K.P APPROXIMATION USING 4×4 LUTTINGER KOHN HAMILTONIAN FOR HETERO-STRUCTURE BAND CALCULATIONS

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Master's Thesis

Department of Physics

Programme in Solid State Physics

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Eskişehir

Eskişehir Technical University

Institute of Graduate Programs

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.

ABSTRACT

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(Co-Supervisor:)

Evaluating the band structure of semiconductors is one of the most important for building quantum lasers, MOS-FETs, bipolar transistors, diodes, semiconductor sensors. This thesis studies generalize k.p method to Compute the band structure of some materials such as zincblende. We calculated the band structure of AlGaAs and GaAs compounds, using both 4×4 Kane's model and Luttinger-Kohn's model approximations. The Kane's model provides incorrect effective mass for heavy hole band, neglected distance between bands and it considered only four bands. However, this model developed basis functions which are useful for Luttinger Kohn model.

Luttinger Kohn model correct all Kane's model errors and classified bands as main interest bands named class A and some other bands called class B which influence the main interest bands (class A). In this master thesis the multi-band effective-mass theory also is used. This approximation is helpful for wide-band-gap semiconductors such has GaAs. This wide energy band gap, isotropic simple parabolic is used for conduction band while 4× 4 Luttinger-Kohn Hamiltonian is used for valence band. Finally, finite-difference method is used to solve numerically results.

Keywords: k.p method, Kane's Model, Luttinger-Kohn Model,

ÖZET

4X4 K.P YÖNTEMİYLE SÜPERÖRGÜ SİSTEMLERİNİN VALANS BAND HESAPLAMALARI

Mustafe Mohamoud BARKAD

Fizik Anabilim Dalı

Katıhal fiziği Bilim Dalı

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Yarı iletkenlerin bant yapısını değerlendirmek, kuantum lazerler, MOS-FET'ler (Metal oksit yarı iletken alan etkili transistörler), bipolar transistörler, diyotlar, yarı iletken sensörler oluşturmak için en önemli faktörlerden biridir. Bu tez çalışmasında, çinkoblend gibi bazı malzemelerin bant yapısını hesaplamak için k.p. (Kadomtsev-Petviashvili Denklemi) yöntemini genelleştirdik. Hem 4×4 Kane modeli hem de Luttinger-Kohn modeli yaklaşımlarını kullanarak GaAsAl ve GaAs bileşiklerinin bant yapısını hesapladık. Kane modeli, ağır delik bandı için yanlış etkin kütle sağlar, bantlar arasındaki mesafeyi dikkate almaz ve sadece dört bandı dikkate alır. Ancak bu model, Luttinger Kohn modeli için faydalı olan temel fonksiyonları geliştirmiştir.

Luttinger Kohn modeli, Kane modelinin tüm hatalarını düzeltir ve bantları, A sınıfı olarak adlandırılan ana ilgi bantları ve A sınıfının ana ilgisini etkileyen B sınıfı olarak adlandırılan başka bir bant olarak sınıflandırır. Bu yüksek lisans tezinde çok bantlı etkin kütle teorisi de kullanılmıştır. Bu yaklaşım,AlGaAs ve GaAs'lara sahip geniş bant aralıklı yarı iletkenler için yararlıdır. Bu geniş enerji bandı aralığı izotropik basit parabolik iletim bandı için kullanılırken, değerlik bandı için 4×4 Luttinger-Kohn Hamiltonian kullanılmıştır. Son olarak, sonuçları sayısal olarak çözmek için sonlu farklar yöntemi kullanılmıştır. r

Anahtar Sözcükler: k.p. Kadomtsev-Petviashvili Denklemi Kane modeli, Luttinger Kohn modeli,..

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Mustafe Mohamoud BARKAD

16/08/2021

STATEMENT OF COMPLIANCE WITH ETHICAL PRINCIPLES AND RULES

I hereby truthfully declare that this thesis is an original work prepared by me; that I have behaved in accordance with the scientific ethical principles and rules throughout the stages of preparation, data collection, analysis and presentation of my work; that I have cited the sources of all the data and information that could be obtained within the scope of this study, and included these sources in the references section; and that this study has been scanned for plagiarism with “scientific plagiarism detection program” used by Eskişehir Technical University, and that “it does not have any plagiarism” whatsoever. I also declare that, if a case contrary to my declaration is detected in my work at any time, I hereby express my consent to all the ethical and legal consequences that are involved.

