**MATLAB Modelling electron energy spectrum in one-dimensional quantum well with infinitely high walls for GaAs solid solution**

E R Kozhanova¹, I M Tkachenko²

¹Yuri Gagarin State Technical University of Saratov, Saratov, Russia
²École de Technologie Superieure, Montreal, Canada

E-mail: kozhanovaer@gmail.com

**Abstract.** The paper presents calculations of electron states in semiconductor nanostructures Al_Ga_1-x_As (x=0) and simulates the energy spectrum of the electron in a one-dimensional quantum well with infinitely high walls of a given width (from 10 to 30 atomic monolayers) using MATLAB application. The data is visualized using a wavelet transform with different wavelet functions.

1. Introduction

Calculations of electronic states in semiconductor nanostructures, performed in the effective mass method, are based on the solution of the stationary Schrödinger equation, which is one-dimensional for the motion of electrons in the perpendicular plane of the layers (excluding cases where the potential relief is a function of time) [1 - 5]:

\[
\frac{-\hbar^2}{2m} \frac{\partial^2 \psi(z,E)}{\partial z^2} + U(z) \cdot \psi(z,E) = E \cdot \psi(z,E),
\]

where \( m \) is the effective mass of the electron, \( E \) is its total energy, \( U(z) \) is the potential relief for the electron along the \( z \) axis directed perpendicular to the plane of the layers.

A solution of this Schrödinger equation is the \( z \) - component of the envelope of the wave function \( \psi(z,E) \) which characterises the motion of electrons in the perpendicular plane of the layers and determines the probability of finding an electron with energy \( E \) of motion along the \( Oz \) axis at a point with coordinate \( z \) within the normalisation [1 - 2].

2. Modelling the energy spectrum of an electron in a one-dimensional quantum well

Consider simulation of the energy spectrum of an electron in a one-dimensional quantum well.

If a thin layer of narrow band material is placed between two quite thick layers of wide-band material, a potential well can be formed for an electron moving in a direction transverse to the planes of the layers (Fig. 1) (the energy is counted from the bottom of the conduction band of the well material). This kind of relief is called a rectangular potential well. For modeling we will consider a symmetric potential well (Fig. 1, b) [1-2].
Figure 1. Energy diagram of a rectangular potential well:
a - asymmetrical, b – symmetrical [1]

Consider the idealized case of a potential well with infinitely high walls, in which case the envelope wave function \( \psi(z,E) \) outside the well is identically equal to zero and inside the well satisfies the Schrödinger equation (1) with boundary conditions [1-5]:

\[
\psi\left(\pm \frac{a}{2}, E\right) = 0
\]

where \( a \) is the width of the potential well (thickness of the middle layer of the three-layer structure). Then \( \pm a/2 \) are coordinates of interfaces between the layers.

The solution at discrete energy \( E \) - eigenvalues of this equation (1) [6] has the form:

\[
E = \frac{\hbar^2}{2m} \left( \frac{\nu \pi}{a} \right)^2
\]

where \( \nu \) is the number of the energy level.

The system has symmetry along the Oz axis with respect to the origin, so the set of eigen solutions of the Schrödinger equation is divided into subgroups of even and odd solutions [1, 3-5]:

\[
\psi(z,E) = \begin{cases} 
C \cos\left( \frac{\nu \pi}{a} \cdot \frac{z}{a} \right) & \text{at } \nu = 1, 3, 5, \ldots \\
C \sin\left( \frac{\nu \pi}{a} \cdot \frac{z}{a} \right) & \text{at } \nu = 2, 4, 6, \ldots 
\end{cases}
\]

where \( C \) is the normalisation factor, depending on \( \nu \).

Plots of the envelope wave functions of electrons use the square of the modulus of expression (4) (Fig. 3):

\[
|\psi(z,E)|^2
\]

This task can be solved for the solid solution \( \text{Al}_x\text{Ga}_{1-x}\text{As} \), the band structure for any \( x \) is shown in figure 2.
3. Modeling of electron energy spectrum in a one-dimensional quantum well with infinitely high walls of solid solution $\text{Al}_x\text{Ga}_{1-x}\text{As}$

As a test case, the authors considered a quantum well with infinitely high walls of 20 atomic monolayers wide (11.3 nm) for the first four allowed energy levels (Fig. 3, a), the energy spectrum of the electron in such a well shown in Fig. 3, b [1]. The well material is GaAs ($x = 0$). The graphs are plotted on the basis of calculations in MathCad.

The next step was written a program in the MATLAB mathematical package to simulate the energy spectrum of the electron in a one-dimensional quantum well with infinitely high walls of solid solution $\text{Al}_x\text{Ga}_{1-x}\text{As}$ for the well material is GaAs ($x = 0$) (Fig. 3, c and d).

