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Comparison of methods for solving the Schrödinger equation for multiquantum well heterostructure applications

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Abstract. Direct numerical approaches for the solution of the time-independent one-dimensional Schrödinger equation are discussed. Applications to multiquantum well (MQW) semiconductor heterostructure potentials need linear dependence of the computer time t_{comp} on the number of spatial grid points N. Although acknowledged as a very effective Fourier grid Hamiltonian (FGH) method, it has cubic dependence on the number of spatial grid points, i.e., $t_{comp} \sim N^3$, which limits its use to problems with a complexity of $N \le 1000$. A simple straightforward shooting method (ShM), which is based on trial stepping over the coordinate and energy, has the necessary $t_{comp} \sim N$ dependence with moderate energy convergence efficiency but the recommended symmetry pre-conditions and the not very clearly defined external boundaries make its application inconvenient. This paper offers a new reliable and effective energy and wave function coupled solution (EWC) method with a Newton iteration scheme and an internal bordered tridiagonal matrix solver. The method has a linear $t_{comp} \sim N$ dependence and may by applied to arbitrary potential energy distribution tasks with complexity up to $N = 10^5$ and beyond. Zero or cyclic boundary conditions may be specified for the wave function. For versatile MQW tasks the combined use of ShM and EWC is illustrated. Detailed accuracy and computer time comparisons show that the combined ShM + EWC method is three orders of magnitude more effective than the FGH method.

Key words: multiquantum well structures, Schrödinger equation, bound states, numerical methods, energy, wave function.

1. INTRODUCTION

In spite of the fact that Erwin Schrödinger formulated his famous equation 80 years ago in 1926 and that for over 70 years scientists have proposed various analytical and numerical methods for the solution of this central quantum

mechanics equation, approaches even to one-dimensional solutions are still a subject of debate. This is confirmed by the continuing appearance of new publications in this field [1–6]. Since 1990s, one of the driving forces in this field has been physical chemistry and its applications. The second spur of motivation has come from the extremely wide application area in semiconductor hetero-structures with quantum wells, wires and dots [7]. Although nowadays the available sophisticated *ab-initio* software tools already make quite realistic three-dimensional calculations possible, almost every research task needs an estimation of static bound states in a one-dimensional (1D) approximation either in spherical or rectangular coordinates. The last case is more typical for semiconductor heterostructures where the calculation of 1D bound states for complex multi-barrier quantum well systems like, e.g. in quantum cascade lasers [8] or digitized quasi-parabolic quantum wells [9], may be a rather time-consuming subtask.

In applications in physical chemistry, the potentials in the atomic subnano-meter scale are rather smooth and relatively small number ($N \leq 100$) of spatial grid points may be sufficient to obtain accurate results. In contrast to that, MQW structures with great numbers of relatively abrupt potential steps over the 10–1000 nm spatial scale may need spatial grid sizes over $N > 10^4$ to achieve acceptable results [7,9]. This means that for the analysis and even more for the optimization of MQW structures the methods of solving the Schrödinger equation must consume computer time no more than proportionally to N.

The FGH method [1–3] has been declared to be very effective and the simplest method for the calculation of bound states from the time-independent 1D Schrödinger equation. It can take as input an arbitrary potential distribution, but its computer execution time t_{comp} scales as N^3. The use of the Fast Fourier Transform in the construction of the Hamiltonian matrix may reduce the last number to $N^2 \times \ln N$ but not more [2]. The internal algebraic solver of the FGH method uses standard procedures from the EISPACK computer package [10].

Actually, the most elementary solution method with the required linear dependence of the computer time on the grid size ($t_{\text{comp}} \sim N$) is the shooting method [7], which finds eigenvalues of the bound state energy by using a trial procedure, based on the condition that an iteration over the spatial coordinate from the centre of the active area into the surrounding barriers must yield a vanishing wave function $\Psi \to 0$. The ShM needs two initial values of the wave function to start the iteration over the spatial coordinate. Those two values may be correctly defined for symmetric potentials but in the general case it needs an approximate auxiliary algorithm [7]. Another problem, troubling the application of the ShM, is associated with the exponentially growing components of the wave function in the outer barrier regions, which can impede the detection of the theoretical boundary condition $\Psi \to 0$.

In the present work we propose an effective iterative coupled energy and wave function method for solving the time-independent one-dimensional Schrödinger equation, which possesses linear $t_{\text{comp}} \sim N$ dependence and may be applied to arbitrary potential energy distributions without any symmetry restrictions. The

method uses an iterative approach in the Newton method and its internal algebraic task involves the solution of a linear system, represented by a bordered tri-diagonal matrix; zero or cyclic boundary conditions may be specified. In the case of arbitrarily complex MQW problems the combined ShM+EWC approach is necessary when approximate wave functions and estimations for the energy eigenvalues for the EWC method are supplied by the ShM. Considering formation of the Jacobi matrix in the Newton method by zero boundary conditions, the EWC method is similar to the known relaxational approach [4]. As one can see below, direct comparison of FGH and ShM+EWC methods reveals that the latter may be over three orders of magnitudes more effective than the FGH method for tasks with $N > 1000$. Some results of application of the present work are published in [9].