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GLOSSARY OF SYMBOLS AND ABBREVIATIONS

LKM	:	Luttınger Kohn Model
QW	:	Quantum Well
P	:	Kane's Parameter
γ	:	Kohn Parameter
MOS-FETs	:	Metal Oxide Semiconductor Flied Effective Transistors
GaAS	:	Galium Arsinide

1. INTRODUCTION

Currently lasers[1], MOS-FETs, bipolar transistors, diodes, semiconductor sensors of various types and other low power semiconductor devices of which the important parameters are: size, shock resistance, reliability etc. play very important role in, medicine, entertainment and industrial technology. Lasers can be construct various ways but the most commonly used are made up of solid-state semiconductors. In this study our focus is quantum wells (QWs).

In semiconductors there are two types of diodes, the laser diode and rectifier diodes. The two diodes are similar but the important difference is rectifier diodes have two regions N-type and P-types on each side of the device while the laser diode has third region on middle of the two other terminals. The middle region of laser diode is made up of different material: p-type doped, un-doped intrinsic and N-type doped semiconductors. The middle region of the laser diode carriers is pumped, if electric current is applied, there are two types of carriers: electrons from N-types region and hole from P-type region. The aim of pumping is to recombine[2] electrons and holes this recombination produce photons. To recombine all electrons and hole which implies converting all energy into radiation, the direct band gap semiconductors are used.

There are two types of photon generation: spontaneous and stimulated are quite different. Spontaneous emission take place randomly (without interaction with other photon) while stimulated emission is driven when excited electron interact with another photon. Stimulated emission is used for lasers whereas spontaneous emission is applied in light emitted diodes (LEDS). The stimulated emission produce pack of photons with same characteristic (frequency, phase and polarization). To generate a laser beam with this pack of photons should amplify its size and produce optical gain. For the Fabry-Perot resonator structure[3] the Gain in laser crystal may be achieved by polishing it on two sides to form mirrors. The two mirrors, one fully is reflective and the other is partial reflective. The output beams of laser propagate through the semi-reflective mirror. The size of cavity region is $20 - 100\mathring{A} = 2 - 10nm$ whereas the wavelength light varies

[1] Laser - acronym for "light amplification by stimulated emission of radiation".

[2] Recombination means disappearance of one pair of carriers in semiconductor with the energy output.

[3] This structure consists of two opposite flat reflecting mirrors

from $\sim 400nm - 3000nm$ therefore the size of cavity is very small compare to the wavelength of light. The semiconductor laser usually requires the optical system at the output, focused on a particular point.

Semiconductor laser is most popular laser it has many advantages including size, efficiency of consuming electricity. In different application required different wavelength so variety of semiconductor material allow to manufacture laser with many different wavelengths. The semiconductor lasers are better than the common gas lasers include helium neon because they are costly change its operational wavelength. Helium neon emitter 633 nm of wavelength but semiconductor laser emitted variety wavelengths.

Quantum well (QW) contains at least two materials with different band gap energies to make a potential barrier. The operational wavelength influenced on the value of band gap energy. The laser output is affected the probability of energy bands which is depend on band structure. Barrier's width, material compositions, and strain and crystal orientation these external factors effect influence on the band structure: well width.

The description of band structure around the extremum Γ point can be used the effective mass or k.p methods. For GaAs/$AL_xGa_{x-1}AS$ band structure of QWs for cubic zinc-blende crystal, which was obtained for (11N) orientation by Xia [1] for hole sub-band structure (4×4 Hamiltonian) and with spin-orbit split-off influence by Seo and Donegan [2] (6×6 Hamiltonian) for $In_xGa_{1-x}As$/InP QWs are described by the effective mass theory. K.p model which Fan [3] obtained for (11N) oriented substrates describe dilute nitride semiconductors, InGaAsN, and the influence of nitrogen concentration on band structures is not negligible. Tight binding analysis of band anti-crossing in GaBiNAS, 12-ban k.p model for dilute bismide alloys and 14-band k.p Hamiltonian for GaBiNAS compound grown on (001) oriented substrates introduced by Brderick et al [4]. 8-and 14-band k.p models from GaInAsBi of QWs which grown on (001) oriented GaAs and InP substrates drived by Gladysiewicz et al [5]. For the band structure of Bi containing semiconductors grown on none (001) oriented substrate is not include these reports in literature.

