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# The Ben Daniel–Duke model in general nanowire structures

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## Abstract

A simple computationally effective method is developed for solving the Ben Daniel–Duke equations for nanowire semiconductor heterostructures. The method allows eigenstates and associated energy levels of nanowires with varying cross-sectional shape and/or varying composition to be obtained, and is based on expanding the envelope function eigenstates on local eigenstates of the corresponding cross-sectional problem. In this way, the original partial differential equation problem is reduced to a set of coupled ordinary differential equations (this set can to a good approximation be limited to a small number of coupled equations). In the first part of the paper, the model equation framework is derived; it can be easily modified to account for a more general set of partial differential equations. In the second part of the paper, three different cases of axisymmetrical nanowire problems are analysed in terms of eigenstates and energy eigenvalues. The cases considered are (a) conical nanowires, (b) a nanowire with a step in radius, and (c) a conical GaAs/GaAlAs nanowire. Comparison with computationally more expensive finite-element results on a two-dimensional domain is made, and good agreement is found.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

With recent advances in semiconductor growth technology [1], possibilities of growing complicated geometrical nanostructures exist [2–6]. In addition, growth-intended simple geometrical nanostructures in reality suffer from size variations, impurities, dislocations, and geometry imperfections. As a consequence, there is a need for understanding the influence of more complicated nanostructure geometries on electron eigenstates and eigenvalues [7, 8]. The present work derives a simple and often effective computational model for solving Ben Daniel–Duke models [9] for nanowires with varying cross-sectional shape. Moreover, the method is easy to implement for more complicated partial differential equation systems. In the first part of

the paper, the Ben Daniel–Duke model is transformed following a procedure originally due to Stevenson [10, 11], who used the method to solve problems in electromagnetics and acoustics. The basis of the model is to expand the envelope function in a set of local basis functions satisfying part of the differential equation. The benefit of the present model is that for the lower-lying states only very few (sometimes one to two) local basis functions are needed so as to obtain the envelope functions and associated energies. In the second part of the paper, the mathematical model is applied to solve three cases of axisymmetric nanowire geometry structures in terms of eigenstates and energy eigenvalues: (a) conical nanowires, (b) a nanowire with a step in radius, and (c) a conical GaAs/GaAlAs nanowire. Comparison with second-order Lagrangian finite-element method calculations on a two-dimensional domain is provided and good agreement is found.

## 2. Theory

Allowing for variations in the effective mass  $m(z)$  and the band edge potential  $V(z)$  along the axial direction being the assumed heterostructure stacking direction, the Ben Daniel–Duke equation for the conduction-band envelope function reads

$$-\frac{\partial}{\partial z} \left( \frac{\hbar^2}{2m(z)} \frac{\partial \psi}{\partial z} \right) - \frac{\hbar^2}{2m(z)} \vec{\nabla}^2 + (V(z) - E) \psi = 0, \quad (1)$$

with  $\psi$  and  $E$  the conduction-band envelope function and its associated energy, respectively. In this work,  $\vec{\nabla}^2$  denotes the two-dimensional (in-plane) Laplacian.

We seek to determine an ordinary set of differential equations in the axial coordinate following the procedure originally proposed by Stevenson [10, 11]. This is done by introducing a set of orthonormal eigenfunctions  $u_n$  and associated eigenvalues  $\alpha_n^2$  defined by

$$\left( \vec{\nabla}^2 + \alpha_n^2 \right) u_n = 0, \quad \text{in } S(z), \quad (2)$$

$$u_n = 0, \quad \text{on } \partial S(z), \quad (3)$$

$$\int_{S(z)} u_n u_m = \delta_{nm}, \quad (4)$$

where  $\partial S(z)$  is the boundary of the cross section  $S(z)$  and  $\delta_{nm}$  is Kronecker's delta ( $\delta_{nm} = 1$  if  $n = m$ ;  $\delta_{nm} = 0$  if  $n \neq m$ ). Rewriting equation (1), multiplying by  $u_n$ , and integrating over the cross-sectional area  $S(z)$  yields

$$-\int_{S(z)} u_n \frac{\partial}{\partial z} \left( \frac{\hbar^2}{2m(z)} \frac{\partial \psi}{\partial z} \right) dS - \frac{\hbar^2}{2m(z)} \int_{S(z)} u_n \vec{\nabla}^2 \psi dS + (V(z) - E) \int_{S(z)} u_n \psi dS = 0. \quad (5)$$

