Al-Mustansiriyah Journal of Science
ISSN: 1814-635X (print), ISSN: 2521-3520 (online)
Volume 30, Issue 2, 2019
DOI: http://doi.org/10.23851/mjs.v30i2.150

Research Article **Open Access**

Finite Element Method Linear Triangular Element for Solving Nanoscale $InAs/GaAs$ Quantum Ring Structures

Eman Ali Hussain, Jamil A. Al-Hawasy, Lamyaa Hussein Ali*
Department of Mathematics, Faculty of Science, Mustansiriyah University, IRAQ.
*Correspondent Author Email: lamya_h2@uomustansiriyah.edu.iq

ArticleInfo

Submitted
24/06/2017

Accepted
01/10/2018

Published
01/10/2019

Abstract

This paper concerned with the solution of the nanoscale structures consisting of the $InAs/GaAs$ with an effective mass envelope function theory, the electronic states of the $InAs/GaAs$ quantum ring are studied. In calculations, the effects due to the different effective masses of electrons in and out the rings are included. The energy levels of the electron are calculated in the different shapes of rings, i.e., that the inner radius of rings sensitively change the electronic states. The structures of $InAs/GaAs$ quantum rings are studied by the one electronic band Hamiltonian effective mass approximation, the energy- and position-dependent on electron effective mass approximation, and the spin-dependent on the Ben Daniel-Duke boundary conditions. In the description of the Hamiltonian matrix elements, the Finite elements method with different base linear triangular element is adopted. The non-linear energy confinement problem is solved approximately by using the Finite elements method with linear triangular element, to calculate the energy of the electron states for the $InAs/GaAs$ quantum ring.

Keywords: nanoscale, Finite elements method, Ben Daniel-Duke boundary conditions, $InAs/GaAs$ quantum rings.

الخلاصة

"تناولت هذه الورقة حل الهياكل النانوية المكونة من $InAs/GaAs$ مع نظرية دالة غلاف الكتلة الفعالة، ودراسة الحالات الإلكترونية للحلقة الكمومية $InAs/GaAs$. في الحسابات، يتم تضمين الآثار الناجمة عن كتل فعالة مختلفة من الإلكترونات داخل وخارج الحلقات. يتم حساب مستويات الطاقة للإلكترون في أشكال مختلفة من الحلقات، أي أن دائرة نصف قطرها الداخلي من حلقات تغيير حساس للحالات الإلكترونية. تدرس هياكل حلقات $InAs/GaAs$ الكمومية من قبل الفرقة الإلكترونية واحدة هاملتونيان تقريب الشامل الفعال، والطاقة، وموقف تعتمد على الإلكترون تقريب الشامل الفعال، وتدور تعتمد على الحدود بن دانيال دوق. في وصف عناصر المصفوفة هاميلتونيان، يتم اعتماد طريقة العناصر المحددة مع العنصر الثلاثي الخطي. يتم حل مشكلة احتجاز الطاقة غير الخطية تقريبا باستخدام طريقة العناصر المحددة مع عنصر ثلاثي خطي، لحساب طاقة حالات الإلكترون للحلقة الكمومية $InAs/GaAs$."

Introduction

The modeling of the electron states in semiconductor nanostructures remains a difficult computational task. The single electron states are advantageous for studying the electron correlations and, the effects of magnetic fields in quantum rings and useful for designing and fabricating the double colors detector by intra band and inter band translations.

In 1990, Paasch *et al.*, [2] used envelope equation and wave function matching for narrow-gap semiconductors. In 1995, Mathine *et al.*, [1] applied computational Fourier series solution of the BenDaniel-Duke Hamiltonian for arbitrary shaped quantum wells. In 2001, Yiming Li *et al.*, [6] used Computer simulation of electron energy levels for different shape $InAs/GaAs$ semiconductor quantum dots. In 2002, Yiming Li *et al.*, [7] used Electron energy state spin-splitting in 3D cylindrical semiconductor quantum dots. In 2003, Melnik *et al.*, [4] applied finite element analysis of Nanowire superlattice structures. Whereas 2005, Yiming Li, [5] using an iterative method for single and vertically stacked semiconductor

quantum dots simulation. In 2016, Deyasi *et al.*, [3] applied numerically computed in presence of electric field using propagation matrix method.

