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Envelope function description of quantum cascade laser electronic states

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In this paper, we present a natural method of finding wavefunctions and energy levels in quantum cascade lasers. The envelope function approximation has been successfully used for modelling electronic structure in conventional semiconductor lasers. Although calculations in the case of polarized potential are more complicated than in non-polarized wells, it is still possible to obtain quickly reliable results.

Keywords: quantum cascade lasers, electronic structure.

1. Introduction

The quantum cascade lasers are very different from the standard semiconductor lasers. In the standard lasers, operating on inter-band transitions, if we know the electronic structure, we immediately know the wavelength and can easily calculate the gain profile. Usually we only need to know the energy levels. However, in quantum cascade structures the question is much more complicated. The energy levels and wavefunctions are only a starting point for further calculations and analysis. So, in order to predict correctly the cascade laser performance we need to be able to calculate the electronic structure very accurately.

In cascade lasers electron travels through a polarized superlattice. To find the electronic properties of such a structure we use envelope function approximation. We have to solve Schrödinger equation with potential consisting of several different quantum wells. Moreover, the wells are polarized. The latter makes the problem more complicated because we need solutions for many different electric fields. Sometimes the potential is approximated by potentials which are easier to analyse [1], but we will show that exact numerical analysis is not difficult.

2. Schrödinger equation for polarized quantum wells

The one-dimensional Schrödinger equation has the following form:

$$-\frac{\hbar^2}{2m}\psi'' + \Big[W(x) + eFx\Big]\psi = E\psi. \tag{1}$$

Function W is the potential of n non-polarized wells (with depth U_0), F is the electric field intensity. In each well or barrier the solution has the following form:

$$\psi_{b_i}(x) = A_i \mathrm{Ai}\Big(k(X_b - x)\Big) + B_i \mathrm{Bi}\Big(k(X_b - x)\Big) \qquad \text{for the } i\text{-th barrier} \tag{2}$$

$$\psi_{w_i}(x) = C_i \mathrm{Ai}\Big(k(X_w - x)\Big) + D_i \mathrm{Bi}\Big(k(X_w - x)\Big) \qquad \text{for the } i\text{-th well} \tag{3}$$

where Ai, Bi are Airy functions, and

$$k = \sqrt[3]{-\frac{2meF}{\hbar^2}}, \qquad X_b = \frac{E}{eF}, \qquad X_w = \frac{E - U_0}{eF}. \tag{4}$$

At the interfaces between barrier and well we use the Ben Daniel–Duke boundary conditions:

$$\psi_i(x_{i,\,i+1}) = \psi_{i+1}(x_{i,\,i+1}), \tag{5}$$

$$\frac{1}{m_i}\psi_i(x_{i,\,i+1}) = \frac{1}{m_{i+1}}\psi_{i+1}(x_{i,\,i+1}). \tag{6}$$

At $-\infty$ the quantization condition gives $B_0 = 0$. Because potential $eFx \xrightarrow{x\to\infty} -\infty$ (assuming $F > 0$) we need to put somewhere an infinite barrier to have normalized eigenfunctions. Although the position of this barrier has generally a significant impact on the equation, it fortunately has little influence on those states which are strongly localized “inside” the wells.

The solution of differential Eq. (1) is reduced to solution of the system of $4n + 1$ homogeneous equations with $4n + 1$ unknowns. The energy levels are given by equation $\det M(E) = 0$, where M is the coefficient matrix of the system of equations. Numerical calculation of determinants is never a good idea. For finding the energy levels we use singular value decomposition algorithm. This method proved to be very accurate and effective. Solving Schrödinger equation for a few structure periods takes reasonably short time.

3. Results of calculations

For the purpose of testing and verifying our program we simulated a part of structure presented in [2]. The structure period consists of a 5-well injector and a 3-well active region. They are separated by a 58 Å wide barrier. Figure 1 shows the simulated structure and the effects of calculations – eigenvalues and eigenfunctions. The infinite barrier is put at position 300 Å. In this figure not all wavefunctions are presented; those localized between the active region and the infinite barrier, or with high energies, have been removed.