Next, using that for every  $z$  the set of functions  $u_n$  constitutes a complete set of functions for our problem, the envelope function can be written as

$$\psi = \sum_n \phi_n(z) u_n(z, \vec{r}), \quad (6)$$

where  $\vec{r}$  are coordinates perpendicular to the  $z$ -direction. A few manipulations lead to the coupled set of ordinary differential equations (ODEs) in the coefficients  $\phi_n$ :

$$-\frac{\partial}{\partial z} \left( \frac{\hbar^2}{2m(z)} \frac{\partial \phi_n}{\partial z} \right) - \sum_m A_{nm} \left( \frac{\partial}{\partial z} \left( \frac{\hbar^2}{2m(z)} \phi_m \right) + \frac{\hbar^2}{2m(z)} \frac{\partial \phi_m}{\partial z} \right) + \sum_m Y_{nm} \phi_m = E \phi_n, \quad (7)$$

$$Y_{nm} = -\frac{\hbar^2}{2m(z)} C_{nm} + \left( V(z) + \frac{\hbar^2}{2m(z)} \alpha_n^2 \right) \delta_{nm}, \quad (8)$$

with

$$\begin{aligned} A_{nm} &= \int_{S(z)} u_n \frac{\partial u_m}{\partial z} dS, \\ C_{nm} &= \int_{S(z)} u_n \frac{\partial^2 u_m}{\partial z^2} dS. \end{aligned} \quad (9)$$

Here, we have used that

$$\begin{aligned} \frac{\partial}{\partial z} \left( \frac{\hbar^2}{2m(z)} \frac{\partial \psi}{\partial z} \right) &= \sum_m \left[ \frac{\partial}{\partial z} \left( \frac{\hbar^2}{2m(z)} \frac{\partial \phi_m}{\partial z} \right) u_m \right. \\ &\quad \left. + \left( \frac{\partial}{\partial z} \left( \frac{\hbar^2}{2m(z)} \phi_m \right) + \frac{\hbar^2}{2m(z)} \frac{\partial \phi_m}{\partial z} \right) \frac{\partial u_m}{\partial z} + \frac{\hbar^2}{2m(z)} \phi_m \frac{\partial^2 u_m}{\partial z^2} \right]. \end{aligned} \quad (10)$$

Equations (7) and (8) are the Stevenson equations for the Ben Daniel–Duke model that are relevant for the case of modulated nanowire structures. It is important to realize that the model equations above allow for any variation in the nanowire cross-sectional shape with axial position as well as heterostructure material modulation along the axis.

In order to get an idea about the order of the error involved by restricting the above infinite set of coupled ODEs to a finite set we turn to perturbative theory in the form introduced by Löwdin [12]. For simplicity, we discuss the case where the infinite set is restricted to one single ODE; however, restrictions to larger sets of ODEs can be handled in a similar manner.

Consider the error introduced by solving the single ODE:

$$-\frac{\partial}{\partial z} \left( \frac{\hbar^2}{2m(z)} \frac{\partial \phi_1^{(l)}}{\partial z} \right) - A_{11} \left( \frac{\partial}{\partial z} \left( \frac{\hbar^2}{2m(z)} \phi_1^{(l)} \right) + \frac{\hbar^2}{2m(z)} \frac{\partial \phi_1^{(l)}}{\partial z} \right) + Y_{11} \phi_1^{(l)} = E_{1l}^{(0)} \phi_1^{(l)}, \quad (11)$$

where superscript  $l$  distinguishes the different eigenvalues and associated eigenfunctions. First, we introduce the differential operator  $\mathcal{D}$  such that equation (7) takes the form

$$D\bar{\phi} = E\bar{\phi}, \quad (12)$$

where  $\bar{\phi} = (\phi_1, \phi_2, \dots)^T$ , i.e.,

$$D_{nm} = -\delta_{nm} \frac{\partial}{\partial z} \frac{\hbar^2}{2m(z)} \frac{\partial}{\partial z} - A_{nm} \left( \frac{\partial}{\partial z} \frac{\hbar^2}{2m(z)} + \frac{\hbar^2}{2m(z)} \frac{\partial}{\partial z} \right) + Y_{nm}. \quad (13)$$