In the present study we discuss neither semi-analytical approaches with specific application areas like [6] nor the new original "random trial" approaches [5].

2. METHODS OF THE NUMERICAL SOLUTION

2.1. The Fourier grid Hamiltonian method

The Fourier grid Hamiltonian method for numerical solution of the time-independent Schrödinger equation was introduced in 1989 by Marston and Balint-Kurti [1]. Initially it was formulated for an odd number of coordinate grid points N in rectangular coordinates [1]. Later it was modified for an even number of grid points and for spherical coordinates with the possibility of applying the Fast Fourier Transform to accelerate the formation of the Hamiltonian matrix [2,3]. The theory behind the method is based on relating the potential energy at the N grid points with the kinetic energy in the momentum space via forward and reverse Fourier transforms between the coordinate and the momentum space. The $N \times N$ symmetric matrix H, obtained by discretization, has elements in the form of cosine sums. The task of calculating the bound state eigenenergies and eigenfunctions is thereby transformed to the task of finding eigenvalues and eigenvectors of the matrix H. As suggested by the authors of the FGH method, this may be accomplished by standard subroutines such as the EISPACK package [10]. The source code of the computer implementation of the method, FGHEVEN [2], for an even number of nodes, is freely distributed via the internet [11]. Subsequently, the method was extended to the three-dimensional case [12]. In the present work we have realized the odd number FGH method in rectangular coordinates and in the SI unit system for testing, following reference [1].

Assuming that the length of the calculation area L is divided into N steps, the discrete grid is defined as

$$x_i = (i - 1/2)\Delta x, \quad \Delta x = L/N, \quad i = 1, 2, ..., N. \tag{1}$$

Equation (1), which defines nodes in the centre of every interval Δx, differs somewhat from the original one $x_i = i\Delta x$ [1] but is more correct in the case of symmetric QW tasks.

Following [1], the spatial discretization and transformations performed yield a symmetric matrix H of size $N \times N$

$$H_{ij} = \frac{2}{N}\sum_{l=1}^{n} \cos(l2\pi(i-j)/N)T_l + V(x_i)\delta_{ij}, \quad n = (N-1)/2,$$
$$T_l = \frac{2}{m}\left(\frac{\pi \hbar l}{L}\right)^2, \tag{2}$$

where $\hbar \equiv h/2\pi$ is the reduced Planck constant, m is the electron rest mass and the Kronecker symbol δ_{ij} ensures that potential energy values at grid nodes $V(x_i)$ are only added to the main diagonal.

The EISPACK subroutines return N eigenvalues and N eigenfunctions with values at all N grid nodes. The eigenvalues, which lie below the potential energy values at the solution area borders $V(0)$ and $V(L)$, may be interpreted as the bound state energies of the system [1]. The other eigenvalues may be interpreted as extraneous solutions, which unfortunately consume computer time for their calculation. On the other hand, the maximum number of eigenvalues is limited by the grid size N. As experience shows, in practical quantum well calculations sufficiently thick outer barrier layers with a sufficiently high potential V must be included to ensure sufficient decay of wave functions and hence remove any uncertainty in the boundary conditions in the FGH method. It should be added that by selecting different subroutines from the EISPACK package, it is possible to calculate the energies without wave functions [11], which reduces the computation time approximately 1.5 times.

2.2. The shooting method

The shooting method is one of the simplest numerical algorithms and its key idea is to replace a boundary condition problem with multiple trial runs of a remarkably simple initial condition task. This is also the most straightforward method for solution of the time-independent Schrödinger equation if the varied trial parameter is the energy E ([7], Chapter 3). The trial energy equals the bound state energy if the wave function vanishes ($\Psi \to 0$) in the surrounding barriers when moving away from the QW area. In spite of the extreme simplicity, ShM has a linear dependence of the computer time on the grid node number $t_{\text{comp}} \sim N$, which makes it efficient for MQW tasks.

The time-independent 1D Schrödinger equation in its classical form, where kinetic energy is defined by the second spatial derivative, reads

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi = E\Psi. \tag{3}$$

In the present study, which is focused on the effectiveness of numerical methods, we ignore the fact that in semiconductor heterostructures, a more sophisticated kinetic energy term [7]

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial}\frac{1}{m}\frac{\partial\Psi}{\partial x} \tag{4}$$

is recommended for tasks with a variable effective mass $m(x)$.

To realize discrete stepping over the spatial coordinate, the second derivative in the Schrödinger equation (3) is replaced by a three-point discretization scheme

$$-\frac{\hbar^2}{2m}\left(\frac{\Psi_{i+1}-\Psi_i}{\Delta x}-\frac{\Psi_i-\Psi_{i-1}}{\Delta x}\right)\frac{1}{\Delta x}+V_i\Psi_i=E\Psi_i, \tag{5}$$

where Ψ_i denotes $\Psi(x_i)$ and $V_i \equiv V(x_i)$.