Understanding the electronic band structure such as energy bands and corresponding wave function simplify, we have to understand optical properties. Semiconductors with direct band gaps are required for application in optical devices and main transition take place around the band edges. The following methods are used to calculate band structure of semiconductors:

1. Free electron approximation
2. Pseudo potential method
3. Green function model (Korringa, Kohn and Rostrocker model)
4. Density-functional theory
5. Tight binding model
6. Kronign-peney model
7. K.p perturbation theory

But our main target is near the band edges such as conduction band and valence band structures. To reach our target we use Kane's model (after Evan O. Kane) and the Luttinger-Kohn model (LKM) (after Joaquin Mazdak Luttinger and Wlter Kohn). Our interest is where $k_0 = 0$ which located extremum point of band structure at the zone center, which is very important for III-V direct band semiconductors. Here k_0 is specific point in k space. [4]Kane model is very useful for finding basic function but it nonrealistic because it gives in correct energy for heavy holes band. To get a correct energy for heavy holes band, Luttinger-Kohn model is used. Using this model proves realistic result for Kane model.

1.1 **Hamiltonian For Schrödinger Equation and Basis Function**

In Kane's model [6], conduction, heavy-hole, light-hole and spin orbit split-off bands are counted to four bands (Fig.1.1). Every band is double degenerate with own spin counterparts. At K=0 the Hamiltonian is written as a following:

[4] K is wave vector

$$H = H_0 + \frac{\hbar}{4m_0^2c^2}(\vec{\nabla}V \times \vec{p}).\vec{\sigma} \tag{1.1}$$

$$H_0 = \frac{p^2}{2m_0} + V(r) \tag{1.2}$$

H_0 is total energy of the system contain both kinetic energy and potential energy, the second term in (1.1) is spin orbit interaction, and the $\vec{\boldsymbol{\sigma}}$ is a vector of Pauli spin matrices with the components below:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.3}$$

Applications for Pauli matrices in (1.3) on the spin operations are:

$\boldsymbol{\sigma_x} \uparrow = \downarrow$, $\boldsymbol{\sigma_y} \uparrow = \boldsymbol{i} \downarrow$, $\boldsymbol{\sigma_z} \uparrow = \uparrow$, $\boldsymbol{\sigma_x} \downarrow = \uparrow$, $\boldsymbol{\sigma_y} \uparrow = \boldsymbol{i} \uparrow$, $\boldsymbol{\sigma_z} \uparrow = \downarrow$ (1.

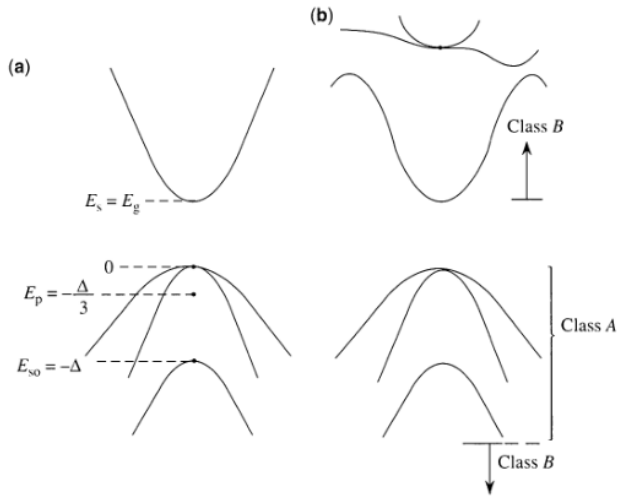


Figure 1.1(a) Kane model with k.p method a conduction, a heavy hole, a light hole and a spin-orbit split-off bands and each band has double degeneracy are only considered: (b) LKM: which interest the heavy hole, light hole, spin-orbit split-off bands with double degeneracy and named class A. all other bands are called class B. this model also consider the effect of class B on class A.