We next define an unperturbed operator  $\mathcal{D}_0$  by

$$[\mathcal{D}_0]_{nm} = \begin{cases} \mathcal{D}_{11} & \text{for } m = n = 1 \\ -\delta_{nm} \left[ \frac{\partial}{\partial z} \frac{\hbar^2}{2m(z)} \frac{\partial}{\partial z} + \left( V(z) + \frac{\hbar^2}{2m(z)} \alpha_n^2 \right) \right] & \text{else.} \end{cases} \quad (14)$$

The remaining part of  $\mathcal{D}$  is denoted  $\mathcal{V}$  and will be treated as a perturbation, i.e.,  $\mathcal{D} = \mathcal{D}_0 + \mathcal{V}$ . According to perturbation theory [12], the error in the energy  $E_{1l}^{(0)}$  is now given by

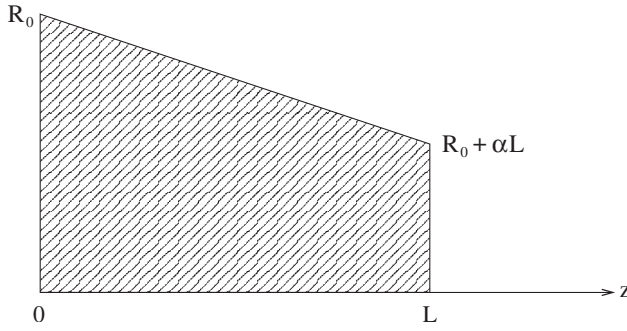
$$\Delta E_{1l} = \sum_{m \neq 1, k} \frac{\langle 1l | \mathcal{V} | mk \rangle \langle mk | \mathcal{V} | 1l \rangle}{E_l^{(0)} - E_{mk}^{(0)}} + \mathcal{O} \left( \left( \frac{1}{E_l^{(0)} - E_{mk}^{(0)}} \right)^2 \right), \quad (15)$$

where

$$\langle nl | \mathcal{V} | mk \rangle = \int \phi_n^{(l)} \mathcal{V}_{nm} \phi_m^{(k)} dz, \quad (16)$$

and  $E_{mk}^{(0)}$  and  $\phi_m^{(k)}$  are solutions to

$$-\frac{\partial}{\partial z} \left( \frac{\hbar^2}{2m(z)} \frac{\partial \phi_m^{(k)}}{\partial z} \right) + \left( V(z) + \frac{\hbar^2}{2m(z)} \alpha_m^2 \right) \phi_m^{(k)} = E_{mk}^{(0)} \phi_m^{(k)}. \quad (17)$$



**Figure 1.** Geometry of the conical nanowire structure.

**Table 1.** Material parameters used.

Material	Effective mass ( $m_0$ )	Band edge (eV)
GaAs	0.067	0
GaAlAs	0.092	0.256

In equation (15), we have assumed that  $\phi_1^{(l)}$  is a non-degenerate solution to  $\mathcal{D}_0$ . The reason why  $\mathcal{V}_{nm}$  appears in expression (16) is that this element alone couples the eigensolutions of  $[\mathcal{D}_0]_{nn}$  with the eigensolutions of  $[\mathcal{D}_0]_{mm}$ . Unfortunately, we do not know the size of the  $\langle nl|\mathcal{V}|mk\rangle$  elements in general but obviously the larger  $E_{1l}^{(0)} - E_{mk}^{(0)}$  is the better our approach will be. Assuming that  $u_1$  is the ground state to the cross-sectional problem, we immediately see that  $E_{1l}^{(0)} - E_{mk}^{(0)}$  will be large as long as we have small cross sections, i.e., our approach is less applicable to structures with larger cross sections as expected. Furthermore, observe that only energies close to the ground state are expected to be well captured. We shall nevertheless demonstrate that extending the number of ODEs to three increases the accuracy substantially when applied to problems where larger cross sections are involved, i.e., problems for which the radius is comparable to the axial length of the structure.

### 3. Numerical results and discussions

In this section, we consider three cases of axisymmetric nanowire geometries to demonstrate the capabilities of the method derived above. The three cases to be examined are (a) conical nanowire structures, (b) a nanowire step structure with a smooth change in radius, and (c) a conical nanowire heterostructure. The material used in the first two examples is GaAs while in the third a GaAs/GaAlAs nanowire heterostructure is considered. Material data used in the computations are given in table 1. These three cases cannot be handled analytically, thus their solution using the present model demonstrates the usefulness of the method.