To initialize the iteration in Eq. (5), two starting values of the wave function are needed. That is facilitated by the obvious fact that the Schrödinger equation (3) and the energy eigenvalues defined by it are insensitive to constant multipliers of Ψ. That means that prior to the wave function normalization with the condition

$$\int_{-\infty}^{+\infty}\Psi^2(x)\,\mathrm{d}x=1, \tag{6}$$

the scale of the wave function has no importance.

Thus for symmetrical QWs, the initial conditions in the QW centre x_c may be specified in the case of symmetrical wave functions by [7]

$$\Psi(x_c)=1, \quad \Psi(x_c+\Delta x)=1+(m\Delta x^2/\hbar^2)(V(x_c)-E),$$

and for antisymmetrical wave functions by [7]

$$\Psi(x_c)=0, \quad \Psi(x_c+\Delta x)=1.$$

In the more general non-symmetrical case, the stepping must start from two adjacent grid points within one barrier, e.g. in the left barrier from coordinates x_{left} and $x_{\mathrm{left}}+\Delta x$:

$$\Psi(x_{\mathrm{left}})=\varepsilon, \quad \Psi(x_{\mathrm{left}}+\Delta x)=\varepsilon\exp(\kappa\Delta x), \tag{7}$$

where ε is a small (but finite) number and κ is the theoretical wave function exponential growth/decay constant, which follows directly from Eq. (3) for the constant barrier height $V > E$ and energy eigenvalue guess E as [7]

$$\kappa=\sqrt{2m(V-E)/\hbar^2}. \tag{8}$$

The condition for energy eigenvalue detection is the vanishing wave function in the opposite external barrier: $\Psi \to 0$ as $x \to \infty$ ([7], p 75). Beside numerical problems, associated with the great range of numerical values of Ψ, the advantage of considering only half of the structure in the symmetrical case is lost in the general non-symmetrical QW case.

One principal inconvenience with the numerical realization of the shooting method is associated with detecting the condition $\Psi \to 0$. The reason for this is

the fact that the Schrödinger equation (3) as a second order differential equation has solutions which contain both growing and decaying exponentials in a uniform potential barrier:

$$\Psi(x) = A\exp(-\kappa\Delta x) + B\exp(+\kappa\Delta x), \tag{9}$$

where the constant κ is defined by Eq. (8). This theoretical form of the wave function in the outer barriers, surrounding the QW, means that every small change in the trial energy from the exact eigenvalues, as well discrepancies in arithmetic operations (rounding errors) are amplified as the stepping iteration proceeds into the barrier. Consequently, in a numerical realization of the ShM algorithm, instead of the theoretical condition $\Psi \to 0$ the energy value must be sought that changes the sign of the "tail" of the wave function ([7], p 77).

The idea of the shooting method of stepping over space and energy is explained in Fig. 1.

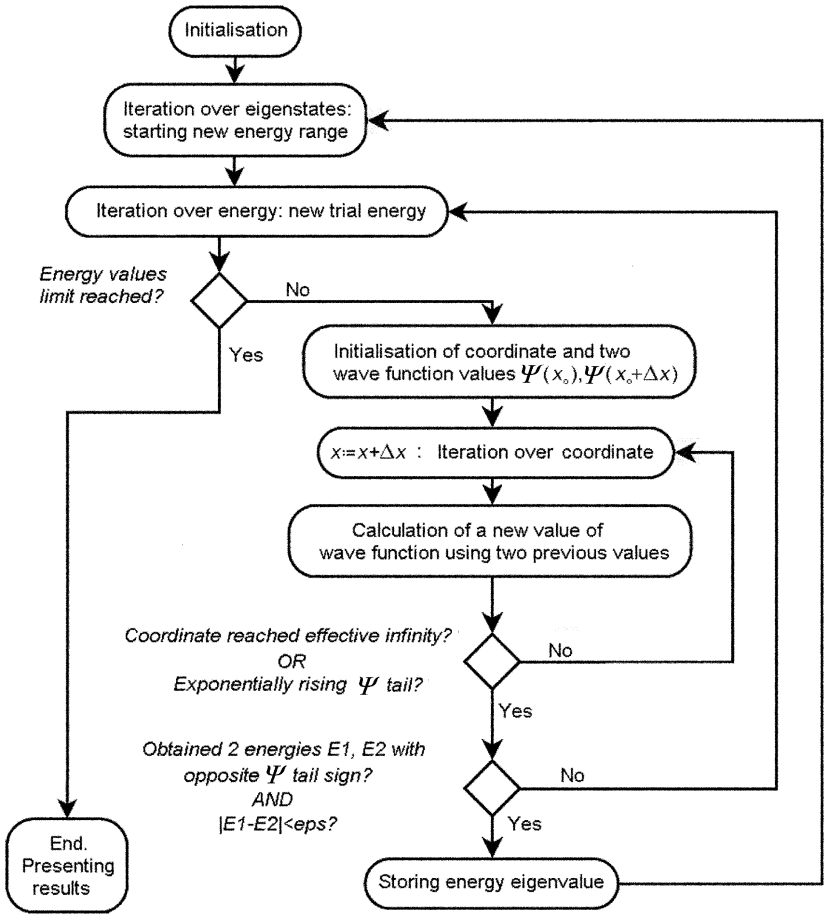

Fig. 1. Algorithm of the shooting method. The internal cycle performs the stepping over space and two external cycles find the eigenvalues of the energy.

