phys. stat. sol. (b) **196**, 63 (1996)

Subject classification: 73.61; 71.15

Department of Electrical and Computer Engineering, Wayne State University, Detroit[1])

Boundary Least Squares Method for the Solution of Schrödinger's Equation in Quantum Wires

By

YU. M. SIRENKO[2]) and V. MITIN

(Received February 2, 1996)

We present a method for the approximate semianalytical calculation of wave functions and eigenenergies in systems consisting of domains with known bulk solutions of the corresponding Schrödinger equation (e.g. with piecewise constant potential). The trial wave function is written as a normalized linear combination of several bulk solutions for the given energy. The coefficients of the linear combination are found by minimization of the integral of square mismatch along the boundaries. Mathematically the problem is equivalent to the minimization of the Rayleigh quotient or solution of the generalized eigenproblem for the vector of coefficients. The value of the residual provides an estimation of the accuracy of the results and gives the possibility to choose an optimal set of trial functions. We illustrate the use of the method by calculation of eigenfunctions of infinitely long triangular and quadrilateral wires.

1. Introduction

Over two decades of research on low-dimensional systems has resulted in the creation of a large variety of artificially grown structures with space quantization that have found numerous applications in high-speed electronic and optoelectronic devices. The growing needs of device designers and manufacturers for full-featured device simulation have brought into existence a fast-growing industry of CAD software allowing to predict the physical behavior of optoelectronic structures with confined geometries, device characteristics, and their circuit performance.

A common feature of these packages is a solution of the set of partial differential equations to find self-consistently the distribution of charge, current, and radiated light in the structure. This complex mathematical problem requires heavy numerical calculations and takes a considerable amount of computer time. Computer simulation of nanostructure devices demands also the solution of the Schrödinger equation for the carriers increasing drastically the computer time consumption. On the other hand, consideration of mesoscopic systems and the problem of electron ballistic transport in confined geometries requires a *semianalytical* solution of the Schrödinger equation which allows calculations for flexible system geometry and accurate treatment of up to several orders of magnitude change in the calculated values, e.g. transmission probabilities.

[1]) Detroit, Michigan 48202, USA.

[2]) Present address: Department of Electrical and Computer Engineering, North Carolina State University, Raleigh, North Carolina 27695-7911, USA. E-mail: sirenko@ccehp1.ncsu.edu.

From the mathematical point of view, the description of the electron systems with space quantization starts with calculation of the eigenfunctions of the system by solution of the corresponding wave equation. Unfortunately, the exact analytical solution of the wave equation exists only for a limited set of geometries (quantum well, rectangular and cylindrical quantum wire, etc.) which do not cover all systems of interest. Numerical solutions result in tables of values which should be processed numerically, in contrast to analytical solutions, for which such quantities as form factors, transition probabilities, etc., can often be evaluated analytically, reducing drastically the amount of calculations.

Therefore, the search of nonconventional numerical techniques allowing to diminish the amount of computation while preserving the accuracy and conveniency of the analytical solutions, is of major importance. Within the proposed boundary least squares method (BLSM) for the solution of the wave equation, a significant reduction of computational time can be achieved at the sacrifice in universality and owing to a proper account of the known bulk solution of the equation.

The rest of the paper is presented as follows. Section 2 provides a brief classification of numerical schemes for numerical solution of the wave equation based on the weighted residuals method. The BLSM is introduced in Section 3 and applied in Section 4 to calculation of eigenfunctions in infinitely deep triangular and quadrilateral quantum wires. Coefficients of overlap matrices required for the solution of the problem are presented in the Appendix.

2. Method of Weighted Residuals

In order to compare advantages and disadvantages of different numerical approaches we provide a brief classification of numerical methods for the solution of partial differential equations based on the *weighted residuals method* [1].

We assume that the linear differential (eigen)equation

$$\mathscr{S}\psi = 0 \tag{1}$$

should be solved in the domain S subject to the linear boundary condition

$$\mathscr{L}\psi = 0 \tag{2}$$

on the boundary L (i.e. perimeter of the domain).

The approximate solution $\tilde{\psi}$ is constructed as a linear combination of the set of *trial* functions $\{\psi_i\}$,

$$\tilde{\psi} = \sum_i c_i \psi_i \,. \tag{3}$$

In a *boundary method* the trial functions satisfy exactly the differential equation (1), $\mathscr{S}\psi_i = 0$, and the *residual* is calculated over the boundary,

$$R = \mathscr{L}\tilde{\psi} = \sum_i c_i \mathscr{L}\psi_i \,. \tag{4a}$$

On the other hand, in an *interior method* the boundary conditions are satisfied exactly, $\mathscr{L}\psi_i = 0$, and the residual is calculated in the interior of the domain,

$$R = \mathscr{S}\tilde{\psi} = \sum_i c_i \mathscr{S}\psi_i \,. \tag{4b}$$

To obtain the approximate solution (3) the coefficients $\{c_j\}$ should be found, minimizing in some sense the residual (4). In the weighted residual method another set of *test* functions $\{\phi_j\}$ is introduced, and the coefficients of the linear combination (3) are obtained from the requirement of orthogonality of the residual R to each test function,

$$\sum_i c_i \langle \mathscr{S}\psi_i, \phi_j \rangle = 0 \quad \text{or} \quad \sum_i c_i \langle \mathscr{L}\psi_i, \phi_j \rangle = 0 \,. \tag{5}$$

Thus, the solution of the eigenproblem (1) is reduced to the system of linear algebraic equations (5). If the set of trial functions coincides with the set of test functions the described procedure is called Galerkin method.

A distinction is made also between the *local* and *global* methods depending on whether the individual trial and test functions span the whole domain or a part of it.