The orthonormality relation of spins are

$$\langle\uparrow|\uparrow\rangle = \langle\downarrow|\downarrow\rangle = \mathbf{1}, \qquad \langle\uparrow|\downarrow\rangle = \langle\downarrow|\uparrow\rangle = \mathbf{0} \tag{1.5}$$

Now let us use the original equation for block functionψ_{nk}:

$$\left(H_0 + \frac{\hbar}{4m_0^2c^2}\left[\vec{\nabla}V \times \vec{p}\right].\vec{\sigma}\right)\psi_{n\vec{k}}(\vec{r}) = E(\vec{k})\psi_{nk}(\vec{r}) \tag{1.6}$$

When written in term $\boldsymbol{u_{nk}(\vec{r})}$ known as Block periodic amplitude, it comes

$$\left\{H_0 + \frac{\hbar}{m_0}\vec{k}\vec{p} + \frac{\hbar}{4m_0^2c^2}\left[\vec{\nabla}V \times \vec{p}\right].\vec{\sigma} + \frac{\hbar}{4m_0^2c^2}\left[\vec{\nabla}V \times \vec{k}\right].\vec{\sigma}\right\}\boldsymbol{u_{nk}(\vec{r})} = E'\boldsymbol{u_{nk}(\vec{r})} \tag{1}$$

Where

$$E' = E_n(\vec{k}) - \frac{\hbar^2k^2}{2m_0} \tag{1.8}$$

The relation between Block function and periodic function is $\psi_{n\vec{k}}(\vec{r}) = e^{ik.r}\mathrm{u}_{n\vec{k}}(\vec{r})$ and the last term in (1.7) is the crystal momentum which is depend on k. this term very small comparing to the atomic momentum p where the most atomic spin-orbit interaction take place. Thus, only other four terms are considered and k dependent spin-orbit interaction term is neglected.

$$H = H_0 + H_1 + H_2 = H_0 + \frac{\hbar}{m_0}\vec{k}.\vec{p} + \frac{\hbar}{4m_0^2c^2}\left[\vec{\nabla}\mathrm{V} \times \vec{p}\right].\vec{\sigma} \tag{1.9}$$

H_1 is the transition from Block function to crystal cell periodic function and H_2 is atomic momentum spin-orbit interaction. At k=0 which correspond the edge of band function of $\mathrm{u}_{n\vec{0}}(\vec{r})$ are: For conduction $|iS\uparrow\rangle$, $|iS\downarrow\rangle$ with Eigen energy E_S and for valance band$|X\uparrow\rangle$, $|X\downarrow\rangle$, $|Y\uparrow\rangle$, $|Y\downarrow\rangle$, $Z\uparrow\rangle$, $|Z\downarrow\rangle$ with Eigen energy E_P. Here the wave function of the bands are degenerate with respect H_0. $H_0|S\uparrow\rangle = E_C|S\uparrow\rangle$, $H_0|S\downarrow\rangle = E_C|S\downarrow\rangle$, $H_0|X\uparrow\rangle = E_P|X\uparrow\rangle, H_0|X\downarrow\rangle = E_P|X\downarrow\rangle$, $H_0|Y\uparrow\rangle = E_P|Y\uparrow\rangle$, $H_0|Y\downarrow\rangle = E_P|Y\downarrow\rangle$ $H_0|Z\uparrow\rangle = E_P|Z\uparrow\rangle$ $H_0|Z\downarrow\rangle = E_P|Z\downarrow\rangle$. Its for simplicity to select the base functions of:

$$|1\rangle = |iS\downarrow\rangle, \qquad |2\rangle = |\frac{X-iY}{\sqrt{2}}\uparrow\rangle, \qquad |3\rangle = |Z\downarrow\rangle, \qquad |4\rangle = |\frac{-X+iY}{\sqrt{2}}\rangle \tag{1.10}$$

$$|\overline{1}\rangle = |iS\uparrow\rangle, \qquad |\overline{2}\rangle = |-\frac{X+iY}{\sqrt{2}}\downarrow\rangle, \qquad |\overline{3}\rangle = |Z\uparrow\rangle, \qquad |\overline{4}\rangle = |\frac{X-iY}{\sqrt{2}}\downarrow\rangle \tag{1.11}$$

