# THE WAVEGUIDE BEHAVIOUR OF THE BALLISTIC CARRIERS IN CONFINED QUANTUM STATES

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## **Abstract**

Peculiar waveguide properties of quantum waveguides are revealed using a new transfer matrix based approach in the numerical analysis of the quantum well structures. The approach is built on the solution of the 2D Schrodinger equation for the oblique incidence of an electron at the semiconductor hetero-interfaces. Both the interface parallel and interface perpendicular complex electron wave numbers are formulated in each layer of the structure. They help us to find bound states of the electron in the quantum structure via an analysis of the global transfer matrix coefficients. Successively, the rigorous curves of the real mode diagram of the quantum waveguide can be evaluated. As a particular result of it a new type of the quantum structures acting as a selectively coupled quantum waveguide pair is shown. A new effect, the longitudinal mezoscopic periodical charge distribution occuring along the waveguide structure, has been predicted.

#### Key words:

#### Introduction

Semiconductor layered microstructures have been used extensively to study many new quantum effects based on the quantum and wave-like nature of fermions. In the crystalline semiconductor heterostructures we

can observe the significant differences in the effective mass and even the distinguishable anisotropic particle mobility due to which the effective mass anisotropy is expectable here [1], [2]. The last seems to have particular importance for behaviour of the confined Bloch electrons in semiconductor layered structures. Recently it has been proposed that heterojunction quantum well structures can act as electron waveguides in which ballistic behaviour along the planes of the heterointerfaces has been predicted [4]. This paper presents an extensive theoretical study of the waveguide nature of slab multilayer semiconductor microstructures. The aims of this work were to establish, within a simple kinetic energy based formalism, a predictive model for the electron waveguiding properties of single and coupled quantum well structures.

## Philosophy of the quantum waveguides

Our approach to the quantum well structures is based on an examination of the behaviour of an electron wave incident at any angle on the confining barriers of single and double quantum well structures as the wave propagates along the planes of the hetero-interfaces. As a ground of our derivation we have the double parallel interface of the three mobility anisotropic semiconductor layers,  $\{1\}$ ,  $\{2\}$  and  $\{3\}$ , with the square shaped band edge potential function V(x) forming the quantum well. The Schrodinger equation for an electron propagating in such a media with potential function V(x) = V has the form

$$\frac{\underline{h}^{2}}{2} \sum_{j} \frac{1}{i_{m_{i}^{*}}} \frac{\partial^{2}}{\partial j^{2}} \psi \left( x, y, z \right) + \left[ E - V_{i} \right] \cdot \psi \left( x, y, z \right) = 0$$

$$i = \{1\}, \{2\}, \{3\}; j = x, y, z$$
 (1)

where  $m_{j}^{*}$  are the effective mass tensor elements for j = x, y, z directions in each of the layers  $i = \{1\}, \{2\}$  and  $\{3\}$ .

It is well known that the electrons can be confined in between the interfaces, obeying perpendicular (x) direction cross-resonance. In the case when the electrons have the non-zero component of velocity in interface-parallel (y) or (z) direction, the electrons are guided along the interfaces by total reflections thar occur even when the electron total energy is higher than the potential edges of the well. How it was shown basically in [4], such the structure has the feature of the waveguide.

# Energy based waveguide analysis

Solution of (1) in x-y plane for an electron incidence at the interface reveals a possibility that the total reflection of the electron at the boundary can occur under

certain conditions. Taking into account the possible differences of the effective masses in the x and y directions the critical angle of the total reflection at the heterointerfaces can be expressed as:

$$\Theta_{c,i} = \tan^{-1} \left| \frac{\frac{i_k}{2k_x}}{2k_x} \right| =$$

$$= \tan^{-1} \left\{ \frac{m_y^* \left( E - V_i \right)}{2m_x^* \left[ E - V_2 - \frac{m_y^*}{2m_y^*} \left( E - V_i \right) \right]} \right\}^{\frac{1}{2}} (2)$$

$$i = 1.3$$

provided  $E \ge V_i$ , where  $V_i$  is the height of the confining barriers and  ${}^ik_x$  are the magnitudes of the wave vector and the vector component respectively. A similar formula, equation (1) in [3], has been derived for the simple mobility isotropic case  $m_x^* = m_y^*$ . The totally reflected electron wave, bouncing in x cross-resonance and propagating along y, must comply the general boundary conditions at the interfaces. They express, in fact, that the variation of all participated wave fields (incident wave, reflected wave and penetrating wave) along the boundary have to be identical. It means in our case:

$${}^{1}k_{y} = {}^{2}k_{y} = {}^{3}k_{y} = k_{y} = \pm \frac{\left(-2 \cdot {}^{2}m_{y}^{*} \cdot \Re_{y}\right)^{\frac{1}{2}}}{\underline{h}}$$