In this paper we propose a Finite element method with different base linear triangular element for solving the nanoscale structures consisting of the $InAs/GaAs$ quantum ring, and the spin-dependent on the Ben Daniel-Duke boundary conditions.

Modeling Energy Stat With Spin-Dependent Boundary Conditions *[4],[5]*

We consider the problem to compute relevant energy states and corresponding wave functions of a three dimensional semiconductor quantum ring. Consider the electrons are confined in system of the three-dimensional quantum ring structures and apply an effective one electronic band Hamiltonian, is given by:

$$\hat{H} = \hat{H}_0 + \hat{V}_{so}(r), \tag{1}$$

where $\hat{H}$ is the Hamiltonian of the system without spin-orbit interaction, $\hat{V}_{so}(r)$ is the spin-orbit interaction for the conduction band electrons, and the expression for $\hat{H}_0$ is as follows:

$$\hat{H}_0 = -\frac{\hbar^2}{2}\nabla_r\left(\frac{1}{m(E,r)}\right)\nabla_r + V(r) \tag{2}$$

where ∇_r is the spatial gradient, $m(E,r)$ is the energy dependent electron effective mass, and $V(r)$ is the confinement potential.

$$\frac{1}{m(E,r)} = \frac{P^2}{\hbar^2}\left[\frac{2}{E + E_g(r) - V(r)} + \frac{1}{E + E_g(r) + \Delta(r) - V(r)}\right] \tag{3}$$

where $E_g(r)$ and $\Delta(r)$ stand for the position dependent band gap and the spin-orbit splitting in the valence band, respectively and, P is the momentum matrix element.

The spin-orbit interaction for the conduction band electrons $\hat{V}_{so}(r)$ is given by

$$\hat{V}_{so}(r) = i\nabla\beta(E,r)\cdot[\hat{\sigma}\times\nabla] \tag{4}$$

where $\beta(E,r)$ is the spin-orbit coupling parameter and $\hat{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$ is the vector of the Pauli matrices. The energy and position dependent $\beta(E,r)$ has the form

$$\beta(E,r) = \frac{P^2}{2}\left[\frac{1}{E + E_g(r) - V(r)} - \frac{1}{E + E_g(r) + \Delta(r) - V(r)}\right] \tag{5}$$

For those quantum ring systems that have sharp discontinuity on the conduction band interfaces between the quantum ring ("$InAs$" material 1) and semiconductor matrix ("$GaAs$" material 2), the hard-wall confinement potential is

$$V(r) = \begin{cases} 0, & r \in \text{material 1} \\ V_0, & r \in \text{material 2}, \end{cases} \tag{6}$$

where V_0 is the structure band offset. Combining the Hamiltonian in equations (1), (2), and (4), the spin dependent Ben Daniel-Duke boundary conditions for the electron wave function $\Psi(r)$ are written as follows:

$$\Psi_{\text{material 1}}(r_s) = \Psi_{\text{material 2}}(r_s)$$
$$\left\{\frac{\hbar^2}{2m(E,r)}\nabla - i\nabla\beta(E,r)[\hat{\sigma}\times\nabla]\right\}_n \Psi(r_s) = \mathrm{C}_0 \tag{7}$$

where V_0 is the some constant, r_s denotes the position of the system interface.

Note (1): We note that the expressions of electron effective mass in equation (3), spin-orbit coupling parameter in equation (5), and the equations of Ben Daniel-Duke boundary condition in equation (7) are all energy and position dependent relationships in this study.