The standard methods in device numerical simulation are *finite difference* and *finite elements* methods (see, e.g. [2 to 7]). In fact, both of them are subclasses of *local* interior weighted residual methods with trial functions defined on the points of the mesh or, usually, relatively small triangular or quadrangular subdomains. A group of boundary element methods [8] is also coming into use.

Main advantages of these methods are universality, existence of ready-to-use packages, and orthogonality of different test functions leading to well-conditioned matrices. However, the solution is obtained in the form of a table and is much less convenient than the analytical form (especially if interpolation, differentiation, and subsequent calculation of the matrix elements of transition are necessary). Moreover, to obtain a reasonable accuracy, a large number of elements N should be used, and the calculation of the eigenvalues of the resulting $N \times N$ matrix is very time consuming. Application of these methods runs into difficulties for problems with singularities.

Obvious benefits of analytical (versus numerical) forms of solution brought into use the *global* methods, where the trial functions ψ_i span the whole domain. In the *interior* version the basis functions satisfy automatically the given boundary conditions and are chosen to possess the proper symmetry of the problem and required asymptotic behavior. With the most popular choice of the trial functions as Gaussians with different exponential factors, this method was applied to the calculation of valence band structure in quantum wires [9], donor [10] and acceptor[11] energy spectrum in low-dimensional structures, etc.

Another version of global interior methods is the Rayleigh-Ritz *variational procedure.* In the case where the variational parameters are just the coefficients of the linear combination (3), this technique is a subclass of the weighted residuals method. In the nonlinear version the parameters enter the argument of a general function, usually as exponent. Though the latter approach is one of the oldest in quantum mechanics and is standard now for the exciton-type problems in confined geometries [12], its applicability is limited to the ground and few first excited states and the accuracy is rather poor.

One of the most successful methods in the semianalytical solution of the Schrödinger equation in restricted configurations is the borrowed from waveguiding theory [13, 14] global boundary method called the *mode-matching technique.* Being essentially a Galerkin-type global boundary technique, the method is applied to a set of subdomains where the wave equation is separable by matching the modes of neighboring subdomains at the boundary.

Over the last seven years the mode-matching technique has been successfully applied to the calculation of transmission coefficients in ballistic electron waveguides, such as nanosize L- and T-junctions [15] and multiple-bend junctions [16], crossed four-terminal junctions [17], coupled parallel waveguides [18], constriction between two two-dimensional [19] and three-dimensional electron gases [20]. Recently other than rectangular subdomains were considered in the problems of sharply bent waveguides [21] and circular bends [22].

3. Boundary Least Squares Method

Despite the obvious success of the mode-matching technique in applications to electromagnetic and electronic waveguides, there is a number of factors which limit its applicability. The most important restriction is the requirement that subdomains should be of the form in which the wave equation is separable (rectangular, sectors, etc.). The method also is inconvenient for the consideration of waveguides with a variable effective mass.

Moreover, the trial wave functions are strictly specified by the geometry of a problem, which quite often leads to slow convergence of the solution and strongly evanescent modes with unphysically large coefficients. At last, there is no built-in criterion of accuracy of the obtained solution, the convergence is estimated from the comparison of the results of calculation with a different number of trial functions.

The global boundary least squares method [1] combines the main advantage of the mode-matching technique – the usage of the known general analytical solution for an infinite domain – with the universality, applicability to almost arbitrary shape of domain, flexibility in the choice of the set of trial functions, and the built-in indicator of the accuracy of the obtained solution, the least-squares deviation from the specified boundary conditions.

In order to introduce the main idea of the method we consider the construction of the approximate solution for a two-dimensional Schrödinger (wave) equation in the *single finite* domain S subject to the zero boundary conditions on the perimeter L of the domain.

We take a set $\psi_i^{(E)}(x, y)$ of linearly independent bulk solutions of the Schrödinger equation corresponding to the energy E. The trial eigenfunctions for the wave equation in the domain S are sought as a linear combination of the bulk solutions

$$\psi^{(E)} = \frac{1}{\sqrt{\mathcal{N}}} \sum_{i=1}^{n} c_i \psi_i^{(E)}, \tag{6}$$

where the positively defined quadratic form

$$\mathcal{N} \equiv \int_S |\psi^{(E)}|^2 \, \mathrm{d}s = \sum_{i,j=1}^{n} c_i c_j N_{ij} \equiv \mathbf{C}^{\mathrm{T}} N \mathbf{C} \tag{7}$$

is introduced for normalization.

Here $\mathbf{C} = (c_1, \ldots, c_n)^{\mathrm{T}}$ is a vector of coefficients in a linear combination (6) and the normalization matrix N is given by

$$\|N\|_{ij} \equiv N_{ij} = \iint \mathrm{d}x \, \mathrm{d}y \, \psi_i^{(E)} \psi_j^{(E)}. \tag{8}$$

The first step in obtaining the approximate eigensolution of the wave equation is to optimize (make minimal) with respect to coefficients $\mathbf{C}$ the functional of square devia-

tion $\mathscr{R}(E)$ from the required boundary conditions for a given energy E. In case of a closed domain with zero boundary conditions (infinitely high well) we have

$$\mathscr{R}(E) = \min_{c_1, \ldots, c_n} \oint_L |\psi^{(E)}|^2 \, \mathrm{d}l \,, \tag{9}$$

or, equivalently,

$$\mathscr{R}(E) = \min_{\mathbf{C}} \frac{\mathscr{F}}{\mathscr{N}} \,, \tag{10}$$

where

$$\mathscr{F} = \sum_{i,j=1}^{n} c_i c_j F_{ij} = \mathbf{C}^{\mathrm{T}} F \mathbf{C} \tag{11}$$

is a non-negatively defined quadratic form with coefficients

$$F_{ij} = \oint_L \mathrm{d}l \, \psi_i^{(E)} \psi_j^{(E)} \,. \tag{12}$$

The second step is to find energies E_n at which a close to zero minimum of $\mathscr{R}(E)$ is reached. These energies should correspond to the spectrum of an electron in a quantum wire.