2.3. The method of coupling the energy and wave functions

As seen above, realization of the shooting method demands a rather small amount of computations but the definition of the boundary conditions and the process of finding the exact energy eigenvalues need special care. Serious numerical problems may arise in the case of relatively thick barriers $(w >> 1/\kappa)$, where exponential growth of the wave function follows from an inaccurately defined energy eigenvalue or discrepancies due to the limited number of significant figures available for the arithmetic operations. To avoid these problems, the EWC method was developed, which solves system of equations with clearly fixed boundary conditions simultaneously for the energy eigenvalue and wave function values across the spatial grid nodes. The 3-point scheme of spatial discretization used corresponds exactly to that of the shooting method in Eq. (5). The exact zero or cyclic boundary conditions for Ψ for the calculations are fixed. The zero boundary conditions actually correspond to the assumption about infinite potential barriers on the external borders of the calculation area. To find the energy eigenvalue together with the values of the wave function on the grid nodes, an additional equation is necessary, besides the discretized Schrödinger equation, which is the normalization condition of the wave function (6). The latter states that the probability of finding an electron over the entire space of the calculation equals unity. With this additional condition the calculated wave functions from the EWC method are automatically normalized.

The unknown vector Y of the EWC method contains N components: the energy eigenvalue E and wave function values $\Psi_i \equiv \Psi(x_i)$ in nodes $i = 2, 3, \ldots, N$ of the grid:

$$x_i = (i-1)\,\Delta x, \quad \Delta x = L/(N-1), \quad i = 1, 2, ..., N, \tag{10}$$

$$Y = (E, \Psi_2, \Psi_3, ..., \Psi_N)^T, \tag{11}$$

where the superscript T denotes transposition.

The value of the wave function in the 1st spatial node is not included in Y since

$$\Psi_1 = \Psi_N \tag{12}$$

is assumed for both boundary condition types.

The zero boundary conditions are then specified simply as

$$\Psi_N = 0. \tag{13}$$

The cyclic boundary condition may be specified by the discrete Schrödinger equation (5) for the boundary node N. Taking into account the translational

symmetry, the node N is equivalent to node 1, node $N+1$ is equivalent to node 2 etc. Thus the necessary three "neighbour" wave function values in the boundary node N are $\Psi_{N-1},\ \Psi_N = \Psi_1,\ \Psi_2$.

Thus the first non-linear equation of the EWC method system is the rewritten normalization condition of the wave function (6) in discrete form

$$F_1(\Psi_2, \Psi_3, ..., \Psi_N) \equiv \sum_{i=2}^{N} \Psi_i^2 \Delta x - 1 = 0. \tag{14}$$

The next necessary $N-2$ equations are the discrete Schrödinger equations (5) for the internal grid nodes $i = 2, 3, ..., N-1$:

$$F_i(E, \Psi_{i-1}, \Psi_i, \Psi_{i+1}) \equiv \frac{\hbar^2}{2m}\left(\frac{\Psi_{i+1} - \Psi_i}{\Delta x} - \frac{\Psi_i - \Psi_{i-1}}{\Delta x}\right)\frac{1}{\Delta x} + (E - V_i)\Psi_i = 0, \tag{15}$$

where for $i = 2$ according to Eq. (12) holds $\Psi_{i-1} = \Psi_N$.

In the case of zero boundary conditions, the last equation of the system is

$$F_N(\Psi_N) \equiv \Psi_N = 0. \tag{16}$$

In the case of the cyclic boundary condition, the last equation of the system is similar to Eq. (15) with the replacement $\Psi_{N+1} = \Psi_2$:

$$F_N(E, \Psi_{N-1}, \Psi_N, \Psi_2) \equiv \frac{\hbar^2}{2m}\left(\frac{\Psi_2 - \Psi_N}{\Delta x} - \frac{\Psi_N - \Psi_{N-1}}{\Delta x}\right)\frac{1}{\Delta x} + (E - V_N)\Psi_N = 0. \tag{17}$$

The system (14)–(17) is non-linear as Eq. (14) contains squares of the values of the wave function and Eqs. (15) and (17) contain products of energy and wave functions. This system may be linearized and solved iteratively using the Newton method. For every iteration, the unknown vector Y may be written as

$$Y = \tilde{Y} + \delta Y, \tag{18}$$

$$[\partial F / \partial Y] \times \delta Y = -\tilde{F}, \tag{19}$$

where $\tilde{Y}$ denotes the approximate unknown vector, δY is the correction vector, $\tilde{F} \equiv (\tilde{F}_1, \tilde{F}_2, ..., \tilde{F}_N)^T$ is the RHS vector of the system calculated by $\tilde{Y}$ and $[\partial F / \partial Y]$ is the $N \times N$ Jacobi matrix with the Newton method derivatives. In the case of normal convergence, both δY and $\tilde{F}$ approach to zero.