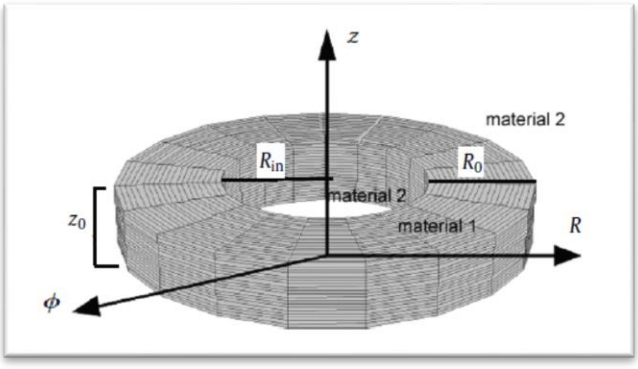


Figure 1: A three-dimensional plot of the disk-shaped semiconductor quantum ring

We now consider the quantum ring as shown in Fig.(1) with the inner radius R_{in}, radius R_0 and the thickness Z_0 in the cylindrical coordinate (R, ϕ, Z). The origin of the system is at the center of the structure and the Z axis is chosen

along the rotation axis. Since the system is cylindrically symmetric, the wave function can be represented as

$$\Psi(r) = \phi(R,Z)exp(il\phi), \quad (8)$$

where l is a constant represents the electron orbital quantum number and the original model remains a two-dimensional problem in (R,Z) coordinate. From equations (1)-(6) and equation (8), we obtain the following equation

$$-\frac{\hbar^2}{2m_1(E)}\left(\frac{\partial^2}{\partial R^2}+\frac{\partial}{R\partial R}+\frac{\partial^2}{\partial Z^2} - \frac{l^2}{R^2}\right)\phi_1(R,Z) = E\phi_1(R,Z), \quad \forall(R,Z) \in \text{material 1} \quad (9)$$

and

$$-\frac{\hbar^2}{2m_2(E)}\left(\frac{\partial^2}{\partial R^2}+\frac{\partial}{R\partial R}+\frac{\partial^2}{\partial Z^2} - \frac{l^2}{R^2}\right)\phi_2(R,Z) + V_0\phi_2(R,Z) = E\phi_2(R,Z), \quad \forall(R,Z) \in \text{material 2} \quad (10)$$

For the same reasons that the problem is symmetry along the Z axis, the spin-dependent boundary conditions in equation (7) are given by

$\phi_1(R,Z) = \phi_2(R,Z),\ Z = f(R)$ and

$$\frac{1}{m_1(E)}\left\{\frac{\partial\phi_1(R,Z)}{\partial R}+\frac{df(R)}{dR}\frac{\partial\phi_1(R,Z)}{\partial R}\right\}_{Z=f(R)} - \frac{1}{m_2(E)}\left\{\frac{\partial\phi_2(R,Z)}{\partial R} + \frac{df(R)}{dR}\frac{\partial\phi_2(R,Z)}{\partial R}\right\}_{Z=f(R)} + \frac{2\sigma(\beta_1-\beta_2)}{\hbar^2}\frac{l}{R_0}\phi_1(R_0,Z) = 0 \quad (11)$$

Finite Element Method

Dependence of the electron effective mass and spin–orbit coupling parameter on each energy state are result in a nonlinear equations (9) and (10). The nonlinear equations complicate the process of analytical solution in the explored quantum ring. Therefore, the numerical approach to the solution of the nonlinear equations is advanced in the calculation of the electronic structure of $InAs/GaAs$ quantum rings. The finite element method is applied to solve the above problem for the nanoscale $InAs/GaAs$ quantum rings. Energy states and spin-splitting are numerically calculated without any fitting parameters. Starting from a given initial energy, the finite element method globally calculates all bounded energies for the corresponding nonlinear algebraic eigenvalue problem. A computational procedure of the finite element method is shown below:

$$-\frac{\hbar^2}{2m_i(E)}\left(\frac{\partial^2}{\partial R^2}+\frac{\partial}{R\partial R}+\frac{\partial^2}{\partial Z^2}-\frac{l^2}{R^2}\right)\phi_i(R,Z) + V\phi_i(R,Z) = E\phi_i(R,Z), \quad \forall(R,Z) \in material\ i \quad (12)$$

