SPECTRAL METHOD FOR SOLVING THE DIFFERENTIAL EQUATIONS INVOLVED IN AB-INITIO TREATMENT OF TUNNEL TRANSISTORS STRUCTURES

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In lucrare este prezentată o nouă variantă a metodei spectrale de rezolvare a ecuațiilor diferențiale cu condiții la limită, aplicabilă la calcule ab-initio pentru tunelarea electronilor. Prin exprimarea potențialului total în care se mişcă electronul ca o dezvoltare în serie după un anumit set de funcții într-un spațiu Hilbert, ecuatiile obtinute prin metoda colocatiei pot admite o integrare analitica initiala. Experimentele noastre numerice au aratat o îmbuntățire importantă a preciziei datorită acestei prelucrări analitice suplimentare, ceea ce, împreună cu propritatea de evanescentă poate conferi metodei avantaje importante pentru calcule ab-initio.

A new variant of the spectral method for solving the boundary conditions ordinary differential equations, suited to the ab-initio tunneling calculus is presented. By expanding the total potential expression in a series in a Hilbert space, the linear equations derived with the collocation method may admit an initial analytical quadrature for certain basis sets. Our numerical experiments showed an important improvement of the precision due to this supplementary analytical treatment which, combined with the evanescence of the method may be a good advantage for ab-initio calculations

Keywords: spectral methods, evanescence, boundary conditions, ab-initio, tunneling transistors.

1. Introduction

As the dimensions of the microelectronic structures continuously decrease, the inherent tunneling current becomes a disturbing part of the various devices design. It seems that the time has come that these tunneling currents to become the active, useful part of the electronic functions of the microelectronic devices, mainly as tunnel transistors structures.

Some major benefits would accompany this new approach in large scale integrated circuits. Among them, the huge increase in operating frequency and the decrease of power consumption, due to the absence of minority carriers and the leakage currents respectively.

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This highly promising achievement has generated an important research effort all over the world and many solutions have been investigated for introducing industrial tunnel transistor structures. Thus, there are some models with simple barrier [1], and others that include one or more quantum wells [2]. The first type is based on the modulation of the Fowler-Nordheim tunneling current by the electric field intensity created by an auxiliary electrode. The second type is based on the resonance effects between the quantum wells, as a significant tunneling current appears only if some quantum states equivalence is satisfied. An auxiliary electrode controls the resonance conditions, starting or stopping the tunneling current, so that the structure is easy to be used as a commutation device.

Concerning the geometry, there are several types of tunnel transistors. Thus, the most promising seems to be the vertical transistor where the electrodes are superposed, which allows a very good control of the thickness of the barrier layer and hence a good reproducibility for large scale integration [1,3,4,7,8].

Also, lateral structures have been proposed, based on a Columbian barrier generated by a lateral p-n junction, which is easier to control by the gate electrode [5,6,14]. There are also some mixed structures [2] where both vertical and horizontal geometries are used, and also some special devices as the magnetic tunnel transistor and the single electron transistor (SET) used as structures in scientific research [9].

Of course, the first step of the process is the mathematical and physical simulation of various configurations using tunnel currents, with both analytical and numerical treatment.

Two main approaches are possible for such models: one that adapts the classical Fowler-Nordheim tunneling equation to the topological and electric characteristics of a particular structure, and another one that uses *ab-initio* calculations on quantum mechanics basis, considering the natural microscopic details.

Although more difficult, the second approach may deliver much more accurate predictions, taking into account that in several situation the ready-made tunneling formulae have been found inappropriate for describing complex configurations, with special topological and materials characteristics. On the other hand, even the *ab-initio* calculations (both Hartree-Fock selfconsistent field theory – SCF [18] and Kohn-Sham density functional theory – DFT [19]) notoriously fail in some situations, especially due to the numerical difficulties involved in some large atomic systems and possibly a subtle loss of precision. It seems that the choice of the numerical method has a considerable importance in complex structure models and some new, better adapted numerical methods have to be considered. The aim of this paper is to exploit the particularities of the equations involved in such calculations for achieving better performances, also trying to preserve a certain amount of generality.

