy of an electron bound to a hydrogenic impurity fixed at the center of a quantum disk is unchanged from the free-impurity energy level unless the disk radius is less than 0.02 μm. The exciton ground state energy shifts significantly, due to quantum confinement, for $L \leqslant 0.1$ μm. Energy shifts of ~ 5 meV occur for $L \approx 0.05$ μm, which is typical of shifts observed in photoluminescence [3,4]. Moreover, shifts in the binding energy and in the ground state energy that occur as L changes are comparable. Thus, any attempt to determine box sizes from the shifts of exciton photoluminescence peaks should account for the shifts of binding energies and single particle levels. The binding energy becomes infinite as

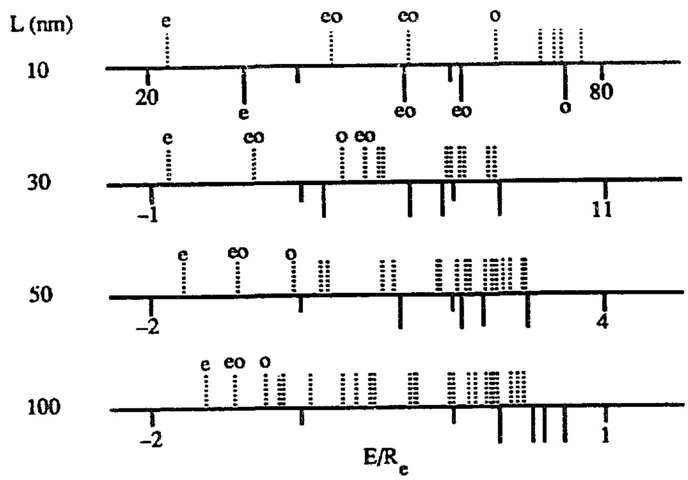

Fig. 2. Energy levels of an exciton (m_h=0.09) confined in a square box of width L. The dashed (solid) lines indicate the levels of an (non)interacting electron–hole pair. The parity relative to the two directions defining the box is shown for the lowest-energy states: e (o) for states even (odd) in both directions; eo for states with even parity in one direction and odd parity in the other. The order of noninteracting levels is independent of box size.

L decreases because the barriers prevent tunneling from the box. In finite-barrier structures, tunneling from the structure reduces the binding energy when $L \leqslant 0.005$ μm [9].

As L decreases and the transition from negligible to complete confinement occures, the exciton state evolves from a state which is a mixture of many electron and hole subbands to a state with the electron and hole in specific subband states. The effect of quantum confinement on the mixing of subband states in the exciton state is shown by fig. 2. For $L \leqslant 0.01$ μm one can clearly identify each exciton state with the specific noninteracting electron–hole pair level that the exciton state is derived from. The exciton states are shifted from the noninteracting states but the ordering of each set of states is the same. This identification becomes more difficult to make as L increases. The finite basis CI calculations for $L \geqslant 0.1$ μm have not been done accurately enough to account for all of the exciton binding; however, the Coulomb mixing of single particle levels that has been included still prevents identification of exciton levels with specific noninteracting levels. The transition from negligible to complete confinement as L decreases is nearly complete when $L \approx R_{2D}$. For $L \approx 0.01$ μm, 92% of the ground-state exciton binding-energy can be accounted for by assuming that the electron and hole occupy the lowest single particle states. For $L \geqslant 0.05$ μm, the mixing of higher levels is crucial; restricting occupation to the lowest level accounts for less than half of the binding energy. As L decreases and the mixing of higher levels becomes insignificant, the difference in light and heavy hole binding energies vanishes (fig. 1).

Several conclusions can be drawn from the results presented. Although the onset of confinement effects occurs for $L \approx 0.1$ μm, the transition to complete confinement does not occur until $L < 0.01$ μm. Quantum structures presently being studied are in this transition regime. Additional reduction in structure size will be needed to reach the regime of complete confinement.

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