$$\left[2 \cdot {}^{i}m_{x}^{*} \left(V_{i} - E - \frac{\underline{h}^{2} \cdot k_{y}^{2}}{2 \cdot {}^{i}m_{y}^{*}}\right)\right]^{\frac{1}{2}}$$

$$i = 1, 2, 3$$

$$0.25$$

$$0.20$$

$$1 \quad 2 \quad 3$$

$$0.10$$

$$2 \quad 3$$

$$0.05$$

Fig. 1

Mode diagram for square-shaped potential well based slab electron waveguide with  $V_1=0.0\,\text{eV};$   $^1\,\text{m}_x=^1\,\text{m}_y=0.2\,\text{m}_e;$   $^2\text{m}_x=^2\text{m}_y=0.1\,\text{m}_e;$   $V_3=0.0\,\text{eV};$   $^3\text{m}_x=^3\text{m}_y=0.2\,\text{m}_e,$   $V_4=0.2\,\text{eV};$   $V_5=0.2\,\text{eV};$   $V_6=0.2\,\text{eV};$   $V_7=0.2\,\text{eV};$   $V_8=0.0\,\text{eV};$ 

E (eV)

0.25

0.15

where symbol  $\Re_y$  refer to the electron kinetis energy of its y-direction motion. Figures (3) can be used for formulating the phase coincidence condition of the electron wave cross-resonance (4).

$$\begin{vmatrix} {}^{2}k_{x} | . d - \tan^{-1} \left[ \frac{|{}^{3}k_{x}| . {}^{2}m_{x}^{*}}{|{}^{2}k_{x}| . {}^{3}m_{x}^{*}} \right] -$$

$$- \tan^{-1} \left[ \frac{|{}^{1}k_{x}| . {}^{2}m_{x}^{*}}{|{}^{2}k_{x}| . {}^{1}m_{x}^{*}} \right] = p . \pi, \ p = 0, 1, 2, ...$$

$$(4)$$

Solution of that complex cross-resonance condition for the integer  $p \ge 0$  gives the allowed longitudinal phase constants  $k_y$  as a function of the total electron energy E. The curves obtained for each p specify the feature of the confined waves in the structure and form an mode diagram of the electron waveguide, see for ex. Fig. 1 and 2. The equation (4) was solved efficiently using a complex transfer matrix method. It was developed from standard transfer matrix approach which is frequently applied to the problems connected with the electron tuneling [5].

#### Results

The mode diagrams  $k_y(E)$  are calculated for the square well shaped potential function V(x) and for two different stepwise effective mass functions  $m^*$  here. The allowed energy sub-bands of our electron waveguide are specified by this way, see figs. 1. and 2. Solid lines show the mode curves while dashed ones depict the margins of the alowed space for the mode propagation constant  $k_y$ . How it is shown, the actual shape of the mode curves weakly approaches parabola and, surpris-

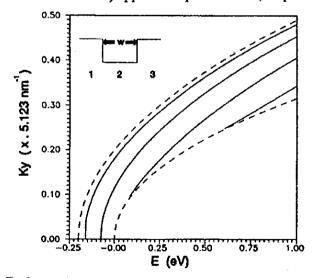


Fig. 2 Mode diagram for square-shaped potential well based slab electron waveguide with  $V_1=0.0$  eV;  $^1m_x=^1m_y=0.1$  m<sub>e</sub>;  $V_2=-0.2$  eV;  $^2m_x=^2m_y=0.2$  m<sub>e</sub>;  $V_3=0.0$  eV;  $^3m_x=^3m_y=0.1$  m<sub>e</sub>, w = 7.0 nm.

ingly, it strongly depends on both the effective mass  $im_{\nu}^*$  differences and the lower cutoff energy level which

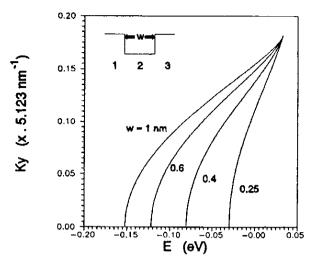


Fig. 3 Mode curve of single subband slab electron waveguide as a function of the potential well width w;  $V_1 = 0.0 \text{ eV}$ ;  $^1\text{m}_x = ^1\text{m}_y = 1.0 \text{ m}_e$ ;  $V_2 = -0.3 \text{ eV}$ ;  $^2\text{m}_x = ^2\text{m}_y = 0.1 \text{ m}_e$ ;  $V_3 = 0.0 \text{ eV}$ ;  $^3\text{m}_x = ^3\text{m}_y = 1.0 \text{ m}_e$ ; w varies from 0.25 to 1.0 nm.

is determined by the pure transversal resonance in the well. To be rigorous, there are cases when the shape of the mode curves fairly differ from the parabolic one, see fig. 3., which have substantial influence to the collective electron behaviour here, namely to the energy density of the electron states in such the electron waveguide. As follows from (3) and (4), there are two basic conditions for allowed  $k_y$  here. They limit the allowed area in the mode curve diagram, see the dash lines in the figs. 1. and 2. If the effective mass component into the well comply with the condition  ${}^2m_v^* < \max({}^1m_v^*, {}^3m_v^*)$  the allowed