It can be shown [23] that the minimum of the ratio of two positively defined quadratic forms (termed Rayleigh quotient) is equal to the minimal eigenvalue of some generalized eigenvalue equation,

$$\min_{\mathbf{C}} \frac{\mathbf{C}^{\mathrm{T}} F \mathbf{C}}{\mathbf{C}^{\mathrm{T}} N \mathbf{C}} = \min \lambda_k \,, \tag{13}$$

where $\{\lambda_k\}$ are the eigenvalues of the matrix equation

$$F\mathbf{C} = \lambda N \mathbf{C} \,. \tag{14}$$

In practice there are two ways to minimize the Rayleigh quotient. First is to find *all* eigenvalues of the equation $F\mathbf{C} = \lambda N\mathbf{C}$ with the help of MATLAB [24] command **eig** (F, N) and choose the minimal eigenvalue λ. The mathematical package MATLAB implements an efficient QZ factorization [25] to find the solutions for the generalized eigenequation. The usage of the built-in function **eig** is very convenient for not very time consuming problems, but for elaborate calculation it is disadvantageous because an overhead of calculation of *all* eigenpairs of the problem.

A second, more efficient procedure is to find the minimum of the Rayleigh quotient directly, using the so-called Rayleigh quotient iteration [26]. The latter procedure is, in fact, a modified shifted power method for solution of the eigenproblems, with the variable shift equal to the previously obtained estimation of the minimal eigenvalue. Due to change of the shift in the process of iteration the conversion of the procedure is not geometrical, as in a power method, but much faster cubical [23]. In practice, usually only few iterations are necessary to find the minimum of the Rayleigh quotient for the given energy E.

We note that a similar method of solution of two-dimensional wave equation has been applied by Heller et al. [27, 28] to a problem of chaotic behavior in quantum billiards. As in the proposed method, Heller [27] seeks a solution of the wave equation as a linear combination of the bulk solutions (sines and cosines) corresponding to the given energy E. However, instead of minimization of the global residual along the boundary, as given by

(9), the author forced the trial function equal to one at an arbitrary chosen point inside the domain, and equal to zero at a *large number of points at the boundary*. Thus, during the first step, instead of dealing with the eigenvalue equation, an inhomogeneous set of linear equations was solved. In the second step the wave function was normalized and evaluated at about four times as many points as were initially set to zero; the residual (termed "tension") was obtained by summing up the squares of the wave function at these points. Finally, as in the proposed method, the eigenstates corresponded to deep minima of the residual as a function of E.

Thus, the approach of Heller [27] is essentially a combination of colloration and least squares methods. With the advantage of an excellent numerical stability, the method was applied to study of semiclassical behavior of quantum billiards, providing an accurate description of states with quantum number exceeding 10^4. However, by definition, in quantum wires and dots only few lowest quantum levels are important, and the proposed method, based on *integrals over the domain and the boundary*, given by (8) and (12), is more simple and efficient. The next section details the implementation of the proposed method to a specific quantum wire geometry.

4. Triangular and Quadrilateral Quantum Wires

Recently a large progress has been reached in the fabrication of GaAs quantum wires [29] and quantum dots [30] using an *in situ* MOCVD selective growth technique on SiO_2 patterned substrates. Triangular, trapezoidal, and arrowhead-shaped GaAs quantum wires have been obtained with lateral widths as small as 100 Å. Using a similar but slightly different selective growth technique, GaAs dots with dimensions of $250 \times 250 \times 120$ Å^3 surrounded by AlGaAs regions were prepared. The photoluminescence and magneto-photoluminescence measurements clearly demonstrated the evidence of carrier quantization in these confined structures.

In this section we apply the proposed boundary least squares method to the calculation of the confined states of quantum wires with triangular and symmetric quadrilateral cross-sections.

Let us consider first a quantum wire of a *triangular* cross-section with vertices in points $(a, 0)$, $(0, \xi a)$, and $(-a, 0)$ in the xy-plane. Due to the symmetry of the structure two independent sets of eigenstates exist, symmetric and antisymmetric with respect to the coordinate x. We choose the trial functions for the *symmetric* states in the form

$$\psi_i = \cos\left(k_i \frac{x}{a}\right) \sin\left(\varkappa_i \frac{y}{\xi a}\right), \tag{15}$$

where $i = 1, \ldots, n_1$ and

$$\begin{cases} k_i = Ka \cos \alpha_i, \\ \varkappa_i = \xi Ka \sin \alpha_i. \end{cases} \tag{16}$$

The trial functions (15) with the wave vectors (16) automatically satisfy the Schrödinger equation for the energy

$$E = \frac{\hbar^2 K^2}{2m}, \tag{17}$$

as well as zero boundary conditions at $y = 0$. Due to the symmetry of the problem the angles α can be chosen from the interval $(0, \pi/2)$.

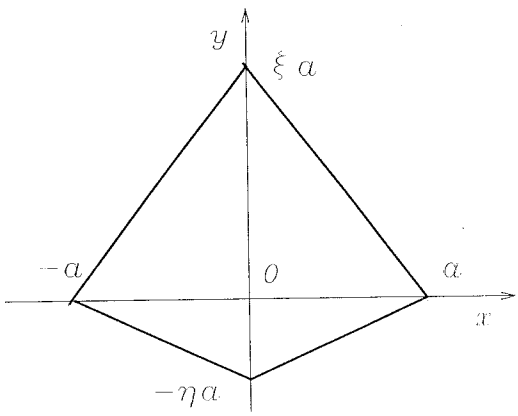

Fig. 1. Cross-section of the quadrilateral wire

To obtain the approximate solution of the Schrödinger equation we need to minimize the square deviation of the wave function along the line $y = \xi(a - x)$, where x belongs to the interval $(0, a)$, while other boundary conditions are satisfied identically by the set (15). The coefficients of the norm matrix $N_{ii'}$ and the deviation matrix $F_{ii'}$, required for the procedure, are calculated in the Appendix.