2. The typical many-body problem for tunneling structures

The ab-initio methods, in the nonrelativistic case, start with the Schrödinger equation for each particle of the many-body problem, taking into account the particularities of the actual system (i.e. the specific potential and boundary conditions):

$$-\frac{\hbar^2}{2m_i}\nabla^2\Psi_i(\vec{r})+V_i(\vec{r})\Psi_i(\vec{r})=E_i\Psi_i(\vec{r}) \tag{1}$$

where $V_i(\vec{r})$ is the function describing the total potential seen by the particle characterized by the wave function $\Psi_i(\vec{r})$. In two or three dimensional systems, this PDE is transformed in a set of ODE by factorizing each wave function in one variable functions and properly manipulating the terms for enabling the variables separation. According to the system's geometry, Cartesian, polar, spherical, etc. coordinates are used trying to obtain standard differential equations, with known analytical solutions. However, such lucky solutions are met only for very special and simple systems, so that in most cases only a numerical treatment is possible.

In the microelectronic devices based on planar technologies one may choose a two-dimensional Cartesian coordinate system so that the wave function may be decomposed as:

$$\Psi_i(\vec{r})=X_i(x)Y_i(y) \tag{2}$$

If the potential may also be decomposed as a sum of one variable function

$$V_i(\vec{r})=V_{xi}(x)+V_{yi}(y) \tag{3}$$

by plugging these relations in (1), the problem can be broken-down into one-dimensional equations.

For the inner shells of atoms, the total potential for each electron is composed by the simply Coulomb potential due to the nucleus $-Z/r$, the Hartree potential due to the repulsion from the other electrons $V_H(r)$ and an exchange-correlation term $V_{XC}(r)$ due to the antisymmetric fermionic nature of the electrons. In a spherical coordinate system imposed by the symmetry of the Coulomb potential of the nucleus in the Born-Oppenheimer approximation, the single electron wave function equations read [18]

$$-\frac{1}{2}y_i''(r)+\left(\frac{\ell(\ell+1)}{2r^2}-\frac{Z}{r}+V_{Hi}(r)+V_{XCi}(r)\right)y_i(r)=E_iy_i(r) \tag{4}$$

Both the repulsion and the exchange-correlation potential have a computational time expensive form, since they are depending on the wave functions of others electrons. The direct evaluation implies solving the integrals [18]

$$V_{Hi}(r) = \sum_j \int \frac{\left|y_j(\mathbf{r}_i)\right|^2}{\left|\mathbf{r}_i - \mathbf{r}'\right|} d\mathbf{r}' \tag{5}$$

$$V_{XCi}(r) = \sum_j \int \frac{\left|y_i(\mathbf{r}_i) y_j(\mathbf{r}_i)\right|}{\left|\mathbf{r}_i - \mathbf{r}'\right|} d\mathbf{r}' + V_C(r) \tag{6}$$

where V_c is the correlation potential, which is not known exactly, but some widely accepted models are available in the literature [20-23].

On the other hand, these potentials obey the Poisson equation

$$\nabla^2 V_{Hi} = -4\pi\rho_{ir}(r) \tag{7}$$

$$\nabla^2 V_{Xi} = -4\pi\rho_{ia}(r) \tag{8}$$

where

$$\rho_{ir}(r) = \sum_j \left|y_j(r)\right|^2 \tag{9}$$

$$\rho_{ia}(r) = \sum_j \left|y_i(r) y_j(r)\right| \tag{10}$$

are the charge densities for the repulsive and the attractive terms respectively[19].

Thus, if the correlation term V_c is separately treated, these potentials may also be calculated from a second order differential equation with boundary condition and with no first derivative term.

We notice that the main problem formulated in eq. (1) may be reduced to solving this kind of differential equations with the general form

$$y''(x) + V(x)y(x) = f(x) \tag{11}$$

$$\begin{aligned} y(a) &= y_i \\ y(b) &= y_f \end{aligned} \tag{12}$$

for a given domain $[a,b]$, usually from about 0 to 10-20 (in Bohr radius if everything is expressed in atomic units). Here the coefficient $V(x)$ is the potential calculated directly using eqs (5)-(6) or using eqs. (7)-(8), divided by the coefficient of the second derivative in the uni dimensional Schrödinger equation.

3. Solving the second order differential equation involved in ab-initio calculations

There are some popular methods for numerically solving the differential equations involved in ab-initio calculations, each of them having various advantages and disadvantages.

The main candidate for atomic systems seems to be the fifth order Numerov method. Its main advantage is the high precision with reasonable speed, but it has the disadvantage of the starting which demands two initial points. If the

wave function normalization is possible the second point may be chosen arbitrary and the result is afterwards adjusted. Unfortunately, for the ending point boundary condition to be satisfied, an additional shooting algorithm is needed, which drastically decreases the speed.

Also, the well known fourth order Runge-Kutta [24] method may be applied, again in conjunction with a slowing shooting algorithm. The problem of shooting is also present for various other very precise schemes that use the Bulrich-Stoer extrapolation [24].