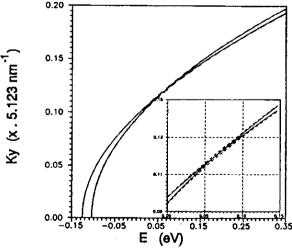


Fig. 4 Intersection of the mode curves for the two electron waveguide to be coupled, dash curves describe the situation under the coupling distance d = 6.0 nm; waveguide  $^{1}$  m<sub>y</sub> =  $^{1}$  m<sub>y</sub> = 0.1002 m<sub>e</sub>, (Al<sub>0.4</sub>Ga<sub>0.6</sub>As); V<sub>2</sub> = -0.149 eV;  $^{2}m_{x} = ^{2}m_{y} = 0.0836 m_{e}; \quad w_{a} = 6 nm,$ (Al<sub>0,2</sub>Ga<sub>0,8</sub>As);  $V_3 = 0.0 \text{ eV}$ ;  ${}^3m_x = {}^3m_y = 0.1002 \text{ m}_e$ ;  $V_1 = 0.0 \text{ eV};$ electron waveguide  $^{1}m_{x} = ^{1}m_{y} = 0.1002 m_{e};$  $V_2 = -0.52 \text{ eV};$  $^{2}m_{x} = ^{2}m_{y} = 0.0541 m_{e}, w_{b} = 1.05 nm, (ln<sub>0.3</sub>Ga<sub>0.7</sub>As);$  $V_3 = 0.0 \text{ eV}$ ;  ${}^3m_x = {}^3m_y = 0.1002 \text{ m}_e$ .

area for the  $k_y(E)$  curves is closed and each mode has its upper cutoff. All mode curves now begin in their lower cutoffs at  $k_y = 0$  with energies  $E < \min(V_1, V_3)$  related to the pure transversal electron resonance like it is shown in fig. 1. In case of  ${}^2m_y^* \ge \max({}^1m_y^*, {}^3m_y^*)$  the upper cutoff does not exist at all and, moreover, there are modes which begin at the energies  $E > \min(V_1, V_3)$  above the edges of the well and which have no origin in pure transversal cross-resonance, see fig 2. Knowledge on the potential and mass relations to the mode curve shape allows us to design the complex electron waveguide structure with predictable performance. Using it, we can design the electron waveguides with different mode curve position and steepness.

As a particular result we report here the possibility of creating an electron waveguide structure with a periodic corrugation in the longitudinal charge distribution. The periodic distribution is attainable even when the broad energy spectrum feeding of the electron waveguide is applied. This effect is produced by the selectively coupled pair of asymmetric electron waveguides (inset of fig. 5) which offer a sharp mutual crossing of their original mode curves. Energy coupling evoked by placing one electron waveguide close to the other causes the coupled mode curves to deviate from the original shape but only closely around the point where the imperturbed mode curve intersects, see fig. 4. This feature brings about the energy selective mode coupling.

#### Conclusion

The charge distribution in the coupled waveguides is shown in fig. 5 for the case of only one electron waveguide (a) is fed with the broadband electron energy spectrum  $E \in (0.02, 0.12)$  eV with constant spectral

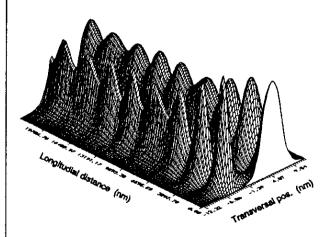


Fig. 5

Charge distribution in coupled electron waveguides, for configuration see fig. 4., electron waveguide a) is fed by the electrons with constant spectral density in range 0.02 to 0.10 eV above the potencial edge of the wells.

distribution. Fig.6. shows the actual shape of selective coupling coefficient. The eventual presence of any elastic scattering mechanisms was neglected there. Discussion of that shows that an additive confinement of the moving electrons in (z) direction can help to solve this problem substantially. Destructive influence of the nonelastic scattering processes can be limited by the

setting the original mode cross-point to the low energy range comparable to the longitudinal phonon energies. The longitudinal periodicity of the charge variation can

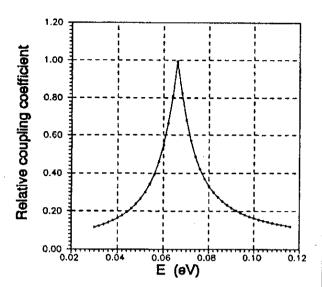


Fig. 6 Plot of the relative coupling coefficient on the energy of the electron wave for the identical case with that in figs. 4. and 5.

be adjusted by the variation of the mutual electron waveguide distance. Coincidence of the periodic charge distribution with an optical wave can be easily arranged and consequently new opto-electronics and electronic devices can be envisaged.

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