Similarly, the *antisymmetric* solution is constructed of the trial functions of the following form $(i = 1, \ldots, n_1)$

$$\psi_i = \sin\left(k_i \frac{x}{a}\right) \sin\left(\varkappa_i \frac{y}{\xi a}\right). \tag{18}$$

For the implicit form of the norm and deviation matrices see the Appendix.

Next we turn to the more complicated problem of a symmetric *quadrilateral* structure consisting of two attached triangles with equal bases of length $2a$ and heights ξa and ηa, see Fig. 1. Note, that the symmetric triangle considered above can be reproduced by putting $\eta = 0$, while bound states of the *nonsymmetric* triangle correspond to the antisymmetric states of the structure on Fig. 1.

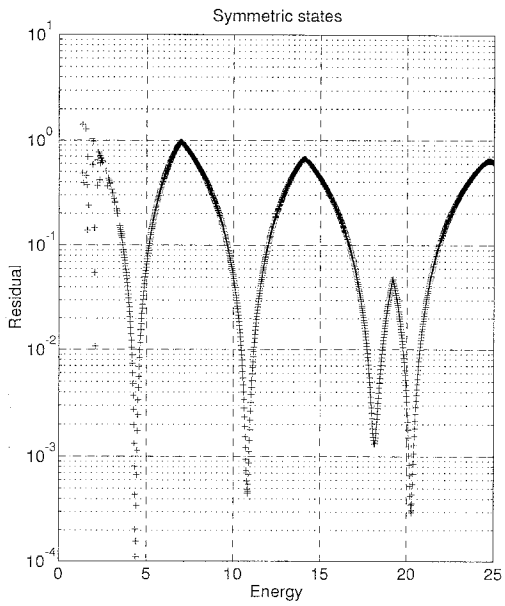

Fig. 2. Dependence of the residual $\mathscr{R}$ on energy E for the *symmetric* wave functions of a quadrilateral wire with $\xi = \sqrt{2}$ and $\eta = \sqrt{2}/3$. Number of trial functions: $n_1 = 7$ and $n_2 = 5$

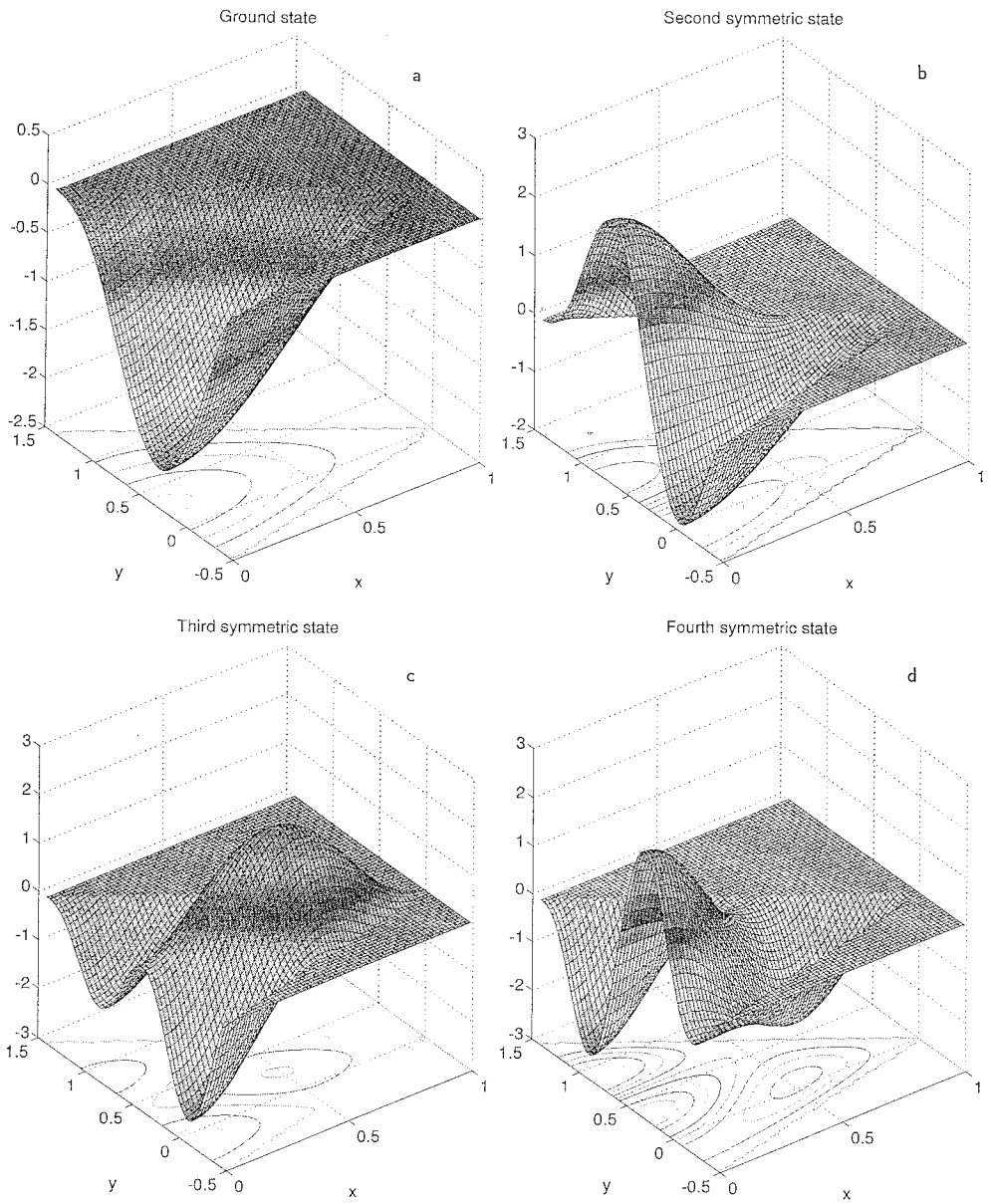

Fig. 3. Wave functions of the four lowest *symmetric* states. Right half of the wire is shown. a) Ground state, energy $E_0 = 4.40$; b) second symmetric state, $E_2 = 10.81$; c) third symmetric state, $E_4 = 18.16$; d) fourth symmetric state, $E_6 = 20.24$