First, consider nanowires with varying radius  $R(z)$  given by

$$R(z) = R_0 + \alpha z, \quad (18)$$

as shown in figure 1. We have made calculations for three different sets of parameters: (a1)  $\alpha = -0.15$  and  $R_0 = 3$  nm, (a2)  $\alpha = -0.3$  and  $R_0 = 6$  nm, and (a3)  $\alpha = -0.6$  and  $R_0 = 12$  nm. The length of the wire is in all three cases 10 nm. We have chosen these geometries in order to study how good the method is for wires of different size. To compare we have also solved the full problem, i.e., solving the eigenvalue problem given in equation (1), using a second-order Lagrangian finite-element method (FEM). As a solver, we use Comsol Multiphysics so as to ensure convergence of eigenvalues to within 0.01 meV, and we refine

**Table 2.** Energies for the first three envelope eigenstates for the structure shown in figure 1 with  $\alpha = -0.15$ ,  $R_0 = 3$  nm, and  $L = 10$  nm.

Eigenstate	$n = 1$ (eV)	$n = 3$ (eV)	FEM (eV)
Ground state	0.639	0.639	0.639
First excited state	0.929	0.928	0.928
Second excited state	1.251	1.249	1.249

**Table 3.** Energies for the first three envelope eigenstates for the structure shown in figure 1 with  $\alpha = -0.3$ ,  $R_0 = 6$  nm, and  $L = 10$  nm.

Eigenstate	$n = 1$ (eV)	$n = 3$ (eV)	FEM (eV)
Ground state	0.222	0.222	0.221
First excited state	0.411	0.408	0.408
Second excited state	0.694	0.686	0.685

**Table 4.** Energies for the first three envelope eigenstates for the structure shown in figure 1 with  $\alpha = -0.6$ ,  $R_0 = 12$  nm, and  $L = 10$  nm.

Eigenstate	$n = 1$ (eV)	$n = 3$ (eV)	$n = 4$ (eV)	FEM (eV)
Ground state	0.104	0.102	0.102	0.102
First excited state	0.276	0.256	0.256	0.254
Second excited state	0.557	0.297	0.297	0.298

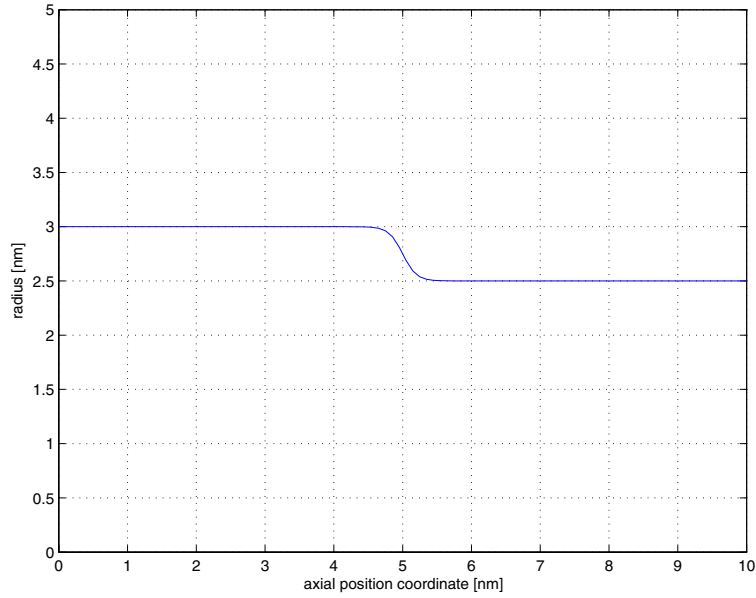
the mesh until this accuracy is obtained. The first three computed energy eigenvalues for the parameter set (a1) using one and three cross-sectional  $u_n$  functions are listed in table 2. Comparing to the FEM eigenvalues also shown in table 2 we see that for nanowires this small we get good agreement using only one cross-sectional function. In table 3, we show the first three eigenvalues for the parameter set (a2). Here we observe that if only one cross-sectional function is used the energy of the ground state is well captured; however, the energy of the first excited state shows some deviation, and for the energy of the second excited state it is even worse. When we use three cross-sectional functions we get agreement with the FEM results to within 1 meV. The eigenvalues obtained when using the last parameter set (a3) are shown in table 4. We see that the energy of the ground state is still reasonably well captured using only one cross-sectional function, but the energy of the first excited state is 22 meV too high, and the energy of the second excited state is completely wrong. However, when we use three cross-sectional functions we again get good agreement with the FEM results for all three states. Hence, we observe that the error introduced using the above method follows the observations made in the previous section.

