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**Abdusalom Umarov**  
 Doctor of Technical Sciences,  
 Professor, Tashkent Institute  
 of Railway Transport  
 Engineers, Uzbekistan

**Mukaddas Ergasheva**  
 Docent, Department of  
 Physics, Namangan State  
 University, Namangan,  
 Uzbekistan

**Anvarjon Soliev**  
 The teacher of Department of  
 Physics, Namangan State  
 University, Namangan,  
 Uzbekistan

## On the dispersion of two dimensional electrons in the heterostructures with a Kane Nonparabolicity

Abdusalom Umarov, Mukaddas Ergasheva and Anvarjon Soliev

### Abstract

In the model of the quantum well of infinite depth a two dimensional electron dispersion is investigated. A bulk semiconductor conduction band describes by simplified Kane model. The simplified approximation of electron spectrum is found. This approximation allows to investigate a number of physical properties of the two dimensional electron gas.

**Keywords:** Heterostructures, quantum well, Kane model, band Nonparabolicity, dispersion curve's of sub bands, two dimensional electron gas

### 1. Introduction

The importance of the study of the properties of two-dimensional electron gas (TDEG) has been known for a long time [1]. The study of nature of TDEG and is currently is actual [2-4]. A large number of studies dedicated to the study of TDEG in the presence of a magnetic field [3-5]. Particularly interesting is also the study of the influence of other factors such as periodic potentials [6], the anisotropy of the spectrum [7], nonparabolicity area [8, 9]. The results of such studies play an important role in understanding the nature of TDEG: subzone structure, electron statistics of subzones etc.

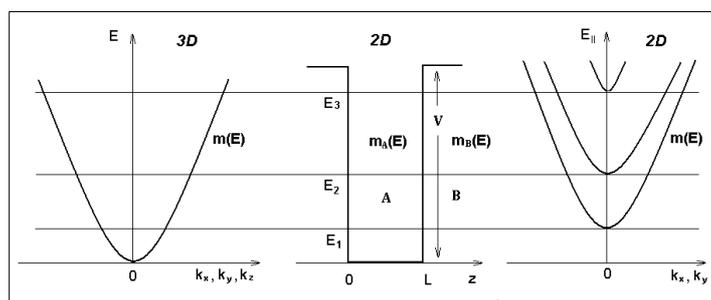
Furthermore, such studies are more relevant in relation with the growing demands for the creation of nanocomposite materials with predetermined properties as nanocomposites consisting of nanoparticles, embedded in a matrix or a heterostructure with nanoparticles of different materials in contact with each other, may form a super lattice quantum well.

The purpose of this work - the calculation of dispersion curves of two-dimensional electrons in the subarea of dimensional quantization. A simplified mathematical model would be created which allows calculating the statistics of TDEG. The presence of such a device allows the theoretical study of a number of physical properties (electrical, magnetic, kinetic, Optical) of quasi-two-dimensional heterostructures.

The calculations will be performed in a single quantum well (QW) of final depth, for example heterostructures In As / AlSb.

### 2. Basic equations

Consider a single quantum well of width  $L$  (region A), lying between the potential barrier height  $V$  (area B). To present the figure shows the potential profile and approximate dispersion curves of an electron in a volume (3D) and two-dimensional (2D) case. The energy is measured from the bottom of the bulk InAs zone.



**Correspondence Author:**  
**Abdusalom Umarov**  
 Docent, Department of  
 Physics, Namangan State  
 University, Namangan City,  
 Uzbekistan

In the effective mass approximation, the three-dimensional Schrödinger equation solution can be represented as  $\psi = e^{i(k_x x + k_y y)} \phi(z)$ . Then, for the area A and B can write the following dimensional equation

$$\frac{\partial^2 \phi_A(z)}{\partial z^2} + q^2 \phi_A(z) = 0, \quad q = \sqrt{\frac{2m_A}{\hbar^2} E - k^2} \quad (1)$$

$$\frac{\partial^2 \phi_B(z)}{\partial z^2} - \chi^2 \phi_B(z) = 0, \quad \chi = \sqrt{\frac{2m_B}{\hbar^2} (V - E) + k^2} \quad (2)$$

