Superlattices and Microstructures 55 (2013) 198–210

Contents lists available at SciVerse ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

New wavefunctions for the excited states of an axial impurity in a quantum wire

I.F.I. Mikhail [a,*], S.B.A. El Sayed [b]

[a] Department of Mathematics, Faculty of Science, Ain Shams University, Cairo, Egypt
[b] Department of Mathematics, Faculty of Girls, Art, Science and Education, Ain Shams University, Cairo, Egypt

ARTICLE INFO

Article history:
Received 27 September 2012
Received in revised form 20 November 2012
Accepted 12 December 2012
Available online 28 December 2012

Keywords:
Quantum wire
Hydrogenic impurity
Variational method
Excited states
Magnetic field

ABSTRACT

The binding energy of a central hydrogenic impurity located in a finite confining potential quantum well wire (QWW) has been calculated within the effective mass approximation. The study is devoted to deal with the first four excited states ($2P\pm$, $2P_z$ and $2s$) in the presence of a uniform axial magnetic field. The different effective masses of the wire and barrier are taken into consideration. New forms of the trial variational wavefunctions have been introduced. These forms are analogous to the new form given in our earlier work on the ground state ($1s$). They are distinct from the conventional forms by the fact that they satisfy the required boundary conditions in the case of different masses of wire and barrier. The resulting new expressions for the energy and binding energy of the four excited states have led to more accurate results for the binding energy and have improved considerably its values. It is also of importance to point out that a new iteration technique has been introduced to perform the minimization procedure for the energy of the state ($2s$). This technique may be applied in similar problems of slow convergence.

1. Introduction

The problem of calculating the binding energy of a hydrogenic impurity located in a quantum well wire (QWW) has attracted a great attention since the early eighties of the last century until now. Spector and his coworkers [1,2] calculated the binding energy of axial and off-axial impurities in an infinite and finite confining potential QWWs. They studied the variation of the binding energy with the wire

* Corresponding author.
E-mail address: ifi_mikhail@hotmail.com (I.F.I. Mikhail).

0749-6036/$ - see front matter
http://dx.doi.org/10.1016/j.spmi.2012.12.009

radius and impurity location. The optical properties of a QWW in the presence of donor and acceptor impurities were investigated by Montenegro et al. [3,4], Santhi and Peter [5] and Santhi et al. [6]. Branis et al. [7] studied the problem in the presence of an axial uniform magnetic field. The effect of the magnetic field intensity in addition to the effect of the other parameters on the binding energy was explored. The same type of calculations was performed in Merchancano and Morques [8], Niculescu et al. [9], Manaselyan et al. [10] Karki et al. [11] and Başer et al. [12].

The diamagnetic susceptibility of hydrogenic impurities in QWWs in the presence of a magnetic field was calculated in Koksal et al. [13]. Moreover, the effect of an external electric field on the binding energy of axial and off-axial impurities in QWWs was investigated in Mikhail and Emam [14] and Wang et al. [15]. The effect of both electric and magnetic fields were further studied in Mughnetsyan et al. [16].

The related problem of exciton binding energy has been considered in a QWW by Brown and Spector [17], Elagoz et al. [18], Wu [19] and Arunachalam et al. [20,21]. Also, Yesilgul et al. [22] and Karki et al. [23,24] have studied the effect of hydrostatic pressure and temperature on some of the parameters (effective mass, wire radius, dielectric constant and confining potential) needed for the calculation of the binding energy.

Also, the excited states of a hydrogenic impurity located in a QWW have been studied by Latge et al. [25], Villamil et al. [26,27] and Mikhail and El Sayed [28]. The donor impurity states in coupled QWWs under hydrostatic pressure and applied electric field have been investigated in Tangarife et al. [29] and Tangarife and Duque [30]. Furthermore, the binding energy of a hydrogenic impurity in a coaxial QWW (CQWW) in the presence of external electric and magnetic fields have been considered by Zeng et al. [31], Mikhailov et al. [32], Aktas et al. [33,34], Boz and Aktas [35] and Mikhail and El Sayed [36]. The effect of an intense high frequency laser field on an off axial impurity in a CQWW has further been explored in Radu and Niculescu [37].

In most of the previous studies the variational method has been applied with a conventional trial wave function that consists of two parts. The first is the exact wavefunction in the absence of impurity of the ground state 1*s* while the second part represents the hydrogenic impurity in the considered state. It is usually taken in the same form as the wavefunction of this state but with a variational parameter included. However, if the effect of the different masses of wires and barriers is taken into consideration it has been found that this form of the trial wavefunction does not satisfy the required boundary conditions.

In Mikhail and El Sayed [28,36] the different masses of wires and barriers have been considered. They introduced a new form of the trial wavefunction which satisfies the boundary conditions where the impurity is in the ground state 1*s* in the cases of QWW and CQWW.

The use of the new form in Refs. [28,36] has led to a considerable improvement in the results of the binding energy. This has persuaded us to introduce analogous new forms for the trial wavefunctions in the excited states $2P\pm$, $2P_z$ and 2*s* of an axial impurity in a QWW. This is the main motivation of the present article. The different effective masses of the wire and barrier are taken into consideration in the presence of a magnetic field parallel to the wire axis and in the case of finite confining potential. By applying the variational method, new analytical expressions for the electron energies and binding energies in the excited states have been obtained. To the best of our knowledge these expressions have not been reported anywhere before.

Also, it is worthwhile pointing out that in the state 2*s* the "FindMinimum" statement of the Mathematica packages converges very slowly and takes quite a long time to give a solution. We have thus introduced a new iteration approach to determine the minimum energy for this state in the case of different masses when the new wavefunction is utilized. We believe that this new approach will be very effective in similar alternative problems of slow convergence.

The paper is organized as follows: In Section 2 the basic equations are given while in Sections 3–5 the new forms for the trial wavefunctions of the first four excited states $2P\pm$, $2P_z$ and 2*s* are presented. Also, new analytical expressions for the binding energies have been derived. Finally, in Section 6 the numerical results obtained in the case of $Ga\ As - Ga_{1-x}\ Al_x\ As$ QWW are displayed and discussed.