Where $i = 1,2$ since the cylindrical is symmetry, $V = V(R,Z)$, and $\phi_i = u(R,Z)e^{il\phi_i}$, where l is an integer. Equation (12) becomes

$$\frac{-\hbar^2}{2m_i(E)}\left[\frac{1}{R}\frac{\partial u}{\partial R}+\frac{\partial}{\partial R}\left(\frac{\partial u}{\partial R}\right)-\frac{l^2}{R^2}u+\frac{\partial}{\partial Z}\left(\frac{\partial u}{\partial Z}\right)\right] + Vu = Eu \quad (13)$$

The electron energy spectra for $InAs/GaAs$ quantum rings the semiconductor band structure governing physical process in a ring nanoscale are described in terms of cylindrical coordinates. When the geometry, loading, and boundary conditions are independent of the circumferential direction (ϕ -coordinate), the electron energy spectra for $InAs/GaAs$ quantum rings of the semiconductor band structure equation become two-dimensional in terms of R and Z.

Weak Form

Assume that Ω is a typical element, whether triangular or quadrilateral, of the finite element mesh, and we develop the finite element model of equation (13) over Ω. Various two-dimensional elements will be discussed in the sequel.

There are three steps in the development of the weak form of equation (13) over the typical element Ω.

The first step is formulated equation (13) by the following weak form.

$$0 = \int_{\Omega} \left[\frac{-\hbar^2}{2} \left[w \frac{1}{m_i(E)} \frac{\partial u}{\partial R} + wR \frac{\partial F_1}{\partial R} - \frac{l^2}{m_i(E)R} wu + wR \frac{\partial F_2}{\partial Z} \right] + VwRu - EwRu \right] dRdZ \quad (12)$$

Where

$$F_1 = \left(\frac{1}{m_i(E)} \frac{\partial u}{\partial R} \right) \quad \text{and} \quad F_2 = \left(\frac{1}{m_i(E)} \frac{\partial u}{\partial Z} \right)$$

In the second step, we note the identities

$$-wR \frac{\partial F_1}{\partial R} = R \frac{\partial w}{\partial R} F_1 - R \frac{\partial}{\partial R} (wF_1) \quad (15a)$$

$$-wR \frac{\partial F_1}{\partial Z} = R \frac{\partial w}{\partial Z} F_2 - R \frac{\partial}{\partial Z} (wF_2) \quad (15b)$$

Next, using equation (15a) and equation (15b) in the equation (14) then applying the divergence theorem, we obtain

$$0 = \int_{\Omega} \left[\frac{-\hbar^2}{2m_i} w \frac{\partial u}{\partial R} + \frac{\hbar^2}{2} R \frac{\partial w}{\partial R} \left(\frac{1}{m_i} \frac{\partial u}{\partial R} \right) + \frac{\hbar^2 L^2}{2m_i R} wu + \frac{\hbar^2}{2} R \frac{\partial w}{\partial z} \left(\frac{1}{m_i} \frac{\partial u}{\partial Z} \right) + wRVu - wREu \right] dRdZ - \oint_{\Gamma} w \left[n_1 \left(\frac{1}{m_i} \frac{\partial u}{\partial Z} \right) + n_2 \left(\frac{R}{m_i} \frac{\partial u}{\partial R} \right) \right] ds \quad (16)$$

where $\vec{n} = (n_1, n_2)$ is an outer unite vector normal on Γ and ds is the length of an infinitesimal line element along the boundary.