Here  $k^2 = k_x^2 + k_y^2$  and  $m_{A,B}$  - are depends on the energies of the effective masses of electrons in the material A or B. Solving the equations (1) and (2) and using the boundary conditions

$$\phi_A(0) = \phi_B(0), \quad \left. \frac{1}{m_A} \frac{d\phi_A(z)}{dz} \right|_{z=0} = \left. \frac{1}{m_B} \frac{d\phi_B(z)}{dz} \right|_{z=0} \quad (3)$$

$$\phi_A(L) = \phi_B(L), \quad \left. \frac{1}{m_A} \frac{d\phi_A(z)}{dz} \right|_{z=L} = \left. \frac{1}{m_B} \frac{d\phi_B(z)}{dz} \right|_{z=L} \quad (4)$$

Can to find the dispersion equation  $E(n, k)$

$$E = E_{||} + E_0 \left[ \pi \cdot n - 2 \operatorname{Arcsin} \left( \sqrt{\frac{\gamma^2 (E - E_{||})}{\gamma(\gamma - 1)E + \gamma V + (1 - \gamma^2)E_{||}}} \right) \right]^2 \quad (5)$$

Where

$$\gamma = m_B/m_A, \quad E_0 = \frac{\hbar^2}{2m_A L^2} = \frac{3,81\text{э}}{m_A (L/\text{А})^2}, \quad E_{||} = \frac{\hbar^2 k^2}{2m_A} = \frac{3,81\text{э}}{m_A} \cdot (k^2 \text{А})^2$$

The nonparabolicity of conductivity band of material In As and AlSb taken into account under the simplified formula

$$m_A = m_A(0)(1 + \alpha_A E), \quad (6)$$

$$m_B = m_B(0)(1 + \alpha_B (E - V)), \quad (7)$$

Where  $m_{A,B}(0)$  и  $\alpha_{A,B}$  - effective masses of the electrons at the bottom of the conduction band (in a unit mass of a free electron) and parameters Nonparabolicity zone in area A and B, respectively.

## 2. Dispersion of minibands and its approximation

To describe the electron statistics the equation (5) is inconvenient, since it is insoluble is relatively  $E$  or  $k$ . The approach of an infinite wall  $V \rightarrow \infty$  this equation takes the simple form

$$E = E_{||} + E_0 \pi^2 n^2$$

This approximation, however, gives higher ratings of energy compared with the equation (5). Suppose that  $k = 0$  and at a given  $n$  numerical solution (5) is equal  $E_n$ . Then, the value of the right side (5) is conveniently represented as a  $E_n(1 + \alpha_A E_n)$ . Leaving this value is constant (not depending on  $k$ ), from (5) we obtain the following approximation

$$E(1 + \alpha_A E) \approx \frac{\hbar^2 k^2}{2m_A(0)} + E_n(1 + \alpha_A E_n) \tag{8}$$

where,  $E_n$  - the bottom of the n-th miniband. Its value can be found from (5) numerically for  $k = 0$  for each  $n = 1, 2, 3, \dots$ , and then we substitute in (8) for further use. Then, the bottom of the miniband each obtained from Equation (5) and approximation of (8) coincide.

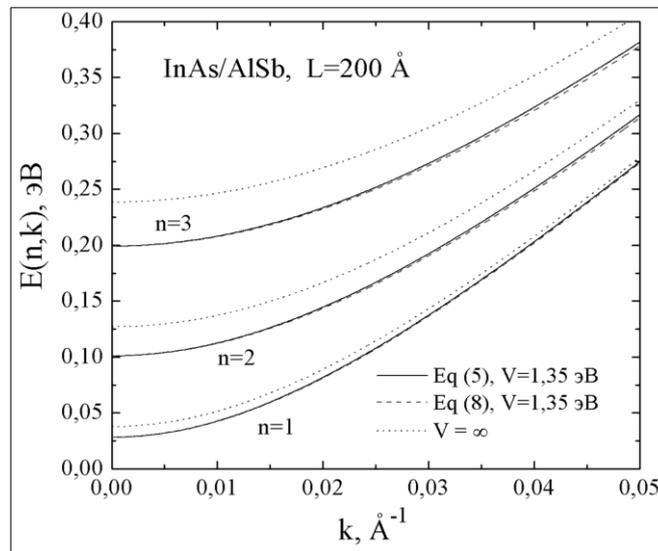
Used in the calculation of the values of the band parameters of In As and AlSb - bandgap  $E_g$ , the effective mass  $m(0)$ , nonparabolicity setting  $\alpha$  and jump conduction band  $V$  are shown in the table.