The Jacobi matrix, obtained by differentiation of Eqs. (14)–(17), has a tridiagonal structure with filled first row and column and zero element in the upper left corner. Four terms in the last line and the last column are not zero in the case of cyclic boundary conditions for Eq. (17):

$$\begin{bmatrix} 0 & 2\Psi_2 & 2\Psi_3 & 2\Psi_4 & 2\Psi_5 & ... & 2\Psi_{N-3} & 2\Psi_{N-2} & 2\Psi_{N-1} & 2\Psi_N \\ \Psi_2 & a_2 & c & 0 & 0 & ... & 0 & 0 & 0 & c \\ \Psi_3 & c & a_3 & c & 0 & ... & 0 & 0 & 0 & 0 \\ \Psi_4 & 0 & c & a_4 & c & ... & 0 & 0 & 0 & 0 \\ ... & ... & ... & ... & ... & ... & ... & ... & ... & ... \\ ... & ... & ... & ... & ... & ... & ... & ... & ... & ... \\ ... & ... & ... & ... & ... & ... & ... & ... & ... & ... \\ \Psi_{N-2} & 0 & 0 & 0 & 0 & ... & c & a_{N-2} & c & 0 \\ \Psi_{N-1} & 0 & 0 & 0 & 0 & ... & 0 & c & a_{N-1} & c \\ \Psi_N & c & 0 & 0 & 0 & ... & 0 & 0 & c & a_N \end{bmatrix}, \tag{20}$$

where $c \equiv \hbar^2/(2m\Delta x^2)$ and $a_i \equiv E - V_i - 2c$.

In the case of zero boundary conditions of Eq. (16), in the last line of the matrix (20) there remains only one non-zero element $a_N = 1$. A more radical way is to solve the problem with the $(N-1)\times(N-1)$ matrix without the last row and column for the respectively reduced unknown vector, since $\Psi_N = 0$ is fixed and must not be considered as an unknown variable.

To solve the linear system (19) with the tridiagonal bordered matrix (20), a special effective Gaussian elimination algorithm ([13], p 90) was applied.

Using approximate form for the wave function and the value of the energy level, the EWC method described here finds iteratively the exact value for energy and wave function for any specified potential. The approximate initial solution may be obtained from theoretical estimations or with any other method. The only drawback of the EWC method is that in the case of a poor initial approximation when, e.g., a wrong number of halfwaves of the wave function within the QW is determined, the convergence process may give a solution for a different eigen-state instead of the one which was wanted. The method was tested in the case of MQW structures with hundreds of abrupt potential barriers [9]. A reliable scan over the whole range of eigenenergies was obtained if rough approximations were precalculated by the shooting method.

Numerical tests showed that in the case of poor initial solutions the EWC method usually needed 5–7 iterations to converge. Divergence was never observed. In a combined use together with the shooting method, the typical number of Newton iterations decreased to 3–4 to reach convergence with practically zero error. Figure 2 illustrates very high quadratic convergence speed of the EWC method.

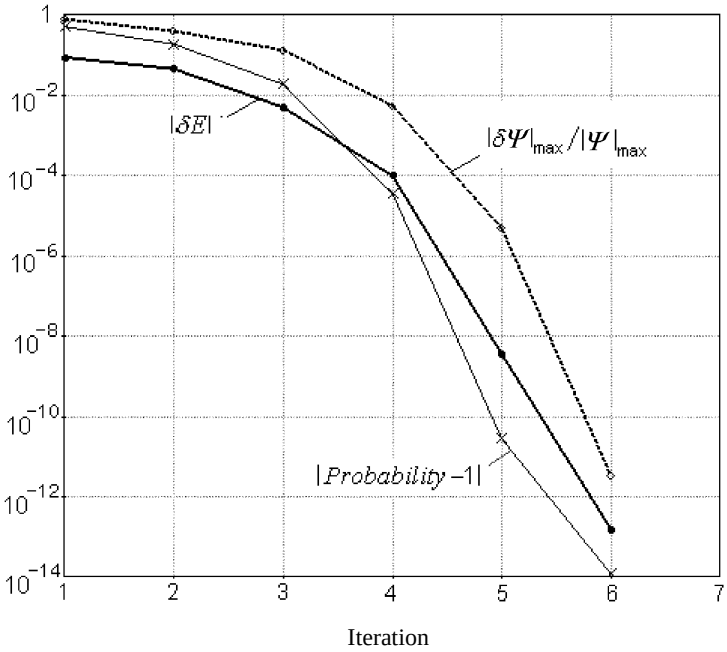

Fig. 2. Typical convergence characteristics of the iteration process of the EWC method. Figure shows in logarithmic scale the decrease of the bound state energy increment δE (eV), the decrease of the maximum relative wave function increment and the approach of the particle finding probability to its theoretical limit of 1.