Since for the geometry shown on Fig. 1 the boundary condition $\psi(x, y) = 0$ at $y = 0$ is absent, we add to (15) and (18) another set of trial functions,

$$\varphi_j = \cos\left(k_j \frac{x}{a}\right) \cos\left(\varkappa_j \frac{y}{\xi a}\right) \tag{19}$$

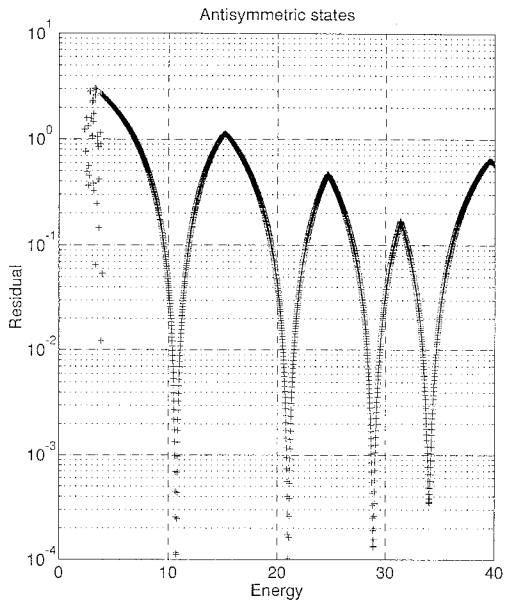

Fig. 4. Dependence of the residual $\mathscr{R}$ on energy E for the *antisymmetric* wave functions of a quadrilateral wire with $\xi = \sqrt{2}$ and $\eta = \sqrt{2}/3$. Number of trial functions: $n_1 = 7$ and $n_2 = 5$

for the symmetric states, and

$$\varphi_j = \sin\left(k_j \frac{x}{a}\right) \cos\left(\varkappa_j \frac{y}{\xi a}\right) \tag{20}$$

for the antisymmetric states, where $j = 1, \ldots, n_2$.

The norm and deviation matrices are equal to the sum of the corresponding matrices for the upper and lower constituting triangles (see Fig. 1). Due to existence of two sets of trial functions, (15) and (19) or (18) and (20), the matrices contain cross terms F_{ij} and N_{ij} (cf. the Appendix).

To illustrate the procedure described above we consider the quantum wire of quadrilateral cross-section as shown on Fig. 1. To eliminate the obvious dependence of all pertinent values on the distance a and concentrate on their dependence on the shape of the structure we will measure all distances in units of a and energies in units of $\hbar^2/2ma^2$.

For the numerical calculations we choose the parameters ξ and η to be equal to $\sqrt{2}$ and $\sqrt{2}/3$. That corresponds to the crystallographic planes (111) and (113).

The results of the calculation of the least squares residual for the symmetric states versus the energy is shown in Fig. 2. The calculation was performed with $n_1 = 7$ trial functions of the form (15) and $n_2 = 5$ functions of the form (19). The angles α_i were chosen to be equidistant in the interval $(0, \pi/2)$.

On Fig. 2 one can see well-pronounced minima of the residual $\mathscr{R}(E)$ corresponding to the eigenenergies of the *symmetric* states. Fig. 3a to d show the three-dimensional plots of the lowest four symmetric wave functions.

The dependence of the residual $\mathscr{R}$ versus energy E for the *antisymmetric* states with $n_1 = 7$ trial functions of the form (18) and $n_2 = 5$ functions of the form (20) is shown in Fig. 4. The normalized wave functions $\psi(x, y)$ of the four lowest antisymmetric states are plotted on Fig. 5a to d.