On the other hand, various methods specific to the boundary conditions problems, especially the finite difference and the finite element methods are currently used but their convergence is poor and hence the speed may be insufficient for reasonably high accuracy [24].

A new class of methods developed in the last years was successfully applied to ab-initio calculations: the spectral methods. They are already used in well known techniques as Hartree-Fock-Roothaan [25] equations and Gaussian software, but the complexity of the calculations (mainly the eigenvalues problems) tends to slow-down the evaluations. The main advantages of these methods are: an exponential decrease of the errors when the number of points in increased (the *evanescence* property) and a natural dealing of the two point boundary problems.

In the spectral methods, the unknown function $y(x)$ is approximated as a finite expansion in a Hilbert space, using a known (chosen) basis set $\varphi_i(x)$ (the *trial functions*)

$$y(x) \simeq \sum_{j=0}^{n} c_j \varphi_j(x) \tag{13}$$

The problem of solving the second order ODE generated by linear differential operator L

$$Ly(x) = f(x) \tag{14}$$

subject to the boundary conditions (12) is reduced to the problem of finding the coefficients c_i in the expression (13).

Taking into account that the expansion (13) is only an approximation, by plugging it in the ODE the relationship (14) will also be an approximation and we may define a residual function $R(x)$ as

$$R(x) := Ly(x) - f(x) \tag{15}$$

Using another set of functions $\left(\chi_0(x), \chi_1(x), ..., \chi_n(x)\right)$ named *test functions* we check the smallness of a residual R, by means of the Hilbert space scalar product:

$$\forall i \in (1, 2, ..., n), \quad \left\langle \chi_i(x), R(x) \right\rangle = 0 \tag{16}$$

Among the spectral methods, the collocation method seems to have the advantage of simplicity in conjunction with precision and speed. It uses the test functions

$$\chi_i(x) = \delta(x - x_i), \quad i = 0,1,...,n \tag{17}$$

where x_i form a set of fixed, chosen points (the collocation points) and $\delta(x)$ is the Dirac distribution. It follows from (16) the equations system

$$R(x_i) = 0, \quad i = 0,1,...,n \tag{18}$$

or, according to the definition (15)

$$Ly(x_i) = f(x_i) \tag{19}$$

If the coefficients of the linear operator are constants, all the equations in the system will have simple forms and any standard method for such systems will determine the unknown function's coefficients in the expansion (13). The most usual trial functions for this procedure are: monomials, orthogonal polynomials (Legendre, Chebyshev, etc.) for non periodic problems, and trigonometric functions for periodic problems.

However, for the case discussed, the general equation (11) does not have constant coefficients, so that the calculus will have an increased volume. Indeed, from eqs (19) and (11) we obtain

$$y''(x_i) + V(x_i)y(x_i) = f(x_i), \quad i = 0,1,...,n \tag{20}$$

In fact, the most cumbersome term is the total potential $V(x)$, calculated in the previous iteration for a given set of wave functions, which must be included in the current iteration.

Our method avoids the increased complexity of the equations system by expanding this term also, using a basis set $\{\xi_j(x)\}$, in a similar way as for the unknown function.

$$V(x) = \sum_{k=0}^{m} d_k \xi_k(x) \tag{21}$$

With one of the usual interpolation methods (as Newton or Lagrange interpolation), we obtain the set of coefficients $\{d_k\}$.

Of course, the multiplication of the two series has to generate an expression as simple as possible for achieving good speed and accuracy. A possible choice for the expansion (21) would be a polynomial one, so that the basis set is monomial

$$\xi_k(x) = x^k \tag{22}$$

If we choose the same basis set for the expansion (13)

$$\varphi_j(x) = x^j \tag{23}$$

from equations (20), (13) and (21) we obtain

$$\sum_{j=0}^{n} c_j \varphi''_j(x_i) + \left[\sum_{k=0}^{m} d_k \xi_k(x_i)\right]\left[\sum_{j=0}^{n} c_j \varphi_j(x_i)\right] = f(x_i), \quad i = 0,1,...,n \tag{24}$$

Using the monomial expansions (22) and (23) we obtain the following system

$$\sum_{j=0}^{n} c_j \left[j(j-1)x_i^{j-2} + \sum_{k=0}^{m} d_k x_i^{k+j} \right] = f(x_i), \quad i = 1,2,...,n-1 \tag{25}$$