In Figure 2, we show results of simplified calculations. Separately calculated injector and active regions are put together. The injector is shifted upwards by energy equal to $|eFw| \approx 0.08$ eV, where $w = 199$ Å is the width of the active region and the

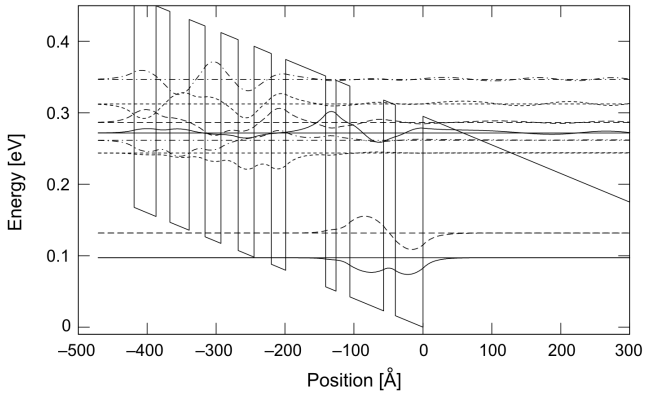

Fig. 1. Energy levels and wavefunctions in a single period of a quantum cascade structure polarized with intensity 40 kV/cm.

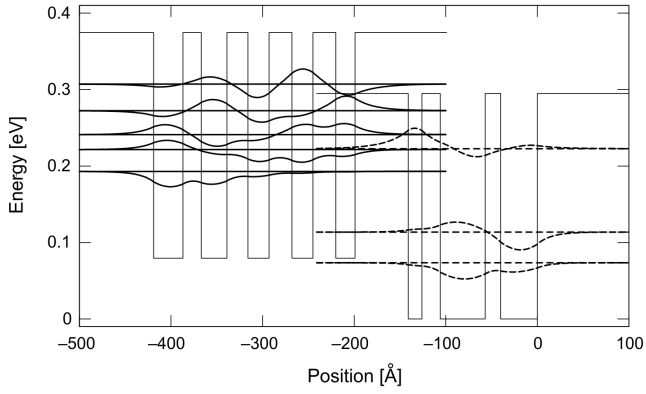

Fig. 2. Non-polarized segments shifted by approximately 0.08 eV.

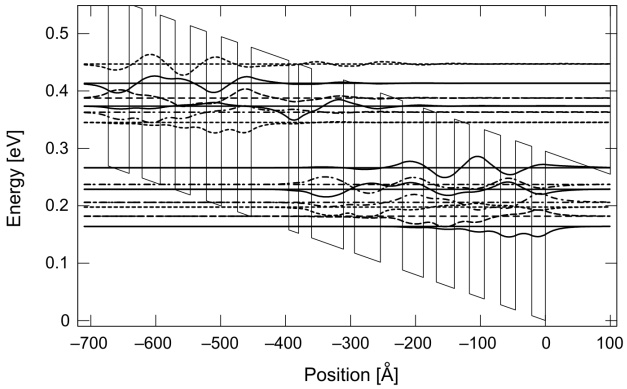

Fig. 3. Energy levels and wavefunctions in structure consisting of an active region and two injectors.

barrier between the segments. The electric field in Figs. 1 and 2 is the same. One can see that such an approximation may give only very simplified information. Both the shape of the wavefunctions and distances between the levels are different from ones calculated before. For example, the distance between the third and the second level in the active region in Fig. 2 is about 109 meV. Their analogs in Fig. 1 are spaced by approximately 140 meV. This is a significant difference, showing that if we want to predict even a basic laser parameter, like the wavelength, we may not use too simplified methods.

Of course, modelling only one injector and active region is not enough. The upper states localized in the active region are modified by the injector, which is on its left side. The lower states depend even stronger on the injector. From Fig. 3, we see that when we add the right injector, the structure gets significantly modified.

4. Conclusions

We have shown that it is possible to effectively calculate electronic structure of large areas of quantum cascade structures. The envelope function approximation can be used without any further simplifications, despite strong electric fields applied to the structure.

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