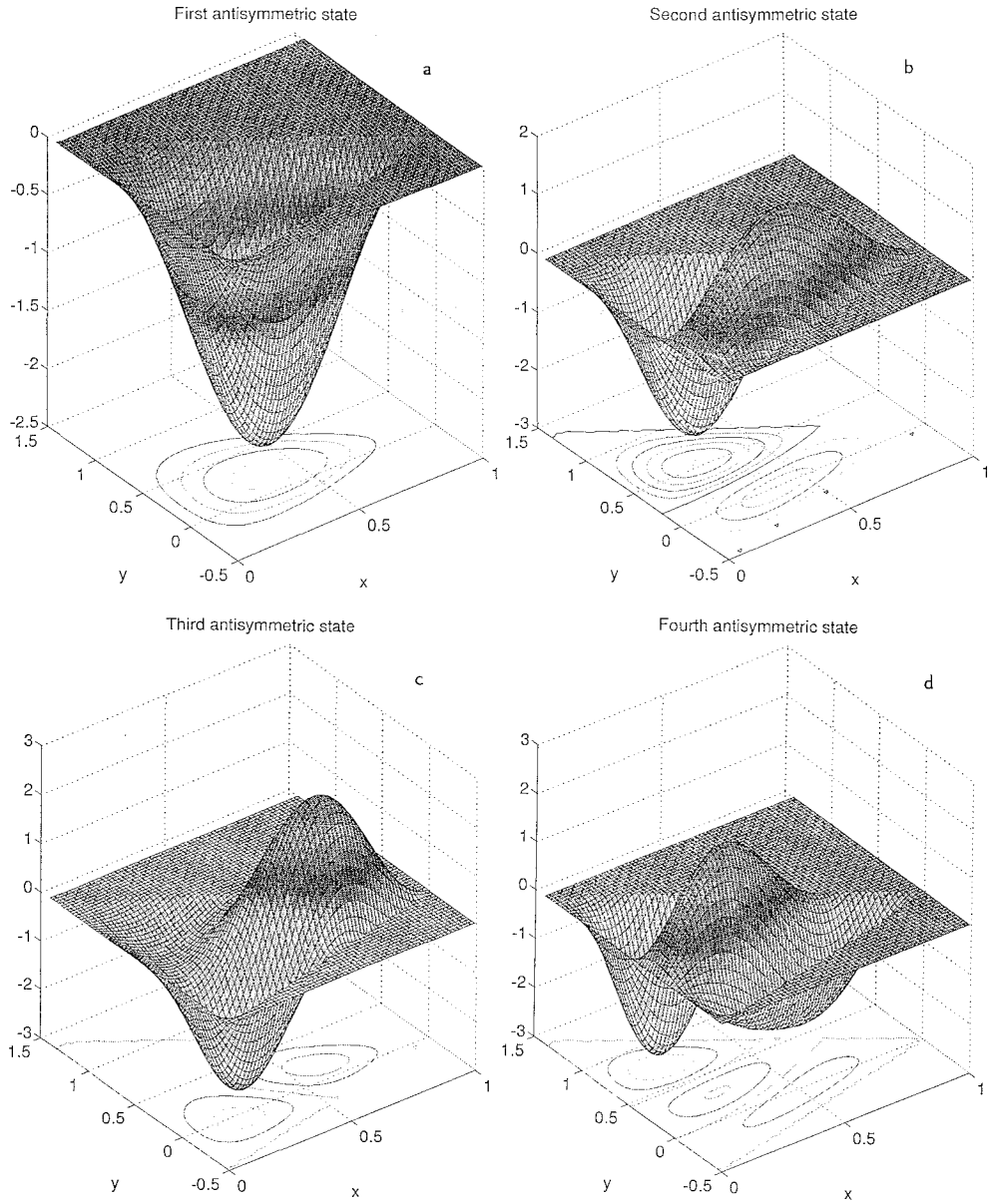

Fig. 5. Wave functions of the four lowest *antisymmetric* states of the quadrilateral wire (right half shown), or, equivalently, the four lowest states of the triangular wire. a) First antisymmetric state, energy $E_1 = 10.72$; b) second antisymmetric state, energy $E_3 = 21.03$; c) third antisymmetric state, energy $E_5 = 28.18$; d) fourth antisymmetric state, energy $E_7 = 34.05$

As seen from Fig. 2 to 5 the proposed boundary least squares method produces very accurate results for the structure under consideration. We emphasize that the approximate solutions are sums of $n_1 + n_2 = 12$ analytical functions of form (15) and (19) or

(18) and (20), which are in fact products of sines and cosines. Calculations show that the obtained wave functions, corresponding to different bound states, are mutually orthogonal with a high accuracy. Thus, we have obtained a very accurate global semianalytical solution of the Schrödinger eigenproblem for the chosen quadrilateral quantum wire.

We note that in general case the quadrilateral structure shown on Fig. 1, or the triangle with arbitrary lengths of sides, does not allow for an analytical solution of the corresponding Schrödinger equation. However, in the important case of a *right triangle*, the analytic solution of the eigenproblem exists and corresponds to the wave functions of a rectangle, antisymmetric with respect to the diagonal. In this case the BLSM reproduces the analytical results for energies and wave functions.

In conclusion, we have presented a boundary least squares method for the solution of the Schrödinger equation in quantum wires. This method takes advantage of known bulk solutions of the Schrödinger equation, and is based on the minimization of the square deviation of the trial function on the *boundary*, while inside the domain the equation in satisfied exactly. Application of the method to triangular and quadrilateral wires produced high accuracy solutions with a small number of global analytical functions.

Acknowledgement This work was supported by the U.S. Army Research Office and National Science Foundation.

Appendix A

Below we calculate the coefficients of matrices N and F, defined by (8) and (12) for the *triangle* with vortices at $(-a,\,0)$, $(a,\,0)$, and $(0,\,\xi a)$.

For the symmetric state, substituting (15) into (8) and (12), we find

$$\begin{aligned} N_{ii'} = \xi\,\frac{a^2}{4}\,&[C(k_i+k_{i'},\,\varkappa_i-\varkappa_{i'})+C(k_i-k_{i'},\,\varkappa_i-\varkappa_{i'}) \\ &-C(k_i+k_{i'},\,\varkappa_i+\varkappa_{i'})-C(k_i-k_{i'},\,\varkappa_i+\varkappa_{i'})] \end{aligned}$$

and

$$\begin{aligned} F_{ii'} = \frac{a}{4}\sqrt{1+\xi^2}\,&[S(k_i+k_{i'},\,\varkappa_i-\varkappa_{i'})+S(k_i-k_{i'},\,\varkappa_i-\varkappa_{i'}) \\ &-S(k_i+k_{i'},\,\varkappa_i+\varkappa_{i'})-S(k_i-k_{i'},\,\varkappa_i+\varkappa_{i'})]\,, \end{aligned}$$

where

$$C(k,\,\varkappa)=\frac{\cos\varkappa-\cos k}{k^2-\varkappa^2}$$

and

$$S(k,\,\varkappa)\equiv\frac{k\,\sin k-\varkappa\,\sin\varkappa}{k^2-\varkappa^2}\,.$$