We have $n+1$ coefficients c_j, so we used only $n-1$ equations in the system (25) and complete them with two equations (13) that include the boundary conditions

$$\begin{aligned} y(a) &= \sum_{j=0}^{n} c_j a^j \\ y(b) &= \sum_{j=0}^{n} c_j b^j \end{aligned} \tag{26}$$

By solving this system we obtain the coefficients c_j and then the unknown function

$$y(x) = \sum_{j=0}^{n} c_j x^j \tag{27}$$

Concerning the collocation points x_i, it is known that uniform sampling of the domain $[a,b]$ is not recommended for polynomial approximations since increasing errors appear at the ends, when the number of points increases (the Runge phenomenon). That is why a non uniform sampling has to be considered here, for example in the roots of a n degree Chebyshev polynomial

$$x_i = \frac{b-a}{2}\cos\left[\frac{\pi}{n}\left(i+\frac{1}{2}\right)\right] + \frac{b+a}{2}, \quad i = 0,1,...,n-1 \tag{28}$$

where the usual scaling of the range from $[a,b]$ to $[-1,1]$ was used.

Of course, some other expansions may be used for the unknown function and its coefficient but this polynomial expansion has an important advantage: it is possible to perform an analytical integration of the whole equation before numerically solving it. One may expect an improvement of the performances due to this supplementary analytical treatment which is not time consuming since the polynomials are easy to integrate.

Indeed, performing integration in eq. (25) from a to x_i the following formula is obtained

$$\sum_{j=0}^{n} c_j \left[j\left(x_i^{j-1} - a^{j-1}\right) + \sum_{k=0}^{m} d_k \frac{x_i^{k+j+1} - a^{k+j+1}}{k+j+1} \right] = \int_a^{x_i} f(x)dx, \quad i = 1,2,...,n-1 \tag{29}$$

We emphasize that the presented method can be extended to equations where first order derivatives are also present. In this case, a supplementary term in eq. **Error! Reference source not found.**, (25) and (29) will occur. This term may be easily calculated if the coefficient of the first derivative is constant, but if it is not, the same procedure used for the coefficient of the free term may be applied. It is an advantage over the Numerov method which is more difficult to be used in such cases.

The disadvantage is the right hand member which demands an integration in the general case. However, the quadrature is a very precise and low cost operation if a Gauss-Legendre or Clenshaw-Curtis method is used.

Moreover, for the special case of ab-initio calculations for the stationary wave functions, we may exploit the particular form of the right hand side of the eq. (20). Indeed, according to the stationary Schrödinger equation it should be

$$f(x) = E_s y(x) \tag{30}$$

where E_s is the eigenvalue and $y(x)$ is the unknown wave function.

This may be included in the left side of the equation, and modifies only the constant term of the potential so that the eq. (25) becomes

$$\sum_{j=0}^{n} c_j \left[j(j-1)x_i^{j-2} + \sum_{k=0}^{m} e_k x_i^{k+j} \right] = 0, \quad i = 1, 2, ..., n-1 \tag{31}$$

where $e_0 = d_0 - E_s$ and $e_i = d_i$ for $i = 1, 2, ..., n$.

This avoids the integration process in eq (29) which becomes

$$\sum_{j=0}^{n} c_j \left[j\left(x_i^{j-1} - a^{j-1}\right) + \sum_{k=0}^{m} e_k \frac{x_i^{k+j+1} - a^{k+j+1}}{k+j+1} \right] = 0, \quad i = 1, 2, ..., n-1 \tag{32}$$

The system (32) with the boundary conditions equations (26) will be solved for the coefficients c_j and then the expansion (27) will provide the solution.

4. Numerical results

As an example for testing the presented method we choose a potential $V(x)$ that often occurs in tunnel transistor structures. The various slopes illustrated correspond to the regions with uniform electric fields in the regions with various dielectric constants. Note that some regions with high-k dielectrics have to be used for reducing the gate leakage currents. The sampling was made in the roots of a Chebyshev polynomial in the rang $[0.01, 2.5]$ i.e. the abscises: $\{0.041214, 0.28162, 0.714815, 1.255, 1.79519, 2.22838, 2.46879\}$, where the values of the potential were (0,3,4,4,6,3,0} as in figure 1.

