Quantum states of a hydrogenic donor impurity in a cubic quantum dot by the finite difference method

C.S. Yang *

Department of Electronic Engineering, Kun Shan University, No. 949, Da Wan Road, Tainan Hsien 710, Taiwan

ARTICLE INFO
Article history:
Received 24 February 2008
Accepted 23 April 2008
Available online 11 June 2008

Keywords:
Quantum dot
Hydrogenic donor impurity
Effective-mass method
Finite difference method
Nonlinear programming

ABSTRACT
The problem of a hydrogenic donor impurity in a cubic quantum dot with finite confinement potential is solved by the finite difference method. The discretized matrix equation needs to be solved for its eigenvalues and eigenfunctions. An algorithm of nonlinear programming is utilized for this problem. The results match references qualitatively in the weak regime, but introduce new problems in the strong and intermediate regimes.

© 2008 Elsevier Ltd. All rights reserved.

1. Introduction

Impurities in semiconductors play an important role in modern semiconductor devices and possess fundamental questions for understanding the performance of quantum devices. Especially in recent man-made meta-atoms, researches are still very active. For example, there are quantum dots [1–3], quantum well [4], and quantum wire [5].

In the computational approaches, there exist exact solutions [6,7], variational solutions [8], and perturbational solutions [9]. Many methods have been proposed including quantum Monte Carlo method, density functional method, non-equilibrium Green function method, effective-mass method [10,11], and so on. They can be divided into two categories. One is first-principle calculation, and the other is the effective-mass method. For a quantum dot of size about 10 nm, the number of atoms is about 100, and the effective-mass method is quite suitable for saving computer memory.

As for a hydrogenic donor impurity in a quantum dot, many factors affect the quantum energies and states. First is the position of the impurity [12,13]. Second is the confinement potential [14]. Third is the size of the quantum dot [15,16]. These three factors are to be simulated here for the results of their influences on the quantum energies and states.

In this paper, the simulation is going to solve the effective-mass time-independent Schrödinger equation for a hydrogenic donor impurity in a cubic quantum dot by the finite difference method (FDM). To derive the eigenvalues of the large matrix, we solve the problem of nonlinear programming by a modified form of Fletcher and Reeves method [17], rather than the Arnoldi method [18] in [2].

2. Computational model

In this paper, the units of length and energy are the effective Bohr radius $a^*$ = $\hbar^2/e^2m^*$ and the effective Rydberg constant $R^*$ = $\hbar^2/(2m^*a^2)$ respectively, where $\hbar$ is Planck constant over $2\pi$, $m^*$ is effective electron mass, $e$ is dielectric constant, and $e$ is electron charge. And the coordinates are all Cartesian coordinates.

A whole domain $D$ of $x$-coordinate from 0 to $b$, $y$-coordinate from 0 to $b$, and $z$-coordinate from 0 to $b$ is set for FDM. The center of $D$ is $(c, c, c) = (b/2, b/2, b/2)$. A hydrogenic donor impurity is situated at $r_0 = (x_0, y_0, z_0)$. The effective-mass time-independent Schrödinger equation is

$$\left(\nabla^2 - \frac{z}{|r - r_0|} + V(r)\right)\psi(r) = E_\psi\psi(r) \tag{1}$$

where $\nabla^2$ is Laplacian operator, $z$ can be 0 or 1, and $V(r)$ is the confinement potential. And for $r = (x, y, z)$,

$$V(r) = \begin{cases} 0 & |x - c| \leq w/2 \\
0 & \text{and } |y - c| \leq w/2 \text{ and } |z - c| \leq w/2 \\
0 & |x - c| > w/2 \text{ or } |y - c| > w/2 \\
0 & \text{or } |z - c| > w/2 \end{cases} \tag{2}$$
The binding energy is defined as

$$E_b = E_0^2 / E_1^0$$

After discretization of $D$ into $N$ grid points, (1) becomes

$$AX = \lambda X$$

where $A$ is an $N \times N$ matrix, $X$ is an $N$-component vector, and $\lambda$ is the eigenvalue.