For the *antisymmetric* state, substituting (18) into (8) and (12), we obtain

$$\begin{aligned} N_{ii'} = \xi\,\frac{a^2}{4}\,&[C(k_i+k_{i'},\,\varkappa_i+\varkappa_{i'})+C(k_i-k_{i'},\,\varkappa_i-\varkappa_{i'}) \\ &-C(k_i+k_{i'},\,\varkappa_i-\varkappa_{i'})-C(k_i-k_{i'},\,\varkappa_i+\varkappa_{i'})] \end{aligned}$$

and

$$F_{ii'} = \frac{a}{4}\sqrt{1+\xi^2}\,[S(k_i+k_{i'},\,\varkappa_i+\varkappa_{i'})+S(k_i-k_{i'},\,\varkappa_i-\varkappa_{i'}) - S(k_i+k_{i'},\,\varkappa_i-\varkappa_{i'})-S(k_i-k_{i'},\,\varkappa_i+\varkappa_{i'})]\,.$$

The expressions for the *quadrilateral* structure of Fig. 1 is given by the sum of the correspondent coefficients for the upper and lower triangular parts. Due to the presence of the additional set of trial functions, given by (19) or (20), we need the following coefficients of block norm and deviation matrices.

In the case of the *symmetric* wave function we have

$$N_{jj'} = \xi\,\frac{a^2}{4}\,[C(k_j+k_{j'},\,\varkappa_j+\varkappa_{j'})+C(k_j-k_{j'},\,\varkappa_j-\varkappa_{j'}) + C(k_j+k_{j'},\,\varkappa_j-\varkappa_{j'})+C(k_j-k_{j'},\,\varkappa_j+\varkappa_{j'})]\,;$$

$$N_{ij} = \xi\,\frac{a^2}{4}\,[S_1(k_i+k_j,\,\varkappa_i-\varkappa_j)+S_1(k_i-k_j,\,\varkappa_i-\varkappa_j) + S_1(k_i+k_j,\,\varkappa_i+\varkappa_j)+S_1(k_i-k_j,\,\varkappa_i+\varkappa_j)]$$

and

$$F_{jj'} = \frac{a}{4}\sqrt{1+\xi^2}\,[S(k_j+k_{j'},\,\varkappa_j+\varkappa_{j'})+S(k_j-k_{j'},\,\varkappa_j-\varkappa_{j'}) + S(k_j+k_{j'},\,\varkappa_j-\varkappa_{j'})+S(k_j-k_{j'},\,\varkappa_j+\varkappa_{j'})]\,;$$

$$F_{ij} = \frac{a}{4}\sqrt{1+\xi^2}\,\{(\varkappa_i-\varkappa_j)\,[C(k_i+k_j,\,\varkappa_i-\varkappa_j)+C(k_i-k_j,\,\varkappa_i-\varkappa_j)] + (\varkappa_i+\varkappa_j)\,[C(k_i+k_j,\,\varkappa_i+\varkappa_j)+C(k_i-k_j,\,\varkappa_i+\varkappa_j)]\}\,.$$

In the case of the *antisymmetric* states we have

$$N_{jj'} = \xi\,\frac{a^2}{4}\,[C(k_j-k_{j'},\,\varkappa_j+\varkappa_{j'})+C(k_j-k_{j'},\,\varkappa_j-\varkappa_{j'}) - C(k_j+k_{j'},\,\varkappa_j+\varkappa_{j'})-C(k_j+k_{j'},\,\varkappa_j-\varkappa_{j'})]\,;$$

$$N_{ij} = \xi\,\frac{a^2}{4}\,[S_1(k_i-k_j,\,\varkappa_i+\varkappa_j)+S_1(k_i-k_j,\,\varkappa_i-\varkappa_j) - S_1(k_i+k_j,\,\varkappa_i+\varkappa_j)-S_1(k_i+k_j,\,\varkappa_i-\varkappa_j)]$$

and

$$F_{jj'} = \frac{a}{4}\sqrt{1+\xi^2}\,[S(k_j-k_{j'},\,\varkappa_j+\varkappa_{j'})+S(k_j-k_{j'},\,\varkappa_j-\varkappa_{j'}) - S(k_j+k_{j'},\,\varkappa_j+\varkappa_{j'})-S(k_j+k_{j'},\,\varkappa_j-\varkappa_{j'})]\,;$$

$$F_{ij} = \frac{a}{4}\sqrt{1+\xi^2}\,\{(\varkappa_i-\varkappa_j)\,[C(k_i-k_j,\,\varkappa_i-\varkappa_j)-C(k_i+k_j,\,\varkappa_i-\varkappa_j)] + (\varkappa_i+\varkappa_j)\,[C(k_i-k_j,\,\varkappa_i+\varkappa_j)-C(k_i+k_j,\,\varkappa_i+\varkappa_j)]\}\,.$$

Here

$$S_1(k,\,\varkappa) = \frac{1}{\varkappa}\left[\frac{\sin k}{k} - \frac{k\,\sin k - \varkappa\,\sin\varkappa}{k^2-\varkappa^2}\right].$$