3. RESULTS OF THE EFFICIENCY TEST

3.1. Comparison of the accuracy of the FGH and EWC methods

Prior to comparing the efficiency on the basis of consumption of the computer time, an estimation of equivalent spatial grid sizes should be performed. Some preliminary calculations in the case of a nearly sine wave function showed that minimal rough accuracy may be achieved with the FGH method if the number of grid nodes per wave of Ψ is 2–3. For EWC method the corresponding number was 4–5. A more accurate comparison was performed for a triple QW task as described in Fig. 3.

The structure in Fig. 3 has three quantum wells of 9 Å width and 10 eV depth, separated by 1 Å barriers. The size of the outer barriers on both sides is 9 Å. The structure has 15 energy levels below 10 eV. The separation of energy levels has peculiarities and the wave functions contain intervals with different spatial frequencies. In tests, the free electron rest mass was used. To achieve maximum compatibility between the FGH and EWC methods, which use slightly different localization of spatial grid nodes, special care was taken. Additionally, for the border nodes in the FGH method a high potential energy

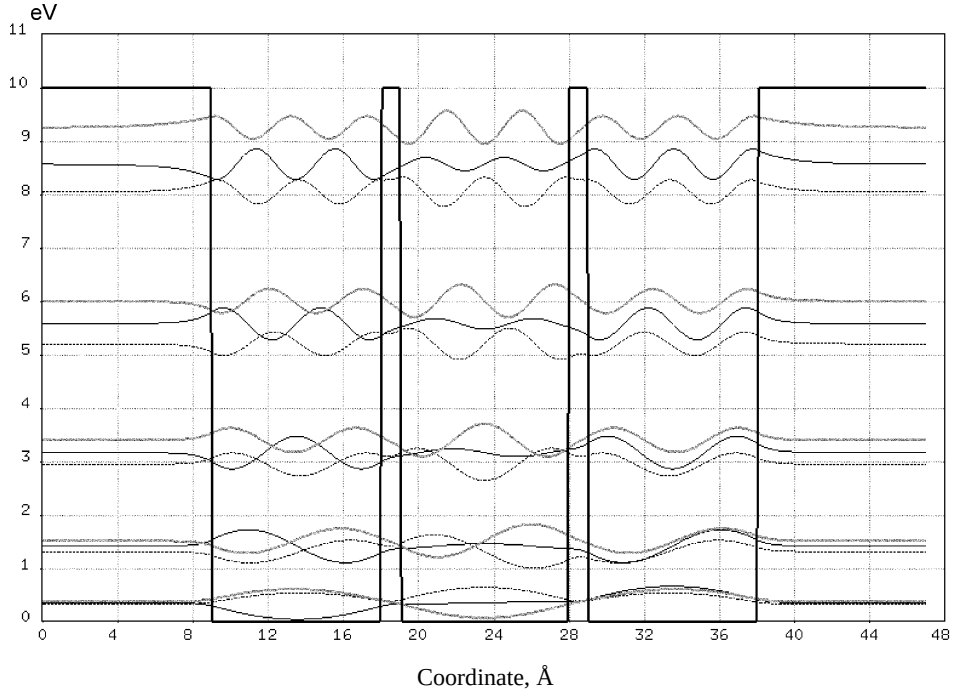

Fig. 3. Potential energy (**—**) and 15 calculated wave functions (—) in the triple quantum well test structure. The variable part of wave functions is presented in an arbitrary scale but the average values are fixed in accordance to the corresponding energy level. Free electron rest mass is used.

value was assigned to model the zero boundary conditions of the EWC method. In this comparison the accuracy of both methods was evaluated by a comparison of the accuracy of the energy eigenvalues calculations. Since the computer time consumption of the FGH method became very high for greater grid point numbers, exact reference numbers were obtained with the EWC method for the grid with $N = 30\,000$. The accuracy criterion for finishing the Newton iterations in the EWC method was practically set to zero ($\delta E \leq 10^{-9}$ eV). The results are presented in Fig. 4.

As Fig. 4 shows, for both methods the error of energy level decreases with the grid step as $\sim \Delta x^2$. However, to achieve a comparable accuracy, the EWC method needs approximately three times more grid nodes. For example, a relatively good accuracy of 0.1 meV needs approximately 1500 nodes in the case of the FGH method and 4500 nodes in the case of the EWC method.

