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Localized donor states in axially symmetrical heterostructures

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ABSTRACT

We present a general method for calculating the energy spectrum of donors confined in heterostructures with axial symmetry in the presence of magnetic and electric fields applied along the symmetry axis. The donor's wave functions are chosen as a product of the Slater orbitals and an envelope function that is a solution of a one-dimensional differential equation, which we derive starting from Schrödinger's variational principle. We calculate the energies of the ground and some excited states of a donor confined in multiple quantum wells and a nanowire superlattice as functions of the donor position, electric and magnetic fields for structures with different numbers and widths of the wells and the barriers. Our method could be applicable to a variety of complex quantum-confined semiconductor structures for which more rigorous approaches require extensive numerical calculations.

1. Introduction

For the past few decades different quasi-two-dimensional semiconductor structures, such as single and double quantum wells (DQWs), multiple quantum wells (MQWs), superlattices (SLs) and nanowire superlattices (NWSLs), have been studied extensively both theoretically and experimentally, and applied to various electronic and photonic devices. Taking electric and magnetic fields applied along to the growth direction together with the effects of the confinement and tunneling across the potential barriers, we have an interesting physical system in which the competition of these factors allows us to manipulate its electro-optical properties conveniently for applications in spintronics, optoelectronics, photovoltaics, and quantum information technologies [1].

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The widespread interest in semiconductor structures with axial symmetry is related to the ability to manipulate the energy splitting between the lowest-lying states or the spatial distribution of carriers by varying the radius (in the case of the NWSL), thicknesses and number of wells and barriers.

The electrical and optical properties of these structures also may be modified by impurities due to alteration of the carriers' spatial distribution, to shift and to splitting of the low-lying energy levels in their presence. The resulting alteration of the electro-optical properties of the heterostructures depends on various factors, such as the donor position, the quantum confinement, the interwell tunneling and the electron–ion attraction. For this reason the elaboration of a simple and accurate method of calculation of the energy spectrum of donors (D^0) confined in different types of the heterostructures has been the subject of intense research since the advent of nanotechnology. The variational [2], Monte Carlo [3], finite difference [4] and other methods [5] have been used for calculating the low lying energy levels of D^0 confined in various types of heterostructures, such as QW [6], MQW [7], QWW and SL [8]. Nevertheless, the elaboration of a unified approach to the theoretical analysis of the localized donor states common to all heterostructures has been difficult due to the additional constraints that are imposed on the electron wave function at short distances by the singularity of the Coulomb potential. If the electron approaches the ion then the potential becomes large and negative. This must be canceled by a corresponding positive divergence in the kinetic energy. This condition can be satisfied only if the corresponding wave functions have a "cusp" at the point of the donor location, identical for all heterostructures independently of their geometries. Any accurate algorithm should take into account this circumstance in order to ensure a rapid convergence of the estimated D^0 energies to their exact values.

In this work a particular emphasis is given to the choice of the optimal wave functions for localized donor states which satisfy the "cusp" condition. We were motivated to analyze this subject by the interest in the elaboration a universal technique for calculating the energies and wave functions of the localized states in nanostructures induced by the presence in them of a shallow donor.

Our main result is a general one-dimensional differential equation for the envelope function derived in Section 2, which allows us to analyze, in a simple form, modifications of the hydrogenic states due to the confinement in any axially symmetrical heterostructure. In Section 3 we compare results obtained with our method for ground state donor energies in different types of heterostructures, such as QW, MQW and SL, with corresponding results obtained previously by using other, more sophisticated techniques. We analyze dependencies of the donor binding energy in these structures on the geometric parameters, donor position, and intensities of the electric and the magnetic fields. Also, we present novel results for some donor s-like states in QW and NWSL.

2. Theory

The object of our analysis is the dimensionless Hamiltonian

$$H = H^{(0)}(Q) + V(z) + \alpha z; \quad H^{(0)}(Q) = -\Delta - \frac{2Q}{\sqrt{\rho^2 + (z-\xi)^2}} + \frac{\tilde{\gamma}^2\rho^2}{4} + \mathrm{i}\gamma\hat{L}_z; \qquad \tilde{\gamma}^2 = \gamma^2 + 4V_0/R_0^2, \tag{1}$$

which describes the on-axis D^0 and the electron confined in a semiconductor heterostructure with axial symmetry for $Q = 1$ and $Q = 0$, respectively: Here lengths are scaled in the units of the Bohr effective radius $a_0^* = \varepsilon\hbar^2/m^*e^2$ and the energy in the effective Rydberg $Ry^* = e^2/2\varepsilon a_0^*$. Parameters $\alpha = ea_0^*F/Ry^*$ and $\gamma = e\hbar B/2m^*cRy^*$ are dimensionless units of the strengths of the applied electric, F, and magnetic, B, fields along the symmetry axis. The electron and the on-axis donor position vectors are given by the cylindrical coordinates (ρ, z, ϕ) and $(0, \xi, 0)$, respectively. For the sake of the mathematical convenience we consider in this work the separable axially symmetrical confinement potential $V_c(\rho, z) = V(z) + V_0\rho^2/R_0^2$ with parabolic confinement in the radial direction in which parameters R_0 and V_0 are associated with the nanostructure radius and the barrier height in the lateral junction, respectively. In the large R_0 limit, this potential is converted into corresponding potentials of the QW, MQW or SL depending on the choice of the potential $V(z)$, which describes the confinement