Electronic Properties of Multi-Ablooms Flower-Like Quantum Dots: a 2- D Finite Element Study

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Research Article

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Electronic properties of Multi-ablooms Flower-Like Quantum Dots: a 2- D Finite Element Study

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Abstract

In this paper, we investigated the electronic properties of two dimensional multi-abloom nanoflower. Also, we approximated a typical form of the Schrödinger equation through an appropriate 2-D finite element approach, and then, we have investigated the effects of different parameters such as number of ablooms, number of rose, variety geometric domain shape and systems size on the energy levels, eigenfunctions, and dipole matrix elements.

Keywords: 2-D multi-abloom nanoflower, 2-D finite element and bilinear method, Galerkin method, electronic properties.

1. Introduction

Because of vast applications in science and technologies, during last few years, quantum dots (QDs) have been an appealing field study. During last few years, a wide variety of shapes, such as quantum dots arrays [1], conical [2], rectangular[3], cylindrical [4], disc-shaped [5], elliptical [6], lens-shaped [7], pyramidal [8], spherical [9], T-shaped [10], Y-shaped [11], etc., for the quantum dot systems have been studied. But as we know up to now, the electronic inter-sub-band structures of nanoflower systems [25] has not so far been addressed. It is clear that due to the complicated form of the quantum dot shapes, the calculation of energy levels and wave functions, analytically, is a nontrivial task [12].

In order to study these quantum dots different methods such as variational method [13, 35], 1/N expansion method [14], quantum cellular automata [15], density functional calculations [16], exact diagonalization [17], finite difference technique [18,36], self-consistent Hartree method [18], k.p theory [19], Monte Carlo [20], molecular dynamics

[21], Green's functions [22, 37], Nikiforov–Uvarov method [23], Transfer matrix method [24] etc. have so far been used.

The finite element method (FEM) is a numerical technique for solving PDEs and was originally applied to problems in engineering, structural mechanics applied sciences and are effective for problems with nonregular and complicated domain geometry. In this method, there is a natural variational approach to the numerical solution of elliptic boundary value problems (BVP) such as Helmholtz form of the Schrodinger, which minimize residual over some suitable finite-dimensional subspace defined on the elements.

The FEM involves four basic steps: first, we must partition the solution region of the PDE into a finite number of nonoverlap elements which the rectangular or triangular shapes and h or p refining are most common for planar and 2-D problems. The collection of all regular or congruent elements should cover and resemble the original region as closely as possible. In the second step, we derive interpolation and governing equations for a typical element by defining a complete polynomial on an element. The smooth degree of assembling elements, determine continuity of global approximation. This step, determine blocks and entries of the problem coefficient stiffness matrix. In the third step, we need assemble all partition elements of the solution region to obtain the global coefficient matrix. Finally, the resulting sparse system of equations will be solved.

Here and in our study, the given polygon region divided into 361 uniform rectangular elements. [29,30,31,32,33,34]

In the present work, we have solved a typical 2-D Schrodinger equation by means of the FEM. We have evaluated the energy eigenvalues and corresponding eigenfunctions of a multi-abloom nano-flower. Then we have computed the corresponding dipole matrix elements M_{12} that is an important parameter in evaluation of optical properties of the semiconducting system through density matrix approach.

2. Finite Element Solution of the 2-D Schrödinger Eq.

In the envelop function approach, we assume a 2-D Schrödinger equation as,

$$\begin{aligned}
H\psi(x, y) &= \frac{\hbar^2}{2m^*} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) \psi(x, y) + V(x, y)\psi(x, y) \\
&= \frac{\hbar^2}{2m^*} \Delta \psi(x, y) + V(x, y)\psi(x, y) \\
&= \alpha \Delta \psi(x, y) + V(x, y)\psi(x, y) \\
&= E\psi(x, y)
\end{aligned} \tag{1}$$

In fact, this 2-D time independent Schrödinger equation is a linear eigenvalue problem with Dirichlet boundary conditions (BCs). The problem domain is rectangular $\Omega = [a_x, b_x] \times [a_y, b_y]$ where in the normalized case, this domain can be scaled and transformed to the form $\Omega = [0, 1] \times [0, 1]$. In equation (1), $\hbar$, m^* and $V(x, y)$ are the Plank constant, effective mass and geometrical confining potential respectively and also set $\alpha = \frac{\hbar^2}{2m^*}$.