**Figure 2.** Zone structure of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ solid solution: a - $x < 0.45$, b - $x > 0.45$ [1]

**Figure 3.** Wave function envelopes (a, c) and quantised energy levels (b, d) of an electron in a rectangular quantum well
First, consider simulations of GaAs \((x = 0)\) at different values of the number of atomic monolayers \(NN\) for the first four resolved energy levels (Table 1, Figure 4).

| Number of atomic monolayers \(NN\) | Width of the quantum well, \(a\), nm | Quantisation levels in the well |
|---|---|---|
| 10 | 5.6533 | 0.0281 e-36 | 0.1125 e-36 | 0.2532e-36 | 0.4502 e-36 |
| 15 | 8.4800 | 0.0125 e-36 | 0.0500 e-36 | 0.1125e-36 | 0.2001 e-36 |
| 20 | 11.3066 | 0.0070 e-36 | 0.0281 e-36 | 0.0633e-36 | 0.1125 e-36 |
| 25 | 14.1333 | 0.0450 e-37 | 0.1801 e-37 | 0.4052e-37 | 0.7203 e-37 |
| 30 | 16.9599 | 0.0313 e-37 | 0.1250 e-37 | 0.2814e-37 | 0.5002 e-37 |

Figure 4. Simulation results of electron energy spectrum in one-dimensional GaAs quantum well with infinitely high walls \((x = 0)\) at different values of number of atomic monolayers \(NN\) for first four resolved energy levels.

4. Wavelet transform

We performed a continuous wavelet transform \([7-9]\) using the following wavelet functions: «Haar» (column 2 of Table 2), capturing inflection points, and «Mexican Hat», capturing points of extremum (column 3 of Table 2), as well as a \(wtmm\) function from the Matlab library \([10]\) (in 0.01 steps; number of samples 1131) for each envelope function of quantised energy levels (Fig. 3,c).

| Energy level | Wavelet «Haar» / \(wtmm\) | Wavelet «Mexican Hat» / \(wtmm\) |
|---|---|---|
| 1 | | |
If we leave the Mexican Hat wavelet function [7-9] for the study and set the step to 0.001 (number of counts 11307), the appearance of the plots will change (Table 3).

| Energy level | Wavelet «Mexican Hat» / wtmm |
|--------------|------------------------------|
|              | step = 0.01                  | step = 0.001                  |
| 1            | ![Plot 1]                    | ![Plot 1]                    |
| 2            | ![Plot 2]                    | ![Plot 2]                    |
| 3            | ![Plot 3]                    | ![Plot 3]                    |
| 4            | ![Plot 4]                    | ![Plot 4]                    |

All wavelet transform results are plotted with respect to the number of reference points with a given step, so the task arises of translating the number of reference points with respect to the coordinate \( z \) defining the width of the quantum well from \(-a/2\) to \(a/2\) (Fig. 5).

**Figure 5.** Conversion from one scale to the other
A formula for conversion from one scale to the other can be derived from this:

\[ z_i^* = -a/2 + shag \times (nN_i - 1) \]  

(6)

where \( shag \) is the step, \( nN_i \) is the number of counts of a given point.

Consider first the errors that arise when converting from one scale to another by summarising the data in Table 4.

| Parameters | \( shag = 0.01 \) | \( shag = 0.001 \) |
|------------|------------------|------------------|
| \( a \)    | 11.3066          | 11.3066          |
| \( a/2 \)  | 5.6533           | 5.6533           |
| \( nN \)   | 1131             | 11307            |
| \( Error \Delta_i \) | 0.0066 | 6e-4 |

Substitute \( nN \) and \( shag \) from Table 4, calculate the last scale value and compare it with the value of \( a/2 \), finding the scale conversion error.

- for step \( shag = 0.01 \):
  
  \[ z_1 = -5.6533 + 0.01 \times (1131 - 1) = 5.6467 \]
  
  \[ \Delta_1 = 5.6533 - 5.6467 = 0.0066 \]

- for step \( shag = 0.001 \):
  
  \[ z_2 = -5.6533 + 0.001 \times (11307 - 1) = 5.6527 \]
  
  \[ \Delta_2 = 5.6533 - 5.6527 = 6e-4 \]

Compare the results obtained with the \textit{wtmm} function for different values of the \( shag \) step (Fig.6).

![Figure 6. Results obtained with the wtmm function](image)

a) \( shag = 0.01 \)  
b) \( shag = 0.001 \)

Use formula (6) to find the values (Table 5).

| Extremes (Fig.6) | \( shag = 0.01 \) | \( shag = 0.001 \) |
|------------------|------------------|------------------|
| sample (Fig.6,a) | \( z_i \)         | \( z_i \)         |
| calculation      |                  |                  |
| 1                | 57               | 567              |
| 2                | -5.0933          | -5.0873          |
| 3                | 566              | 5654             |
| 2                | -0.0033          | -3.0000e-04     |
| 3                | 1074             | 10740            |
| 5.0767           | 5.0857           |
5. Conclusion

The authors present the results of a program written using the MATLAB application for solving the task of modeling the energy spectrum of an electron in a one-dimensional quantum well with infinitely high walls of the Al$_x$Ga$_{1-x}$As ($x=0$) solid solution. As a result of the wavelet transform the wave function envelopes of quantised energy levels, wavelet spectrograms were obtained using the wavelet functions «Haar» and «Mexican Hat» at different values of the number of atomic monolayers (from 10 to 30). The authors have proposed a formula (6) to convert the number of $nN_i$ counts obtained by dividing the width of quantum well by the calculation step $shag$, into a $z$ scale with a range from $-a/2$ to $a/2$. In further research, the authors plan to use a function $w	ext{mm}$, which captures points of extremum and outputs a table with their values.

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