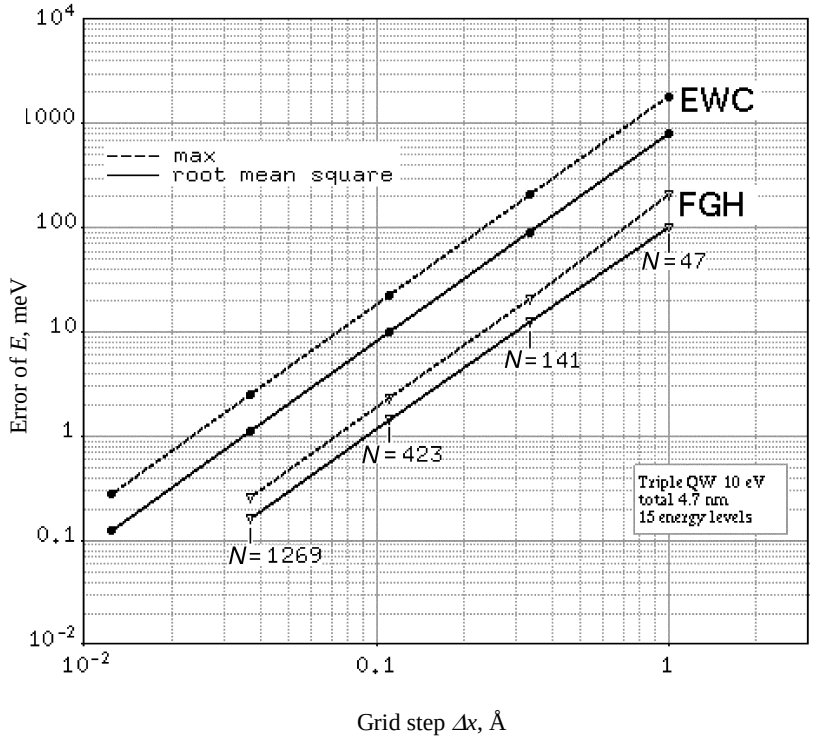

Fig. 4. The accuracy of calculated energy eigenvalues versus grid step for FGH and EWC methods. The triple QW structure (Fig. 3) is tested. The maximum error and the root mean square error for the set of 15 energy levels are shown.

3.2. Comparison of computation times of the FGH and EWC methods

The computer times for both approaches are compared in Fig. 5. The calculations were performed for a triple QW structure with 15 energy levels according to Fig. 3. As the approximate wave functions and energy eigenvalues for the EWC method were calculated by shooting method, the corresponding results are marked as ShM+EWC in Fig. 5. In the case of the FGH method, the computer time practically depends only on the number of grid points and not on the form of the potential. In the case of the EWC method, the amount of computer time is also proportional to the number of energy levels. Numerical experiments were performed on a desktop PC with a 3 GHz Pentium-4 processor on Windows XP platform using GNU-Fortran-77 programming language.

Figure 5 shows the $t_{\text{comp}} \sim N^3$ dependence of the FGH method. That limits the practical use of this method to the grid sizes from 2000 to 3000. It is interesting that the reduced version of the FGH, which does not calculate the wave functions, does not significantly reduce the computational time. In contrast to the FGH, in the case of the EWC method t_{comp} depends linearly on N. Although the EWC method needs roughly three times more grid nodes for the same accuracy,

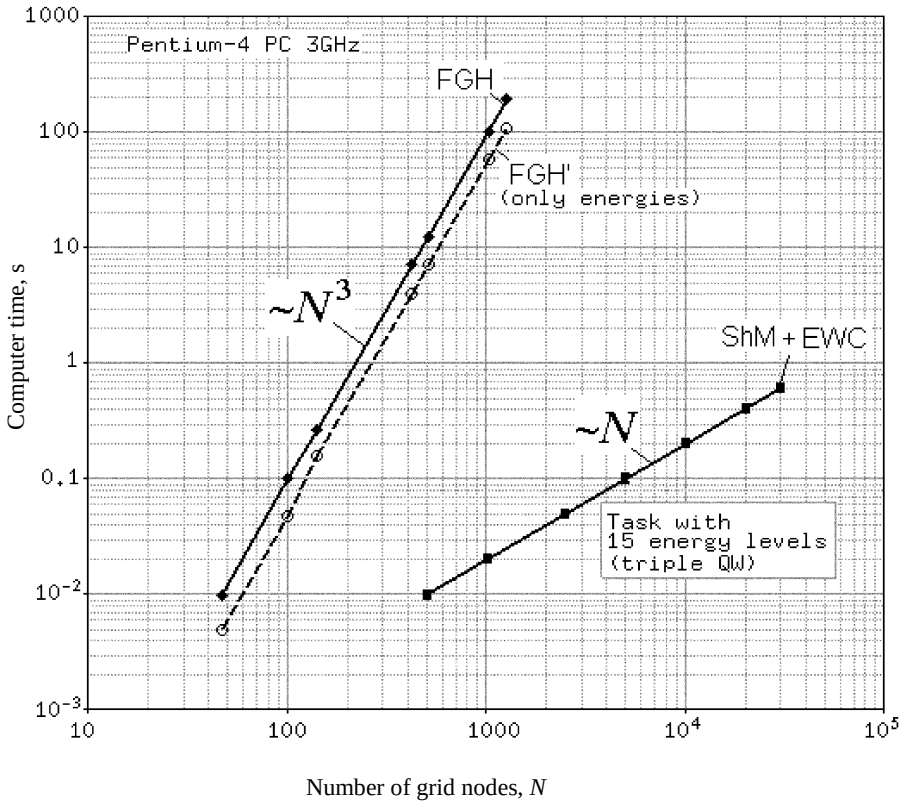

Fig. 5. Comparison of the computer times versus grid size for FGH and EWC methods. The latter is completed with ShM, which provides approximate energy values and wave functions. Triple QW structure with 15 bound state energy levels (Fig. 3) is tested.

the comparison proves clearly that the ShM + EWC approach is more than three orders of magnitudes more effective than the FGH method. Computer times of subsecond range show that the ECW method may be easily applied to very complex MQW problems that demand 10^5 and more grid nodes.