As explained, in the FEM, we discretize domain space into some rectangular element subdomains and build bilinear base functions. If we assume n_x and n_y number of discretization points along x and y direction axes, the steps along the x and y directions will be $h_x = \frac{1}{n_x}$, $h_y = \frac{1}{n_y}$. Then, we have $0 = x_0 < x_1 < \dots < x_{n_x} = 1$, $0 = y_0 < y_1 < \dots < y_{n_y} = 1$, $x_i = a_x + ih_x$, $y_j = a_y + jh_y$. The bilinear polynomial basis functions defined on the rectangular element can be written as,

$$\varphi_{i,j}(x, y) = \begin{cases} \frac{x_{i+1} - x}{x_{i+1} - x_i} \frac{y_{j+1} - y}{y_{j+1} - y_j}, & x_i \leq x \leq x_{i+1}, y_j \leq y \leq y_{j+1} \\ \frac{x_{i-1} - x}{x_{i-1} - x_i} \frac{y_{j+1} - y}{y_{j+1} - y_j}, & x_{i-1} \leq x \leq x_i, y_j \leq y \leq y_{j+1} \\ \frac{x_{i-1} - x}{x_{i-1} - x_i} \frac{y_{j-1} - y}{y_{j-1} - y_j}, & x_{i-1} \leq x \leq x_i, y_{j-1} \leq y \leq y_j \\ \frac{x_{i+1} - x}{x_{i+1} - x_i} \frac{y_{j-1} - y}{y_{j-1} - y_j}, & x_i \leq x \leq x_{i+1}, y_{j-1} \leq y \leq y_j \\ 0, & \text{Otherwise} \end{cases} \tag{2}$$

where $i = 0, 1, 2, \dots, n_x$ and $j = 0, 1, 2, \dots, n_y$. The total number of points are equal $(1+n_x)(1+n_y)$. Since the wave functions degenerate on the boundaries, the boundary

nodes delete from computing and are not necessary. Therefore, the number of unknown variables (and hence the number of algebraic equations) are equal to number of internal discretization points $(n_x - 1)(n_y - 1)$.

Now, we construct the finite element approximation of the wave-function through linear combination of basis functions Eq. (2) on all internal nodes,

$$\psi(x, y) = \sum_{i=1, j=1}^{n_x-1, n_y-1} u_{i,j} \varphi_{i,j}(x, y) \quad (3)$$

where $u_{i,j}$ are unknowns. For simplicity, we use normalized and iso-parametric elements

by scaling $\xi = \frac{x - x_i}{h_x}$ and $\eta = \frac{y - y_j}{h_y}$. Therefore, we can rewrite the equation (2) as an alternative,

$$\varphi_{i,j}(\xi, \eta) = \begin{cases} (1 - \xi)(1 - \eta) & , 0 \leq \xi \leq 1, 0 \leq \eta \leq 1 \\ (1 + \xi)(1 - \eta) & , -1 \leq \xi \leq 0, 0 \leq \eta \leq 1 \\ (1 + \xi)(1 + \eta) & , -1 \leq \xi \leq 0, -1 \leq \eta \leq 0 \\ (1 - \xi)(1 + \eta) & , 0 \leq \xi \leq 1, -1 \leq \eta \leq 0 \\ 0 & , \text{ Otherwise} \end{cases} \quad (4)$$

Since, in the vicinity of the point (x_i, y_j) there are only 9 neighborhood points and naturally 4 proper related elements, thus in matrix form of the Hamiltonian, there are only 9 non-zero diagonal layers of elements and we will have a resulting tri-diagonal block Hamiltonian matrix. Each of these blocks is 3 by 3 and they are symmetric. Now, we define residual through substituting the linear expansion (3) into the equation (1),

$$R(x, y) = \alpha \Delta \psi(x, y) + V(x, y) \psi(x, y) - E \psi(x, y), \quad x \in \Omega \quad (5)$$

The approximated wave-function $\psi(x, y)$ is in the generalized and distributional form [31], thus we can use the Galerkin weighted residual method as,

$$\iint_{\Omega} R(x, y) \varphi_{i,j}(x, y) dx dy = 0, \quad (6-a)$$

where, in a more precise manner we have,

$$\int_{y_{j-1}}^{y_{j+1}} \int_{x_{i-1}}^{x_{i+1}} R(x, y) \varphi_{i,j}(x, y) dx dy = 0, \quad (6-b)$$

And in the normalized space we have,

$$\int_{-1}^1 \int_{-1}^1 R(\xi, \eta) \varphi_{i,j}(\xi, \eta) d\xi d\eta = 0, \quad (6-c)$$

In order to evaluate the equations (6), we need to use green theorem of second kind as [31,34],

$$\iint_{\Omega} \Phi \Delta U d\Omega + \iint_{\Omega} \nabla \Phi g \nabla U d\Omega = \iint_{\Gamma} \Phi \frac{\partial U}{\partial n} d\Gamma, \quad (7)$$

Due to homogeneous Dirichlet boundary condition, this equation can be simplified into,

$$\iint_{\Omega} \Phi \Delta U d\Omega = - \iint_{\Omega} \nabla \Phi g \nabla U d\Omega, \quad (8)$$

Figure (1) represents a simple description about the relating basis functions in the neighborhood of the point (x_i, y_j) .