References

[1] C. A. J. Fletcher, Computational Galerkin Methods, Springer-Verlag, New York 1984.
[2] S. Selberherr, H. Stippel, and E. Strasses (Ed.), Simulation of Semiconductor Devices and Processes, Springer-Verlag, New York 1993.
[3] W. H. Press, S. T. Teukolsky, W. T. Vetterling, and B. P. Flannery, Numerical Recipes in Fortran: the Art of Scientific Computing, Cambridge University Press, 1992.
[4] R. Kircher and W. Bergner, Three-Dimensional Simulation of Semiconductor Devices, Birkhäuser, Boston 1991.
[5] J.-M. Jin, Finite Elements in Electromagnetics, Wiley, New York 1993.
[6] O. Axelsson, Finite Elements Solution of Boundary Value Problems, Academic Press, New York 1984.
[7] Z. Shao, W. Porod, and C. S. Lent, J. appl. Phys. **78**, 2177 (1995).
[8] C. A. Brebbia, Boundary Elements in Mechanical and Electrical Engineering, Computational Mechanics, Boston 1990.
[9] D. S. Citrin and Y.-C. Chang, Phys. Rev. B **40**, 5507 (1989).
[10] R. L. Greene and P. Lane, Phys. Rev. B **34**, 8639 (1986).
R. L. Greene and K. K. Bajaj, Phys. Rev. B **34**, 951 (1986).
[11] S. Fraizzoli and A. Pasquarello, Phys. Rev. B **44**, 1118 (1991).
Y.-C. Chang, Physica (Utrecht) **146B**, 137 (1987).
[12] G. Bastard, Wave Mechanics Applied to Semiconductor Heterostructures, Halsted Press, New York 1988.
[13] E. Kühn, Arch. Elek. Übertragung **27**, 511 (1973).
W. Menzel and I. Wolff, IEEE Trans. Microwave Theory Tech. **25**, 107 (1977).
A. K. Saad and K. Schünenmann, IEEE Trans. Microwave Theory Tech. **30**, 2125 (1982).
A. Weisshaar and V. K. Tripathi, Electronics Letters **25**, 1138 (1989).
[14] R. Mittra, Analytical Techniques in the Theory of Guided Waves, Macmillan, New York 1971.
[15] A. Weisshaar, J. Lary, S. M. Goodnick, and V. K. Tripathi, Appl. Phys. Letters **55**, 2114 (1989).
K.-F. Berggren and Z. Ji, Superlattices and Microstructures **8**, 59 (1990).
J. Martorell, S. Klarsfeld, D. W. L. Sprung, and H. Wu, Solid State Commun. **78**, 13 (1991).
R. Akis, P. Vasilopoulos, and P. Debray, Phys. Rev. B **52**, 2805 (1995).
[16] T. Kawamura and J. P. Leburton, Phys. Rev. B **48**, 8857 (1993).
[17] Y. Avishai and Y. B. Band, Phys. Rev. Letters **62**, 2527 (1989).
R. L. Schult, D. G. Ravenhall, and H. W. Wyld, Phys. Rev. B **39**, 5476 (1989); **41** 12760 (1990).
K.-F. Berggren and Z. Ji, Phys. Rev. B **43**, 4760 (1991).
Y. Takagaki and D. K. Ferry, Phys. Rev. B **44**, 8399 (1991); **45**, 6715, 13494 (1992).
[18] J. Wang, Y. J. Wang, and H. Guo, Phys. Rev. B **46**, 2420 (1992).
Y. Takagaki and K. Ploog, Phys. Rev. B **49**, 1782 (1994).
[19] G. Kirczenow, Solid State Commun. **68**, 715 (1988); Phys. Rev. B **39**, 10452 (1989).
E. Castaño and G. Kirczenow, Solid State Commun. **70**, 801 (1989).
E. Tekman and S. Ciraci, Phys. Rev. B **43**, 7145 (1991).
Y. Takagaki and D. K. Ferry, Phys. Rev. B **46**, 15218 (1992).
[20] H. Xu, Phys. Rev. B **48**, 8878 (1993).
[21] J. P. Carini, J. T. Londergan, K. Mullen, and D. P. Murdock, Phys. Rev. B **48**, 4503 (1993).
[22] F. Sols and M. Macucci, Phys. Rev. B **41**, 11887 (1990).
H. Wu, D. W. L. Sprung, and J. Martorell, Phys. Rev. B **45**, 11960 (1992).
J. Wu, M. N. Wybourne, A. Weisshaar, and S. M. Goodnick, J. appl. Phys. **74**, 4590 (1993).
K. Vacek, A. Okiji, and H. Kasai, Phys. Rev. B **47**, 3695 (1993).
[23] B. N. Parlett, The Symmetric Eigenvalue Problem, Prentice-Hall, Inc., Boston 1980.
[24] MATLAB User's Guide, Math Works, Natick (Mass.) 1992.
[25] C. B. Moler and G. W. Stewart, SIAM J. Numer. Anal. **10**, 384 (1973).
[26] G. H. Golub and C. F. Van Loan, Matrix Computations, Johns Hopkins University Press, Baltimore 1989.

[27] E. J. Heller, in: Chaos and Quantum Physics, Ed. M.-J. Giannoni, A. Voros, and J. Zinn-Justin, Elsevier Publ. Co., Amsterdam 1991 (p. 547).
[28] S. Sridhar and E. J. Heller, Phys. Rev. A **46**, R1728 (1992).
[29] T. Kono, S. Tsukamoto, Y. Nagamune, F. Sogawa, M. Nishioka, and Y. Arakawa, Appl. Phys. Letters **64**, 1564 (1994).
D. Bertram, B. Spill, W. Stolz, and E. O. Göbel, Solid State Electronics **37**, 591 (1994).
S. Tsukamoto, Y. Nagamune, M. Nishioka, and Y. Arakawa, Appl. Phys. Letters **62**, 49 (1993); **63**, 355 (1993).
D. Bertram, W. Stolz, and E. O. Göbel, J. Crystal Growth **132**, 179 (1993).
[30] Y. Arakawa, Solid State Electronics **37**, 523 (1994).
Y. Nagamune, M. Nishioka, S. Tsukamoto, and Y. Arakawa, Solid State Electronics **37**, 579 (1994).
Y. Arakawa, Y. Nagamune, M. Nishioka, and S. Tsukamoto, Semicond. Sci. Technol. **8**, 1082 (1993).
Y. Nagamune, S. Tsukamoto, M. Nishioka, and Y. Arakawa, J. Crystal Growth **126**, 707 (1993).