From an inspection of the boundary integral in (16), we note that the specification of u constitutes the essential boundary condition, and hence u is the primary variable. The specification of the coefficient of the weight function in the boundary expression, i.e. we can let

$$d_n \equiv n_1 \left(\frac{1}{m_i} \frac{\partial u}{\partial Z} \right) + n_2 \left(\frac{R}{m_i} \frac{\partial u}{\partial R} \right) \quad (17)$$

The third and last step of the formulation is to substitute the definition (17) in (16) and write the weak form of (13) as

$$0 = \int_{\Omega} \left[\frac{-\hbar^2}{2m_i} w \frac{\partial u}{\partial R} + \frac{\hbar^2}{2} R \frac{\partial w}{\partial R} \left(\frac{1}{m_i} \frac{\partial u}{\partial R} \right) + \frac{\hbar^2 L^2}{2m_i R} wu + \frac{\hbar^2}{2} r \frac{\partial w}{\partial Z} \left(\frac{1}{m_i} \frac{\partial u}{\partial Z} \right) + wrVu - wrEu \right] dRdZ - \oint_{\Gamma} w d_n ds \quad (18)$$

Now, $u(R, Z)$ is approximated over a typical finite element Ω by the expression

$$u(R, Z) \approx u_h^e(R, Z) = \sum_{j=1}^{n} u_j^e \psi_j^e(R, Z) \quad (19)$$

where $u_j^e(R, Z)$ is the value of $u_h^e(R, Z)$ at the j^{th} node (R_j, Z_j) of the element .

Substituting the finite element approximation (19) for u into the weak form (18), we get

$$0 = \int_{\Omega}\left[\frac{-\hbar^2}{2m_i}w\sum_{j=1}^{n}u_j^e\frac{\partial\psi_j^e}{\partial R} + \frac{\hbar^2}{2}R\frac{\partial w}{\partial R}\left(\frac{1}{m_i}\sum_{j=1}^{n}u_j^e\frac{\partial\psi_j^e}{\partial R}\right) + \frac{\hbar^2 l^2}{2m_i R}w\sum_{j=1}^{n}u_j^e\,\psi_j^e + \frac{\hbar^2}{2}R\frac{\partial w}{\partial Z}\left(\frac{1}{m_i}\sum_{j=1}^{n}u_j^e\frac{\partial\psi_j^e}{\partial Z}\right) + wRV\sum_{j=1}^{n}u_j^e\,\psi_j^e - wRE\sum_{j=1}^{n}u_j^e\,\psi_j^e\right]dRdZ - \oint_{\Gamma}wd_n ds \quad (20)$$

This equation must hold for every admissible choice of weight function w. Since we need n independent algebraic equations to solve for the n unknowns, $u_1^e, u_2^e, \dots, u_n^e$, we choose n linearly independent functions for $w: w = \psi_1^e, \psi_2^e, \dots, \psi_n^e$. For each choice of w we obtain an algebraic relation among $(u_1^e, u_2^e, \dots, u_n^e)$. We label the algebraic equation resulting from substitution of $w = \psi_i^e$ into (20):

$$0 = \sum_{j=1}^{n}\left\{\int_{\Omega}\left[\frac{-\hbar^2}{2m_i}\psi_i^e\frac{\partial\psi_j^e}{\partial R} + \frac{\hbar^2}{2}R\frac{\partial\psi_i^e}{\partial R}\left(\frac{1}{m_i}\frac{\partial\psi_j^e}{\partial R}\right) + \frac{\hbar^2 L^2}{2m_i R}\psi_i^e\psi_j^e + \frac{\hbar^2}{2}R\frac{\partial\psi_i^e}{\partial z}\left(\frac{1}{m_i}\frac{\partial\psi_j^e}{\partial Z}\right) + RV\psi_i^e\psi_j^e - RE\psi_i^e\psi_j^e\right]dRdZ\right\}u_j^e - \oint_{\Gamma}wd_n ds;\ i,j = 1,2,\dots,n \quad (21)$$

Linear Triangular Elements:

In this section, the solution u of equation (18) is approximated by a linear function of R and Z, $u_h^e(R,Z)$ in Ω (by complete linear polynomial in R and Z), i.e.

$$u_h^e(R,Z) = \sum_{i=1}^{3}u_i^e\psi_i^e(R,Z) \quad (22)$$

when

$$\psi_i^e = \frac{1}{2A_e}(\alpha_i^e + \beta_i^e R + \gamma_i^e Z) \quad (i = 1,2,3) \quad (23)$$