A Lagrange interpolation of these values has been performed, generating the following polynomial approximation

$$V(x) = 0.660318 + 16.2613x - 4.35161x^2 + 37.5901x^3 - 47.8981x^4 + 21.0653x^5 - 3.11488x^6$$

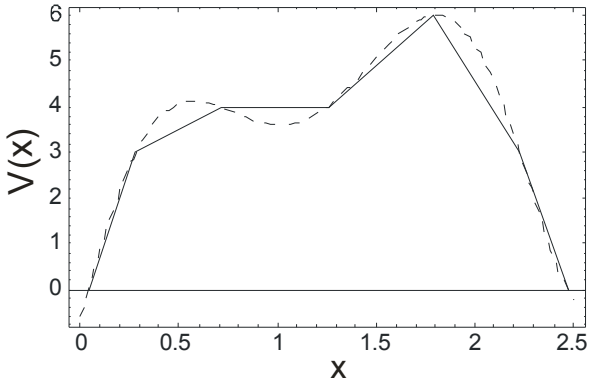

Fig 1. Approximation of a potential $V(x)$ (continuous line) using a 6^{th} degree polynomial (dashed line)

We used the described method with $f(x) = 0$ and obtained the unknown function presented in Fig. 2.

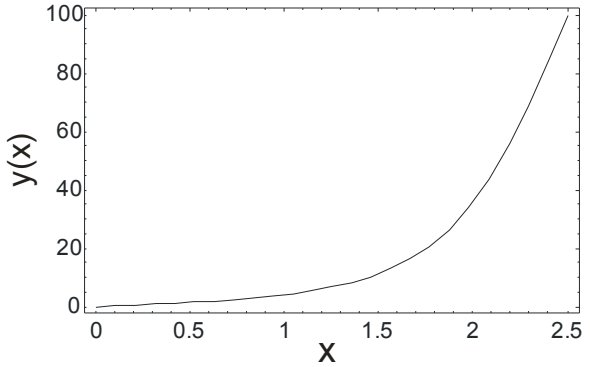

Fig. 2. The solution of the ODE with the potential as in figure 1

We checked the obtained solution in 100 points in the range and choose the maximum error (defined as the residual *R*). The errors are presented in table 1 and Fig. 3.

One may see the fast decrease of the absolute error with the increase of the order of the interpolation polynomial (theoretically exponential) up till $n \approx 22$. Above this value, the terms of the equations become excessively great and the condition number of the system's matrix increase, generating increasing round-off

errors. The evanescence property is very clear in figure 3 and the loss of precision due to the increasing condition number is revealed also.

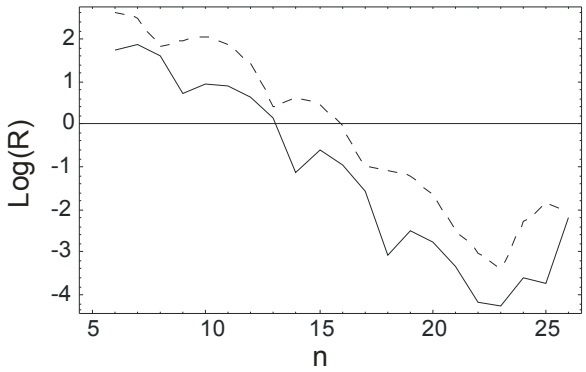

Fig. 3. The logarithm of the residual function of the polynomial's degree for integrated method (continuous line) and simple method (dashed line)

Table 1

The error (residual) as a function of the polynomial's degree

Maxim polynomial degree (n)	Maximum error	
	Without integration	With integration
5	401.169	55.8884
6	315.819	77.5812
7	65.7409	41.6716
8	93.6927	5.16428
9	114.981	8.50767
10	73.0407	8.36208
11	27.9325	4.52969
12	2.5058	1.38072
13	4.39118	0.072402
14	2.98162	0.252796
15	0.96174	0.113378
16	0.101266	0.0277998
17	0.0847201	0.000890848
18	0.0632824	0.00323763
19	0.0221895	0.00181579
20	0.00337523	0.000468068
21	0.000986964	0.0000662559
22	0.000406731	0.0000484947
23	0.00534406	0.000263804
24	0.0140926	0.000179443
25	0.00956485	0.00676438

5. Conclusions

The described method ensures errors lower than 10^{-6} % by solving a linear equations system with 20-22 unknowns, much less than the finite difference or finite element methods. However, the system's matrix is dense and for higher degree polynomials the condition number increases inevitably, so that the round-off errors become dominant.

An important conclusion is that for any approximating polynomial's degree, the errors of the method with integration are several times lower than the errors of the method without integration, due to the supplementary analytical treatment.

This is particularly important in the self-consistent field calculations where the potential involved by an equation depends on its solution and this implies an iterative procedure until the convergence of the solution is achieved. Taking into account the necessity of repeatedly applying the described procedure, the precision and speed achieved at each step may be very important.

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