Where the basis wave function of conduction band is s-state wave function and valence band basis wave function are taken from the p-state wave function of hydrogen atom model. These basis function relate spherical harmonics as.

$$Y_{00} = \frac{1}{\sqrt{4\pi}} = |S\rangle \tag{1.12}$$

$$Y_{10}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r} = |Z\rangle$$

$$Y_{1\pm0}(\theta,\varphi) = \pm\sqrt{\frac{3}{4\pi}}sin\theta e^{\pm i\varphi} = \sqrt{\frac{3}{4\pi}}\frac{z}{r} = \frac{1}{\sqrt{2}}|X \pm iY\rangle$$

The expressions of spherical harmonic are given by

$$Y_{lm}(\theta,\varphi) = (-1)^{\frac{m+|m|}{2}}\sqrt{2l+1\left(\frac{l-|m|!}{l+|m|!}\right)}P_m^l(cos\theta)e^{i\varphi} \tag{1.13}$$

Where $P_m^l(cos\theta)$ are Legendre polynomials. The Legendre polynomials in explicit form are

$$P_m^l(cos\theta) = \sin^{\mathrm{m}}\theta\frac{d^m}{d(cos\theta)^m}P_l cos\theta \tag{1.14}$$

Where P_l for $l = 1$

$$P_l = cos\theta \tag{1.15}$$

The spin is not including this spherical harmonic the basis functions with spin are discussed in chapter 2. The reason that we choose the spherical harmonic [7] is that in crystal potential of the atom states are overlap with each and forming bands, as shown on fig 1.2. Since our main interest is around the band gap, we should use the lowest conduction band and highest valance band. As it seen the wave function near the top of

valance band is p-like state and near the bottom of the conduction band is s-like state which fine structure of the of the energy levels in atomic physics is originated.

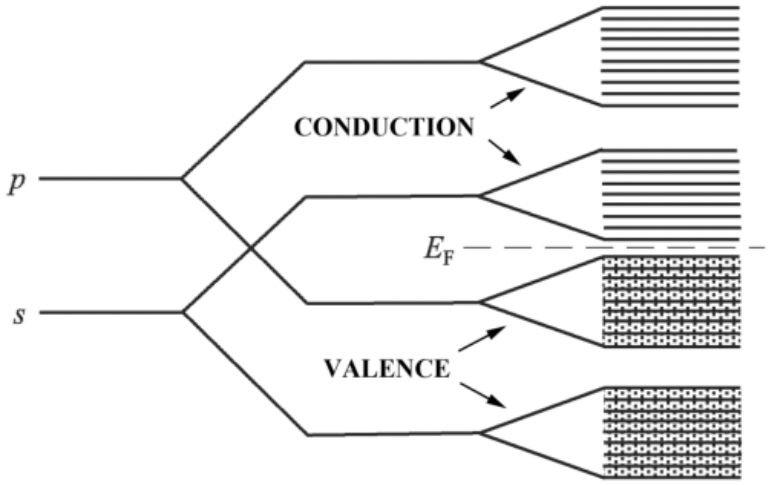


Figure.1. 2 valence and conduction band

Figure1.2 to form valence and conduction zone there is evolution s-and p-state of the In semiconductors; E_f −fermi level which lies at the middle , valence band is below the Fermi level which is bonding p- and s-state and above the Fermi level there conduction band which formed by bonding p- and s-state

Let us assume $\vec{k} = k\hat{z}$, the Kane's parameter P and spin-orbit split off energy ∇ are defined as:

$$P = i\frac{\hbar}{m_o}\langle S|p_z|Z\rangle \tag{1.16}$$

$$\nabla = i\frac{3\hbar}{4m_0^2c^2}\left\langle X\left|\frac{\partial V}{\partial x}p_y - \frac{\partial V}{\partial y}p_x\right|Y\right\rangle$$

