

Effective-mass approximation for electrons in ultrathin heterolayers

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Abstract. It was shown that the usually employed model of rectangular potentials in the effective-mass equations generally fail for ultrathin layers, of width of the order of the lattice constant. There are additional terms, which play minor role for thick quantum wells and barriers, that may have drastic influence on electron states in semiconductor nanostructures with ultrathin layers. The terms are defined with details of the microscopic structure of heterointerfaces. It was shown that allowance for these terms may turn a barrier layer into an effective quantum well binding electrons, and vice versa.

Presently the progress in crystal growth technology allows to compose high-quality heterostructures containing ultrathin layers, of width of the order of the lattice constant a , and experimentally investigate the electron states in such structures (see e. g. [1]). The effective-mass approximation (EMA) based on the envelope-function method is not applicable for description of electron states in quantum wells (or barriers) of width of the order of a is a commonly held view (see e. g. [2]). On the other hand, it is received that EMA works "surprisingly well" for nanostructures composed of thick layers even with atomically abrupt heterointerfaces (see e. g. [3]). Accepting these standpoints, one still may set at least two questions: "What are the reasons leading to the first statement?" and "What is the accuracy of EMA when it is used to consider electron states in a quantum well of some width L ?" The main goal of the work is to answer these questions and formulate envelope-function equations applicable for ultrathin heterolayers.

In [4] it has been shown that the usually employed model of rectangular potentials (just a set of Heaviside step-functions $\Theta(z - z_i)$) and position-independent effective mass parameters in the effective-mass equations describing electron states in semiconductor nanostructures may be used as a *zero-order* approximation, with the small parameter $a\bar{k}$, where $1/\bar{k}$ is the characteristic size of the envelope function. Thus the only input parameters needed to solve the problem of electron states within the accuracy are the bulk effective masses of one of the constituents and the band offsets. The EMA of such grade of accuracy does not allow to describe some fine effects like 2D Brillouin zone-center mixing of light and heavy holes in (001) A_3B_5 nanostructures, mixing of different valleys induced by broken translation symmetry of the structures, *etc.* But for eigenvalues of the electron states it provides one with an approximately correct solution. This takes place only for heterostructures composed of layers of width $L \gg a$ each.

It is evident that the rectangular profile of the heterostructure potential is an approximation. As the width of the layers decreases, the number of atoms in the layers become comparable with the number of heterointerface atoms, and the simple model will inevitably fail even for the eigenvalues. The detailed microscopic structure of the heterointerface is unknown. So it is desirable to describe it with a set of a few parameters that should be taken from the experiment along with other parameters like effective masses and band offsets. Of course, the parameters will definitely depend on the heterostructure growth process, but

similar situation exists for the band offsets: the heterointerface dipole may affect it considerably. From this point of view the properly constructed EMA that takes into account real heterointerface structure, being still very simple and allowing plain inclusion of external potentials, would have no drawbacks when compared to other empirical instruments like tight-binding or pseudopotential methods [5].

The appropriate solution to the problem may be found if we pay attention to the *first*-order EMA in small parameter $a\bar{k}$ that allows for microscopic structure of heterointerfaces (we considered lattice-matched A_3B_5 materials only). This approximation grade will play a role of the basic EMA for structures with ultrathin layers. The structure of the proper equations is the following. The kinetic energy operator has its usual bulk form, but the effective potential energy consists of the “usual” rectangular term and some Dirac δ -functions at the heterointerfaces. For example, for conduction band Γ -states in a symmetric quantum well (or barrier) of width L it has the following form:

$$U_c(z) = \Delta U_c [\Theta(z) - \Theta(z - L)] + d_1 [\delta(z) + \delta(z - L)]. \quad (1)$$

Here ΔU_c is the band offset, for the barrier $\Delta U_c > 0$ and for the quantum well $\Delta U_c < 0$, and the parameter d_1 is defined with details of the microscopic structure of the heterointerface. This parameter may be roughly estimated as $d_1 \sim a\Delta U_c$. For its experimental evaluation it may be important that d_1 should take different values for different nanostructure growth crystal orientations. To illustrate this, we will consider its microscopic structure. If we put down the potential of the heterostructure with a single heterojunction in the following model form [6]:

$$U(\mathbf{r}) = U_1(\mathbf{r}) + G(z) [U_2(\mathbf{r}) - U_1(\mathbf{r})] \equiv U_1(\mathbf{r}) + G(z)\delta U, \quad (2)$$

where $U_1(\mathbf{r})$ and $U_2(\mathbf{r})$ are the periodic potentials of the semiconductors forming the heterojunction, and $G(z)$ is the form-factor appearing like a smeared step-function (Oz is the growth axis), then

$$d_1 = \Delta U_c \int_{-\infty}^{+\infty} (G(z) - \Theta(z)) dz - \sum_{j=\pm 1, \pm 2, \pm 3 \dots} \frac{\langle c | \delta U \cos(Kjz) | c \rangle}{Kj} \int_{-\infty}^{+\infty} \frac{dG(z)}{dz} \sin(Kjz) dz, \quad (3)$$

where $|c\rangle$ is the periodic part of the band edge Bloch function of one of the materials (from (2) it follows that $\Delta U_c = \langle c | \delta U | c \rangle$), and value of K depends on the heterostructure growth crystal orientation:

$$K = \begin{cases} 4\pi/a, & Oz \parallel [001]; \\ 4\pi\sqrt{2}/a, & Oz \parallel [110]; \\ 2\pi\sqrt{3}/a, & Oz \parallel [111]. \end{cases} \quad (4)$$

The effective potential energy written in the form (1) may be used both for thick and ultrathin layers. In the former case the term proportional to d_1 plays a role of a small correction, but in the latter case this term is important, and as $L\bar{k}_z \ll 1$, the potential energy may be written in the form where only one parameter describes both the usual and interface contributions:

$$U_c(z) = b_1 \delta(z - L/2), \quad (5)$$

where

$$b_1 = 2d_1 + \Delta U_c L. \quad (6)$$

Phenomenologically such form of the potential energy of ultrathin quantum wells has been proposed to use in [7].

The sign of d_1 has nothing in common with the sign of ΔU_c , and, as a consequence, it is possible that while the potential of a thick layer does not produce a bound state (that is $\Delta U_c > 0$), there will be such states in a similar structure with an ultrathin layer (so that $b_1 < 0$).

In conclusion, we have shown that the model of rectangular potentials in the effective-mass equations generally fail for ultrathin layers, of width of the order of the lattice constant. The reason of this lies in its over-simplified treatment of the heterointerfaces. Allowance for additional interface potentials may have drastic influence on eigenvalues of electron states in such nanostructures. These interface potentials are defined with details of the microscopic structure of heterointerfaces as well as the heterostructure growth crystal orientation. The potentials may reveal themselves in the following: it is possible that while the potential of a thick layer does not produce a bound state, there will be such states in a similar structure with an ultrathin layer, and vice versa.

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