Zone parameters In As and In Sb at 4.2K

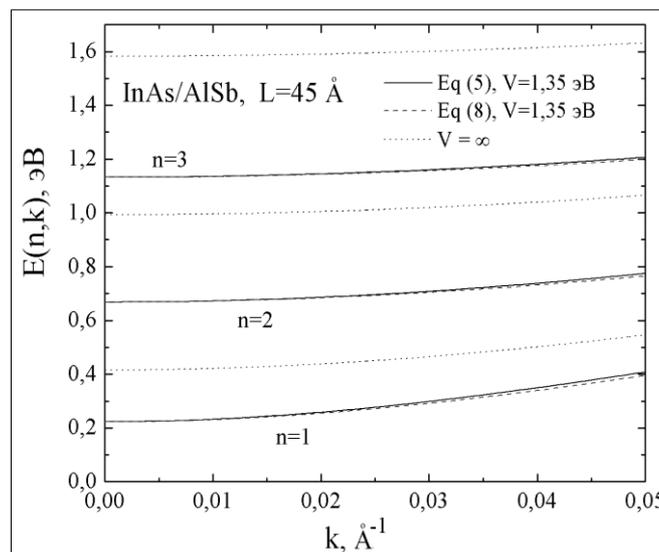
	In As (A)	AlSb (B)
$E_g, \text{eV}$	0,42	2,37
$m(0)$	0,023	0,11
$\alpha, \text{eV}^{-1}$	2,27	0,334
$V(z), \text{eV}$	0	1,35

For structures In As/AlSb a quantum well with a width  $L = 200 \text{ \AA}$ , from (5) we have:  $E_1 = 0,028 \text{ eV}$ ,  $E_2 = 0,1 \text{ eV}$ ,  $E_3 = 0,2 \text{ eV}$  and the width of the quantum well at  $L = 45 \text{ \AA}$  have:  $E_1 = 0,223 \text{ eV}$ ,  $E_2 = 0,668 \text{ eV}$ ,  $E_3 = 1,133 \text{ eV}$ .

Calculated dispersion curves  $E(n, k)$  obtained from equations (5) and approximations (8) are compared in Figures 1 and 2.



**Fig 1:** Dispersion curves  $E(n, k)$  of the first three miniband ( $n = 1, 2, 3$ ) in the QW In As/AlSb with  $L = 200 \text{ \AA}$ : solid line - according to the equation (5), the dashed - by approximation (8) and the point - if  $V = \infty$



**Fig 2:** Dispersion curves  $E(n, k)$  of the first three minibands ( $n = 1, 2, 3$ ) in the QW In As/AlSb with  $L = 45 \text{ \AA}$ : solid line - according to the equation (5), the dashed - by approximation (8) and the point - if  $V = \infty$

From figures 1 and 2 shows that the approximation (8) is sufficiently accurate. Its disadvantage that  $E_n$  to depend on the parameters of the structure  $L, V, m_{A,B}(0), \alpha_{A,B}$ , and therefore every time when changing the value  $n=1,2,3\dots$  of these parameters again recalculated numerically from equation (5) for  $k=0$ .

### 3. Conclusion

In this paper we obtain a useful approximation for miniband dispersion (8). It can be used to calculate the kinetic, magnetic and optical properties DEG. The above mathematical model of the electron dispersion can be applied to other heterostructures with quantum well based on semiconductor group  $A_3B_5$ .

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