Second, consider a nanowire step structure with a varying radius  $R(z)$  as follows:

$$R(z) = R_0 + \frac{1}{2} (R_1 - R_0) \left[ 1 + \tanh \left( \frac{z - z_0}{\delta} \right) \right],$$

$$R_0 = 3.0 \text{ nm}, \quad R_1 = 2.5 \text{ nm}, \quad \delta = 0.1 \text{ nm}, \quad z_0 = 5 \text{ nm}, \quad (19)$$

as shown in figure 2. In figure 3 we show the  $z$ -dependence of the first two modal contributions to the first three eigenfunctions. As expected, we see that the main contribution comes from the first modal function ( $n = 1$ ). In addition, we see that the number of nodes equals the solution number minus 1, i.e., the groundsheet has zero nodes, the first-excited state one node, etc. The ground state is tilted towards the nanowire structure end with the largest radius, i.e., where the geometric confinement is weakest. The eigenvalues are listed in table 5.



**Figure 2.** Geometry of the nanowire step structure.

**Table 5.** First three eigenvalues for the nanowire step structure shown in figure 2.

Eigenstate	Energy (eV)
Ground state	0.496
First excited state	0.695
Second excited state	0.971

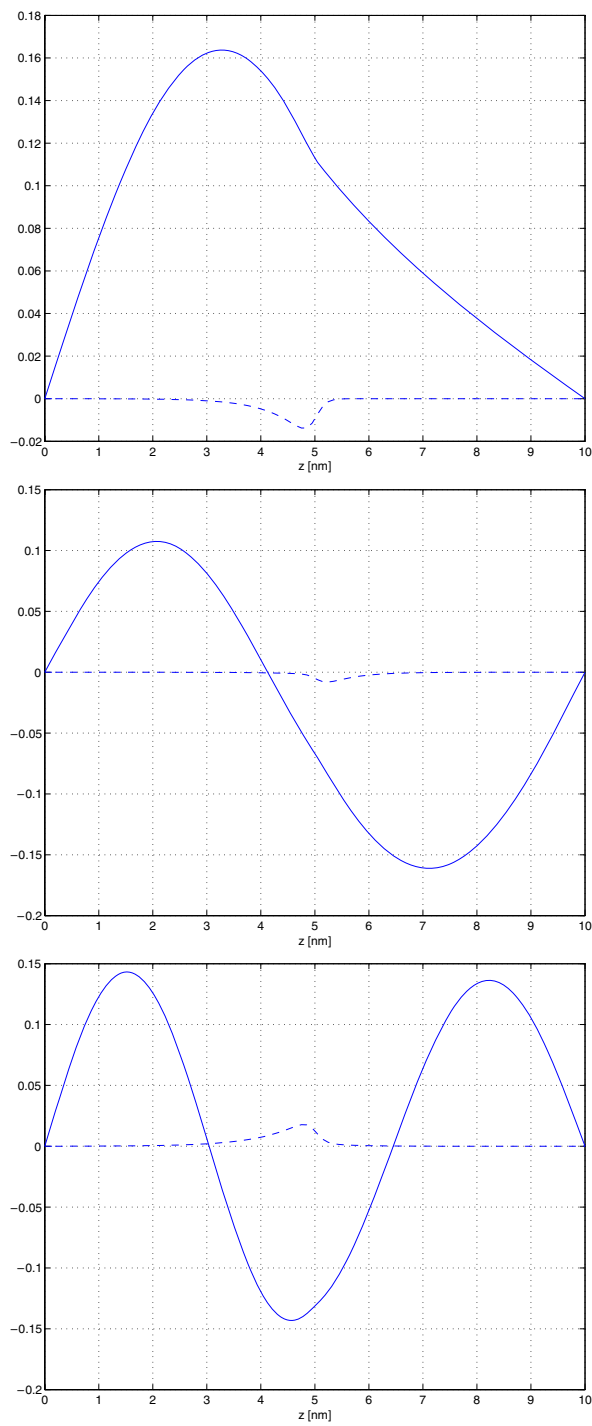
**Table 6.** Energies for the first three envelope eigenstates for the GaAs/GaAlAs heterostructure nanowire with the geometry shown in figure 1. Parameters  $\alpha = -0.1$ ,  $R_0 = 3$  nm, and  $L = 10$  nm are used and the heterostructure effect on effective mass is shown in figure 4 (a similar behaviour is imposed for the potential).