With

$$2A = \alpha_1 + \alpha_2 + \alpha_3,\quad \left.\begin{matrix}\alpha_i = r_j z_k - r_k z_j\\ \beta_i = z_j - z_k\\ \gamma_i = -(r_j - r_k)\end{matrix}\right\}(i \neq j \neq k), \quad (24)$$

Now, to solve equation (13), using linear triangular element, the problem will reduce to the following generalized eigenvalue problem.

$$Ku = \lambda Mu \quad (25)$$

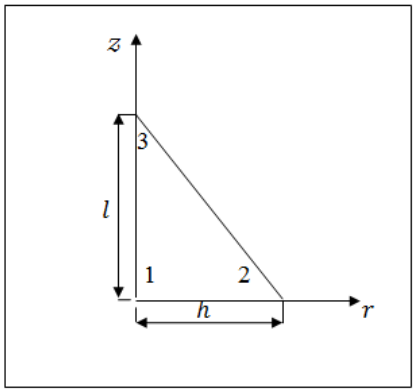
Where matrices *K and M are* n × n *matrices*, u *is the vector of unknowns of dim*ensionality *n, and n is the number of nodes*, with

$K = [K_{ij}^e]$ and $M = [M_{ij}^e], i = 1,2,\dots,n, j = 1,2,\dots,n.$

$$K_{ij}^e = \int_{\Omega}\left[\frac{-\hbar^2}{2m_i}\psi_i^e\frac{\partial\psi_j^e}{\partial R} + \frac{\hbar^2}{2}R\frac{\partial\psi_i^e}{\partial R}\left(\frac{1}{m_i}\frac{\partial\psi_j^e}{\partial R}\right) + \frac{\hbar^2 \mathrm{L}^2}{2m_i \mathrm{R}}\psi_i^e\psi_j^e + \frac{\hbar^2}{2}R\frac{\partial\psi_i^e}{\partial \mathrm{Z}}\left(\frac{1}{m_i}\frac{\partial\psi_j^e}{\partial \mathrm{Z}}\right)\right]dRd\mathrm{Z} \quad (26)$$

$$M_{ij}^e = \int_{\Omega}[V - E]R\psi_i^e\psi_j^e\,dRd\mathrm{Z} \quad (27)$$

To determine the element coefficient matrices K and M in (26) and (27), consider the right angle triangle show the Fig (2).



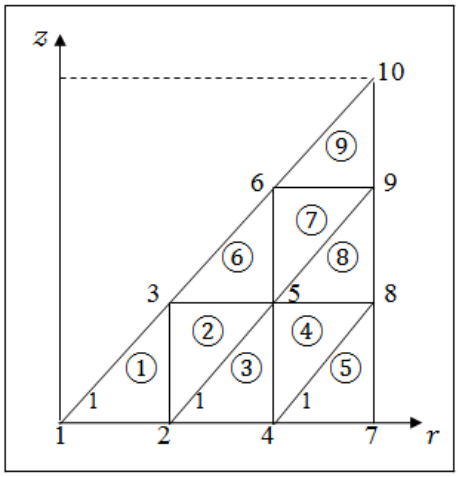
Figure(2) The right angle triangular element

As a first choice the uniform mesh are used by nine linear triangular element, as shown in Fig.(3) to represent the domain (mesh Tri1), to determine the element coefficient matrices K and M of Eq. (26) and Eq. (27) respectively.
The elements 1, 3, 5, 7, and 9 as shown in Fig.(3) are identical in orientation as well as geometry. Elements 2, 4, 6, and 8 are geometrically identical to element 1, except that it is oriented differently. If we number the local nodes of element 2 or (4, 6, and 8) to match those of element 1, then all nine elements have the same element matrices, and it is necessary to compute them only for element 1.
To evaluation of the integral in Eq. (26) and Eq. (27), it is possible to obtain the closed form for the K and M matrices by carrying out the integrals in Eq. (26) and Eq. (27) exactly respectively. We consider element 1 as the typical element. Hence, the element coefficient K and M matrices are

$$[K^e] = \frac{k_e}{2hl}\begin{bmatrix} h^2+l^2 & -h^2 & -l^2 \\ -h^2 & h^2 & 0 \\ -l^2 & 0 & l^2 \end{bmatrix} \qquad (28)$$

$$[M^e] = \frac{k_{e1}}{2hl}\begin{bmatrix} h^2l^2-2hl^2-2h^2l+h^2+2hl+l^2 & -h^2 & -l^2 \\ -h^2 & h^2 & 0 \\ -l^2 & 0 & l^2 \end{bmatrix}$$