Figure 1: 4 neighborhood normalized elements of arbitrary internal point (x_i, y_j)

Now, through integral (6), we have three types of blocked tri-diagonal matrices. For the matrix M_1 we have the matrix elements as figure (2).

i	$i+1$	$j+1$
		j
		$i+1$

$$\begin{array}{cc}
\frac{1}{6h_x^2} - \frac{1}{3h_y^2} & -\frac{1}{6h_x^2} - \frac{1}{6h_y^2} \\
\frac{1}{3h_x^2} + \frac{1}{3h_y^2} & -\frac{1}{3h_x^2} + \frac{1}{6h_y^2}
\end{array}$$

Figure 2: M_1 matrix elements

and M_2 matrix elements are as figure (3).

i	$i+1$	$j+1$
		j
		$i+1$

$$\begin{array}{cc}
\int_0^1 \int_0^1 V(\xi, \eta) \eta (1-\eta) (1-\xi)^2 d\xi d\eta & \int_0^1 \int_0^1 V(\xi, \eta) \eta \xi (1-\eta) (1-\xi) d\xi d\eta \\
\int_0^1 \int_0^1 V(\xi, \eta) (1-\eta)^2 (1-\xi)^2 d\xi d\eta & \int_0^1 \int_0^1 V(\xi, \eta) \xi (1-\xi) (1-\eta)^2 d\xi d\eta
\end{array}$$

Figure 3: M_2 matrix elements

And M_3 matrix elements are as figure (4).

i	$i+1$	$j+1$
		j
		$i+1$

$$\begin{array}{cc}
\frac{1}{3.6} & \frac{1}{6.6} \\
\frac{1}{3.3} & \frac{1}{6.3}
\end{array}$$

Figure 4: M_3 matrix elements

When we evaluate the above mentioned sub-matrices, we will have the following eigenvalue equation system,

$$-\alpha M_1 \psi + M_2 \psi = EM_3 \psi, \quad (9)$$

where, E are the energy eigenvalues.

3. Results and Discussions

By using a finite element method and compact density matrix formalism, we have investigated the electronic properties of multi-abloom nano-flowers. Figure (5) shows the few multi abloom potential profile.

Figure 5: confining potential of the systems with 2 to 8 number of ablooms. ($r^2 = \cos(2\theta)$ for 2 ablooms, $r = \cos(3\theta)$ for 3 ablooms, $r = \cos(2\theta)$ for 4 ablooms, and so on.)

In the figure (6) we have presented the variation of the first 20 lowest eigen-energies of a 5-abloom nano-flower as a function of the domain size. In this figure, we see that, as the domain size increases the energies decreases.

Figure 6: variation of the first 20 lowest eigen-energies as a function of the domain size. Also, in the figure (7), we have given the variation of the first 20 lowest eigen-energies of a 5-abloom nano-flower as a function of the number of ablooms. Here, we see a nonlinear behavior in the energy values when the number of ablooms increases.

Figure 7: variation of the first 20 lowest eigen-energies as a function of the number of ablooms.

In the next four figures (8-1) to (8-4), we have presented the 9 eigen-functions of the system with 2, 3, 5, and 8 number of ablooms. These figures indicate the distribution of the probability densities inside the quantum structure. This probabilities show the probability of finding an electron in an assumed structures and therefore can provide us information about the free careers distribution.

Figure 8-1: First 9 eigen-functions of the system with 2 ablooms. (the 2 ablooms rose can be depicted by $r^2 = \text{Cos}(2\theta)$)

Figure 8-2: First 9 eigen-functions of the system with 3 ablooms. (the 3 ablooms rose can be found by $r = \text{Cos}(3\theta)$ or $r = \text{Sin}(3\theta)$)

Figure 8-3: First 9 eigen-functions of the system with 5 ablooms.

Figure 8-4: First 9 eigen-functions of the system with 8 ablooms.

Figure (8) and (9) also show the effects of the system length and number of ablooms on

the dipole matrix elements $M_{21} = \int_{a_y}^{b_y} \int_{a_x}^{b_x} |x| \psi_1(x, y) \psi_2(x, y) dx dy$, respectively. As figure (8)

shows, when the system length increases, the dipole matrix elements M_{21} also increases.

However, the figure (9) indicates that the variation of the dipole matrix elements M_{21} as a function of the number of ablooms is an oscillatory function.

Figure 8: variation of the dipole matrix elements M_{21} as a function of the system length.

Figure 9: variation of the dipole matrix elements M_{21} as a function of the number of ablooms.

Conclusion

In this work, we investigated the electronic properties of multi-abloom nanoflower. By using detailed finite element method, we showed that as the domain size increased, the energies decreased. A nonlinear behavior in the energy values observed

when the number of ablooms increased. When the system length increased, the dipole matrix elements M_{21} also increased. The variation of the dipole matrix elements M_{21} as a function of the number of ablooms was an oscillatory function.

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Figures

j+1	$-\eta\xi$	$\eta(1+\xi)$	$\eta(1-\xi)$	$\eta\xi$
j	$-\xi(1-\eta)$	$(1+\xi)(1-\eta)$	$(1-\xi)(1-\eta)$	$\xi(1-\eta)$
j-1	$-\xi(1+\eta)$	$(1+\xi)(1+\eta)$	$(1-\xi)(1+\eta)$	$\xi(1+\eta)$
	$\eta\xi$	$-\eta(1+\xi)$	$-\eta(1-\xi)$	$-\eta\xi$
	i+1	i	i-1	

Figure 1

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Figure 2

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Figure 3

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Figure 4

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Figure 10

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