Eigenstate	$n = 1$ (eV)	FEM (eV)
Ground state	0.618	0.620
First excited state	0.797	0.805
Second excited state	1.024	1.023

Finally, we study a conical GaAs/GaAlAs nanowire heterostructure with geometric parameters  $\alpha = -0.1$ ,  $R_0 = 3$  nm and  $L = 10$  nm. Instead of assuming a abrupt interface we use the smooth step function given by

$$\Theta(z) = \frac{1}{2} \left( 1 + \tan \left( \frac{z - z_0}{\delta} \right) \right), \quad (20)$$

with  $\delta = 0.2$  nm. We consider a five-layer structure, i.e., the effective mass is given according to the function shown in figure 4 and the potential has a similar behaviour. In table 6 we show the first three eigenvalues found using one cross-sectional function and the corresponding results obtained when employing the FEM. Here we see, that the above method gives good results also for the case of a heterostructure.

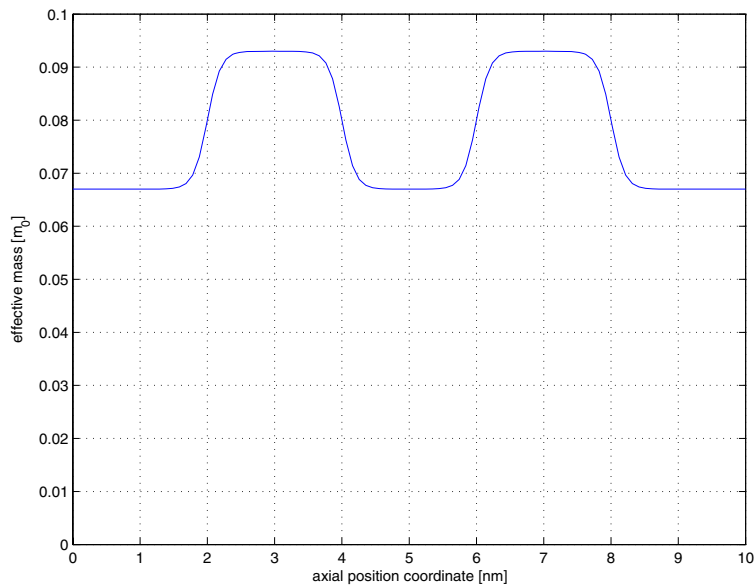


**Figure 3.** Plots of the first two modal contributions (i.e.,  $\phi_1$  and  $\phi_2$ ) to the first three eigenstates (solid—mode 1; dashed—mode 2) as a function of the axial coordinate corresponding to the nanowire step structure shown in figure 2. The upper, middle, and lower plots are the ground state, the first excited state, and the second excited state, respectively.

#### 4. Conclusions

The Ben Daniel–Duke model for semiconductor nanowire heterostructures is solved using a computational effective method due to Stevenson [10, 11] who originally applied the method





**Figure 4.** The functional  $z$ -dependence of the effective mass.

to problems in electromagnetics and acoustics. In the first part of the paper, the general set of coupled ordinary differential equations is obtained from the Ben Daniel–Duke partial differential equation. Output of the model include the envelope eigenstates and associated energy eigenvalues. A strong asset of the present method is that only a small number of coupled ordinary differential equations is needed so as to obtain good accuracy in the solutions. Moreover, also problems without axisymmetry conditions can be handled and the method is easily extendable to other partial differential equation problems. In the second part of the paper, three cases of nanowire structures are analysed in terms of eigenstates and energy eigenvalues. These include: (a) conical nanowires, (b) a nanowire with a step in radius, and (c) a conical GaAs/GaAlAs nanowire. Comparison with computationally more extensive second-order Lagrangian finite-element method calculations on a two-dimensional domain shows good agreement.

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