Where $k_e = \frac{\hbar^2}{2\mathrm{m}}\frac{1}{12A}$ and $k_{e1} = [\mathrm{V}-\mathrm{E}]\frac{1}{12A}$



Figuer(3) The uniform mesh Tri1 of nine linear triangular element.

Then the mesh shown in Fig. (3), will be as

$$K = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}$$

where

$$A_{11} = \begin{bmatrix} k_{11}^1 & k_{12}^1 & k_{13}^1 \\ k_{21}^1 & k_{22}^1+k_{33}^2+k_{11}^3 & k_{23}^1+k_{32}^2 \\ k_{31}^1 & k_{32}^1+k_{23}^2 & k_{33}^1+k_{22}^2+k_{11}^{12} \end{bmatrix},$$

$$A_{12} = \begin{bmatrix} 0 & 0 & 0 \\ k_{12}^3 & k_{31}^2+k_{13}^3 & 0 \\ 0 & k_{21}^2+k_{12}^6 & k_{13}^6 \end{bmatrix},$$

$$A_{13} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

$$A_{21} = \begin{bmatrix} 0 & k_{21}^3 & 0 \\ 0 & k_{13}^2+k_{31}^3 & k_{12}^2+k_{21}^6 \\ 0 & 0 & k_{31}^6 \end{bmatrix},$$

A_{22}

$$= \begin{bmatrix} k_{22}^3+k_{33}^4+k_{11}^5 & k_{12}^1 & 0 \\ k_{21}^1 & k_{11}^2+k_{33}^3+k_{22}^4+k_{22}^6+k_{33}^7+k_{11}^8 & k_{23}^6+k_{32}^7 \\ 0 & k_{32}^6+k_{23}^7 & k_{33}^6+k_{22}^7+k_{11}^9 \end{bmatrix} \qquad (29)$$

$$A_{23}=\begin{bmatrix} k_{21}^{5} & k_{31}^{4}+k_{13}^{5} & 0 & 0 \\ 0 & k_{21}^{4}+k_{12}^{8} & k_{31}^{7}+k_{13}^{8} & 0 \\ 0 & 0 & k_{21}^{7}+k_{12}^{8} & k_{13}^{9} \end{bmatrix},$$

$$A_{31}=\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

$$A_{32}=\begin{bmatrix} k_{21}^{5} & 0 & 0 \\ k_{13}^{4}+k_{31}^{5} & k_{12}^{4}+k_{21}^{8} & 0 \\ 0 & k_{13}^{7}+k_{31}^{8} & k_{12}^{7}+k_{21}^{9} \\ 0 & 0 & k_{31}^{9} \end{bmatrix},$$

$$A_{33}=\begin{bmatrix} k_{22}^{5} & k_{23}^{5} & 0 & 0 \\ k_{32}^{5} & k_{11}^{4}+k_{33}^{5}+k_{22}^{8} & k_{23}^{8} & 0 \\ 0 & k_{32}^{8} & k_{11}^{7}+k_{33}^{8}+k_{22}^{9} & k_{23}^{9} \\ 0 & 0 & k_{32}^{9} & k_{33}^{9} \end{bmatrix}.$$

The above assembled coefficient matrix for finite element mesh is of order 10×10. In this case the sub matrices (the integrals) of k_{ij}^{e} compute by an analytic method. The MATLAB program is used to solve the sub matrices (the integrals) of k_{ij}^{e}.
It is important to mention that the elements of the above sub matrices (the integrals) of $k_{\mathrm{ij}}^{\mathrm{e}}$ are calculated by an analytic method