Some tests were also performed with the shooting method on its own. However, the exact results of a comparison between the ShM and the combined ShM + EWC method depend on the specific finishing criteria for the coordinate and energy iteration processes in the ShM. The EWC method is rather insensitive in the sense that its boundary conditions are clearly fixed and the energy convergence speed is very high (Fig. 2). Numerical experiments showed that by careful selection of the accuracy criteria and using the benefit of a symmetric structure, it was possible to obtain 30–40% shorter computer times with the pure ShM. However, in the general case of a non-symmetrical structure and guaranteed high accuracy the combined ShM + EWC approach was approximately 1.5–2 times more effective than the use of the ShM only.

4. DISCUSSION AND CONCLUSIONS

We have discussed and tested qualitatively some practical approaches to the solution of the time-independent 1D Schrödinger equation without any restrictions on the potential energy distribution. The comparison was centred around two effective methods: the Fourier grid Hamiltonian method known from the field of physical chemistry and the shooting method often applied to semiconductor quantum well calculations. We established cubic computer time dependence on the number of grid points in the FGH method and concluded that it is very difficult to use this method for complex tasks which need more than 2000 grid points.

We also critically analysed the drawbacks of extremely simple trial-and-correction type shooting methods and offered a more general and reliable coupled energy and wave function method (EWC) with a Newton iteration scheme and an internal linear task with a tridiagonal bordered matrix. We formulated this EWC method for two types of boundary conditions: zero wave function (hard wall) or cyclic. A survey of the literature showed that the EWC method was actually an extended version of a relaxational approach [4] published in 2001.

For versatile multiquantum well problems we developed an effective and reliable combined approach (ShM + EWC) where at first the shooting method is used for a rough estimation of the energy eigenvalues and approximate wave functions. Secondly, the fast-converging EWC method is applied for reliable calculation of more exact results. Detailed investigation of the grid error and computer time on the basis of a triple quantum well task for both the FGH and ShM + EWC approaches was performed. The results show that although the ShM + EWC method needs approximately three times more grid nodes than the FGH method, it is still several orders of magnitudes more effective than the FGH method. On modern computers, MQW tasks with grid point numbers over 10^5 may be easily solved with the EWC method.

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Schrödingeri võrrandi lahendusmeetodite võrdlus mitmik-kvantaukudega heterostruktuuride jaoks

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On võrreldud otseseid numbrilisi lahendusmeetodeid ajast sõltumatu ühemõõtmelise Schrödingeri võrrandi lahendamiseks. Mitmik-kvantaukudega (MQW) pooljuht-heterostruktuuride arvutused nõuavad meetodeid, mille puhul arvutusaeg t_{comp} sõltub ruumivõrgu sammude arvust N lineaarselt. Tuntud ja väga efektiivseks peetav Fourier Grid Hamiltoniani (FGH) meetod (Fourier' teisenduse ja ruumivõrgu alusel moodustatud hamiltoniaani analüüsiv meetod) omab aga kuupsõltuvust $t_{\mathrm{comp}} \sim N^3$, mistõttu selle meetodi rakendusala on piiratud probleemidega, kus $N \leq 1000$ on piisav. Lihtsaim otsene lahendusmeetod on nn tulistamismeetod (ShM), mis põhineb katselisel astumisel üle ruumikoordinaadi ja energiaväärtuste. Tulistamismeetod omab vajalikku lineaarset sõltuvust $t_{\mathrm{comp}} \sim N$ ja rahuldavat energiaväärtuste koondumiskiirust, kuid ebaselgelt määratletud piiritingimused teevad meetodi kasutamise ebamugavaks. Artiklis on esitatud energianivoode ja lainefunktsioonide kooslahendamise meetod (EWC), mis on töökindel ja efektiivne ning omab lineaarset sõltuvust $t_{\mathrm{comp}} \sim N$. Meetod põhineb mittelineaarsete võrrandisüsteemide lahendamiseks sobival Newtoni iteratsioonimeetodil, kusjuures sise-

mise lineaarse ülesandena lahendatakse kolmediagonaalse ääristatud maatriksiga süsteem. Esitatud meetod on rakendatav suvalise potentsiaalse energia jaotusega ülesannetele keerukusega $N = 10^5$ ja üle selle nii nulliliste kui ka tsükliliste piiritingimuste puhul. Praktiliste MQW-ülesannete jaoks on realiseeritud võimalus kasutada meetodeid kombineeritult, mille puhul arvutatakse ShM-i abil energiate ja lainefunktsioonide ligikaudsed alglähendid väga kiirelt koonduvale EWC-meetodile. Kolmik-kvantaugu näitel formuleeritud testülesande lahendamise teel on võrreldud vaadeldud meetodite ruumilist täpsust ja arvutiaega. Tulemused näitavad, et kombineeritud meetod ShM + EWC on FGH-meetodist mitu suurusjärku efektiivsem.