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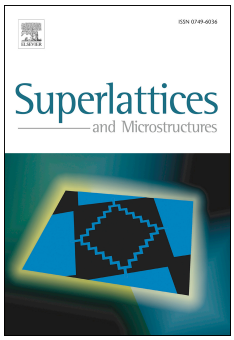

Electronic states in low-dimensional nano-structures: Comparison between the variational and plane wave basis method

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Electronic states in low-dimensional nano-structures: comparison between the variational and plane wave basis method

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Abstract

A comparison is made between the plane wave basis and variational method. Within the framework of effective-mass approximation theory, the variational and plane wave basis method are used to calculate ground state energy and ground state binding energy in low-dimensional nano-structures under the external electric field. Comparing calculation results, the donor binding energies of ground state display the consistent trend, both of them are strongly dependent on the quantum size, impurity position and external electric field. However, the impurity ground state energy calculated using variational method may be larger than the real value and it results in the smaller binding energy for variational method. In addition, the binding energy is more sensitive to the external electric field for the variational method, which can be seen more clearly from Stark shift.

Keywords: Low-dimensional nano-structures, Hydrogenic impurity, External electric field, Variational method, Plane wave basis method

1. Introduction

During the past few years, the low-dimensional semiconductor nano-structures, such as quantum wells (QWs) [1, 2, 3, 4], quantum well wires (QWWs) [5, 6, 7, 8] and quantum dots (QDs) [9, 10, 11, 12, 13, 14] have attracted much interest. The physical property of donor impurity in the low-dimensional nano-structures is a subject of significant technical and scientific relevance due to their potential device applications.

The calculation of electronic states of a hydrogenic donor impurity in the low-dimensional nano-structures has gained special attention. In the framework of effective-mass approximation theory, the variational method has been adopted to calculate the electronic states for a hydrogenic donor impurity in low-dimensional nano-structures [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]; the plane wave basis method has also been adopted in QWs, QWWs and QDs [15, 16, 17, 18, 19, 20, 21, 22, 23]. In addition, many other approaches, such as the fourth-order Runge-Kutta method, the finite-difference method and exact (numerical) integration have been used to calculate the binding energy of a hydrogenic donor impurity [24, 25, 26].

The plane wave basis method is the simplest method since various kinds of symmetric basis functions can be selected according to the shape of the nano-structures. Li et al. [17] proposed the

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