The nonlinear programming problem is to minimize $\lambda$ for deriving $X$ and to use $X$ to calculate $\lambda$, according to

$$\lambda = (X, AX) / (X, X)$$

where the parentheses mean vector inner product.

The next higher-energy eigenvector may be derived by imposing a constraint or by shifting $A$.

### 3. Results

The size $b$ of domain $D$ is set as 5.6, and the grid step $k$ is 0.2. So there are total of $N = (5.6/0.2 + 1)^2 = 21952$ grid points.

In Fig. 1, $v = 40$ and $z = 1$. The ground state distribution $|\psi|^2$ on the $x$–$y$ plane $(x = 1.8–3.8, y = 1.8–3.8)$ at $z = 2.8$ is plotted for four values of $w$ ($w = 0.6, 1.0, 1.4, 1.8$). As the $w$ increases, the distribution broadens. This method converges very well and fast, and saves very much memory.

In Fig. 2, the binding energy as a function of the size $w$ for four positions of the impurity $(r_0 = (c, c, c), (c + w/2, c, c), (c + w/2, c + w/2, c), (c + w/2, c + w/2, c + w/2))$ is plotted. According to these results, we can divide the binding energy into three regimes:

![Fig. 1](image1.png)

**Fig. 1.** $v = 40$ and $z = 1$. The ground state distribution $|\psi|^2$ on the $x$–$y$ plane $(x = 1.8–3.8, y = 1.8–3.8)$ at $z = 2.8$.

![Fig. 2](image2.png)

**Fig. 2.** The binding energy as a function of the size $w$ for four positions of the impurity $(r_0 = (c, c, c), (c + w/2, c, c), (c + w/2, c + w/2, c), (c + w/2, c + w/2, c + w/2))$.

![Fig. 3](image3.png)

**Fig. 3.** The ground state impurity energy as a function of the size $w$ for four positions of the impurity.

![Fig. 4](image4.png)

**Fig. 4.** The binding energy as a function of the size $w$ for four values of the confinement potential $v$ ($v = 20, 40, 60, 80$).
strong confinement regime (about $w < 1.4$), intermediate confinement regime ($1.4 < w < 1.6$), and weak confinement regime (about $w > 1.6$). In the strong confinement regime, the more outer the impurity position is, the more large the binding energy becomes. In the weak confinement regime, the more outer the impurity position is, the more small the binding energy becomes. In the intermediate regime, the influence of the impurity position is small. In Fig. 3, the ground state impurity energy as a function of the size $w$ for four positions of the impurity is plotted. As $w$ increases, the energy decreases. There is little distinction for three regimes. Therefore, the three regimes are the results of the combination of impurity and environment (confinement), not just impurity.

In Fig. 4, the binding energy as a function of the size $w$ for four values of the confinement potential $v$ ($v = 20, 40, 60, 80$) is plotted. In the weak regime, the binding energy increases as the confinement potential increases. In the strong and intermediate regimes, the situations are not monotone. The effects of impurity and confinement compete and induce crossings of the profiles. But in Fig. 5, the ground state impurity energy increases as the confinement potential increases. And in this case, there is little distinction for three regimes. Compared to those in [1–3], only the results in the weak regimes match qualitatively.

4. Conclusions

The Hamiltonian of the system (1) is not definitely positive because of the impurity term. If there is no confinement potential, the problem is like a hydrogen atom. Its eigenenergies are purely negative. The confinement potential will push the eigenenergies toward the positive direction; therefore, ground state impurity energy may be negative for insufficient confinement potential. This effect can be checked in Figs. 3 and 5. Some numerical methods may implicitly assume the matrix $A$ in (4) to be definitely positive and produce some differences for unequal bases. If $E_1^0$ is definitely positive, then it is doubtful. In summary, the results in the weak regime match qualitatively. But the present data in the strong and intermediate regimes is not enough and needs more researches.

References