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Exciton binding energy in an infinite potential semiconductor quantum well–wire heterostructure

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ABSTRACT

An interacting electron–hole pair in a quantum well–wire is studied within the framework of the effective-mass approximation. An expansion to a 1 dimensional, quantum well model is presented to include another confinement dimension for a quasi-2 dimensional, quasi-1 dimensional quantum well–wire heterostructure. The technique is applied to an infinite well–wire confining potential. The envelope function approximation is employed in the approach, involving a three parameter variational calculation in which the symmetry of the component of the wave function representing the relative motion is allowed to vary from the one- to the two- and three-dimensional limits. Results to such a numerical calculation are presented. Quantitative comparisons with previous calculations for quantum wells is made (in the wire limit where $Lz \to \infty$) to find a good agreement between finite and infinite potential models up to a size of 100 Å.

1. Introduction

At the beginning of the 1980s, advances in technology, especially in very accurate lithographic techniques, made it possible to confine electrons in a quasi-one-dimensional structure known as a quantum wire [1–3]. In these semiconductor heterostructures correlated electron–hole pairs will form Wannier-excitons. For the past three decades, the study of confined excitons in quantum well and wire heterostructures has been a subject of great interest and an enormous amount of literature has been devoted to this field [4–20]. Semiconductor based heterostructures have been widely used for the manufacture of electronic and opto-electronic devices [21]. The nonlinear optical properties of low-dimensional semiconductor heterostructures have been a subject of great interest in recent years [22]. It is well established that the confinement of excitons in quantum wells yields enhanced excitonic effects such as the binding energy and oscillator strength. Energy transitions between confined states in these systems usually associate with significant values of the oscillator strength as well as small relaxation times [22]. This can be exploited in the design of novel optoelectronic devices [23–26]. For example blue and ultraviolet light emitting diodes (LEDs) and blue laser diodes (LDs) have been developed using InGaN quantum wells (QWs) as the active layers [27–32]. Another important new physical phenomenon that has attracted much attention is the condensation of excitons at low temperatures [27,33–35].

Characteristic of the optical spectra of quantum wells and wires is the occurrence of excitons [36]. In a real solid, many complicating effects inhibit a simple comparison of the experimental observation of the exciton emission energy with the theoretical estimate of this value, arising from the uncertainty in the knowledge of a range of parameters like the exact

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widths of the potential wells and barriers, the relevant effective mass parameters and the degenerate nature of the valence band states [37]. For excitons in most III–V quantum wells, for example, both the electron and the hole are strongly confined within the well region by the bandgap discontinuities in the valence band (VB) and conduction band (CB). This is the case in GaAs/(Al,Ga)As among others [38]. A quasi-two-dimensional behaviour occurs on reducing the well width as the average electron–hole distance decrease leading to an increase in the binding energy. However, when the well width is smaller than a critical value, the leakage of the wave function into the barriers becomes more important and the binding energy is reduced until it reaches the value appropriate to the bulk barrier material for which $L = 0$.

Recent advances in the synthesis and growth of nano-tubes and nano-wires has allowed for the confinement of excitons in ever decreasing dimensions of both width and length and so the study of exciton confinement in quantum wire structures are not without merit.

As we progress from nanotechnologies to even smaller feature sizes by manipulating single atoms and electrons, it becomes increasingly necessary to address the concern of the exciton losing its enhanced effects in the ultra-small quantum structures, due to the increased penetration of the exciton wave function into the barrier regions in the direction of diminishing spatial confinement [39]. It is also very important not just to consider a potential system that has 2 degrees of freedom, but one that can, dynamically or kinetically change during operation to a 1-D system. Therefore, it will be most useful to describe such a dynamic, quasi-2D-quasi-1D system mathematically.

It is the aim of the present work to introduce a mathematical technique to investigate the quasi-two-dimensional, quasi-one-dimensional behaviour of a confined exciton inside a semiconductor as the bulk material is reduced in dimensions to form a quantum well and wire. We draw on the previous work proposed by Harrison et al. and Hilton et al. [36,37] and expand the model to include 2D confinement. It is standard in literature to employ trial wave functions, written as a product of three wave functions: the first two are corresponding to the single particle wave function of an electron and a hole in the quantum well–wire and the third represents a *free* exciton whose radius is adjusted as a variational parameter [40]. This method can be suitably adapted for any particular choice of variational wave function.

2. Theoretical formulation and method

The validity of the envelope function approximation (which takes the wave function of the interacting system of an electron and hole in a semiconductor to be written as the product of a Bloch function appropriate to the bottom of the associated (electron) conduction or (hole) valence band states together with an envelope function describing the relative electron – hole motion) is assumed [37] as well as the effective mass approximation, in the single band scheme, allowing the use of relevant effective masses for the charge carriers in the CB and VB respectively.

Consider a Wannier exciton in a rectangular quantum well–wire of infinite extent in the x-direction but having a width, Ly, and height, Lz, in the y- and z-direction respectively. Using the variational scheme, the Hamiltonian of a correlated electron–hole pair can be written as:

$$\boldsymbol{H} = H_e + H_h + H_r \tag{1}$$

where

$$H_e = -\frac{\hbar^2}{2m_e^*}\nabla^2_{z_e,y_e} + V_e \tag{2}$$

$$H_h = -\frac{hbar^2}{2m_h^*}\nabla^2_{z_h,y_h} + V_h \tag{3}$$

are the single-particle Hamiltonians of the electron (hole) and V_e (V_h) is the confining potential due to the valence-(conduction-) band offsets, m_e^* (m_h^*) is the effective mass of the electron (hole) appropriate to the VB (CB) of the semiconductor material under consideration, and

$$H_r = -\frac{\hbar^2}{2\mu}\nabla^2_x + V_{\text{Coulomb}} \tag{4}$$

is the relative motion Hamiltonian for the electron–hole pair with μ the reduced mass of the electron–hole pair:

$$\mu = \frac{m_e^* m_h^*}{m_e^* + m_h^*} \tag{5}$$

and V_{Coulomb} is the Coulombic interaction between the electron and the hole:

$$V_{\text{Coulomb}} = \frac{e^2}{4\pi\varepsilon r} \tag{6}$$

with r being the electron–hole separation distance and ε the dielectric constant for the semiconductor material under consideration.