Notes (1):
In the following example, the representative set of parameters were used for the calculations as:
For $InAs$, the energy gap $E_g = 0.42$ eV, $\Delta_1 = 0.38\, eV$, $m_1(0) = 0.024\, m_0$.
For $GaAs$, the energy gap $E_g = 1.52$ eV, $\Delta_1 = 0.34\, eV$, $m_1(0) = 0.067\, m_0$. The band offset parameter is taken as $V_0 = 0.55$ eV.

Example (1):

Consider the Nanoscal $InAs/GaAs$, quantum ring model, with using the above date to solve $InAs/GaAs$, nanostructures quantum ring.

In this example the linear triangular element we used to solve equation (13).

Equation (13) is solved using MATLAB program at $\boldsymbol{n = 1296}$. The results are shown in Fig (4).

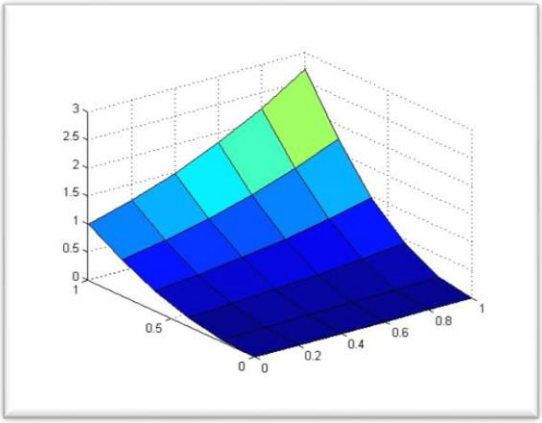


Figure. (4) The calculators of equation (13).

Conclusions

The finite element method using different base linear triangular elements are used for solving the nanoscale structures consisting of the InAs/GaAs quantum ring, and the spin-dependent on the Ben Daniel-Duke boundary conditions. The results of numerical example are gives a good accuracy and efficiency of this method.

References

[1] D. L. Mathine, S. K. Myjak and G. N. Maracas ‘‘A Computational Fourier Series Solutin of the BenDaniel-Duke Hamiltonian for Arbitrary Shaped Quantum Wells’’ IEEE Journal of Quantum Electronics, Vol. 31, (1995), pp. 1216-1222.

[2] G. Paasch, P. H. Nguyen and G. Gobsch ‘‘Envelope Equation and Wave Function Matching for Narrow-Gap Semiconductors’’ Physica Status Solidi (b), Vol. 162, No. 1 (1990), pp. 155–163.

[3] D. Sarkara, A. Deyasib ‘‘Field Induced Tuning of DOS and Eigenstates in Double Quantum Well Structure having Gaussian Geometry’’ American Scientific Publishers , Vol. 5, No. 1, (2016), pp. 138-143.

[4] M. Willatzence, R. Melnik, C. Galeriu and

L. C. Lew Yan Voon ‘‘Finite Element Analysis of Nanowire Superlattice Structures’’ Springer, Vol. 31, (2003), pp. 755‑763.

[5] Yiming Li, ‘‘An Iterative Method for Single and Vertically Stacked Semiconductor Quantum Dots Simulation’’ Mathematical and Computer Modelling, Vol. 42, (2005), pp. 711‑718.

[6] Yiming Li, O. Voskoboynikov, C.P. Lee, S.M. Sze ‘‘Computer simulation of electron energy levels for different shape InAs/ GaAs semiconductor quantum dots’’ Computer Physics Communications, Vol. 141, (2001), pp. 66-72.

[7] Yiming Li, O. Voskoboynikov, C.P. Lee, S.M. Sze O. Tretyak ‘‘Electron energy state spin-splitting in 3D cylindrical semiconductor quantum dots’’ THE EUROPEAN PHYSICAL JOURNAL B, Vol. 28, No. 8 (2002), pp. 475–481.