CHAPTER TWO: CONSTRUCTION OF KANE'S MODEL HAMILTONIAN

In this chapter we will discuss matrix element of the Hamiltonian H as a given (1.9), using the base functions of (1.10) and (1.11). Since matrix is symmetric, we will evaluate only upper block half of the matrix element in (1.10)[5]. The result of Hamiltonian matrix has the following structure:

$$H = \begin{matrix} \widehat{H} & 0 \\ O & \widehat{H} \end{matrix} \tag{2.1}$$

2.1 Explicit Calculations Of Matrix Elements Of H

With the lower and upper block, the form

$$\mathrm{H} = \begin{bmatrix} \mathrm{H}_{11} & \mathrm{H}_{12} & \mathrm{H}_{13} & \mathrm{H}_{14} \\ \mathrm{H}_{21} & \mathrm{H}_{22} & \mathrm{H}_{23} & \mathrm{H}_{24} \\ \mathrm{H}_{31} & \mathrm{H}_{32} & \mathrm{H}_{33} & \mathrm{H}_{34} \\ \mathrm{H}_{41} & \mathrm{H}_{42} & \mathrm{H}_{43} & \mathrm{H}_{44} \end{bmatrix} \tag{2.2}$$

The matrix element which relevant the above Hamiltonian will be evaluated below.

2.1.1 Matrix element $\mathbf{H_{11}}$

The value of matrix element relevant of $\mathbf{H_{11}}$ is defined below

$$\langle 1|H|1\rangle = \langle -iS\downarrow|H|iS\downarrow\rangle = E_s \tag{2.3}$$

Since H in (1.19) consist three parts, separate evaluation of each term of Hamiltonian is required

$$\langle -iS\downarrow|H_0|iS\downarrow\rangle = \langle S|E_S|S\rangle = E_s \tag{2.4}$$

[5] For lower block, the matrix elements should be evaluated between states (2.11), but it will give same results

$$\langle -iS\downarrow|H_1|iS\downarrow\rangle = \left\langle S\left|\frac{\hbar k}{m_0}p_z\right|S\right\rangle = 0 \tag{2.5}$$

Where p_z is angular momentum z direction $p_z = -i\hbar\frac{\partial}{\partial z}$

$$-\langle S|H_2|S\rangle_z = \left\langle S\left|\frac{\hbar}{4m_0^2c^2}\left(\frac{\partial V}{\partial x}p_y - \frac{\partial V}{\partial y}p_x\right)\right|S\right\rangle = 0 \tag{2.6}$$

The reason that matrix element in (2.5) and (2.6) are zero due to the fact that derivative of a constant number is zero.

2.1.2 Matrix element H_{12}

As same as H_{11}, the matrix element of H_{12} is defined below

$$\langle 1|H|2\rangle = \left\langle -iS\downarrow\left|H\right|\frac{X-iY}{\sqrt{2}}\uparrow\right\rangle = 0 \tag{2.7}$$

Due to the spin relation (1.5) the matrix element of H_0 and H_1 Hamiltonians are vanished. The non-zero term is H_2 Hamiltonian which correspond the spin-orbit interaction.

$$\left\langle -iS\downarrow\left|H\right|\frac{X-iY}{\sqrt{2}}\uparrow\right\rangle = \left\langle -iS\downarrow\left|H\right|\frac{X-iY}{\sqrt{2}}\downarrow\right\rangle_x + i\left\langle -iS\downarrow\left|H\right|\frac{X-iY}{\sqrt{2}}\downarrow\right\rangle_y \tag{2.8}$$

Here the subscripts x and y describe that none vanish term in H_2 are $\sigma_x and\ \sigma_y$ respectively. Before we explain the above matrix element and other related matrix elements which contains integral, let us evaluate the integral itself. The first parts of the typical integrals do not contain potential related terms and have the form[6]:

$$\int_{-\infty}^{-\infty}\frac{x}{r^n}dr = \int_{-\infty}^{-\infty}\frac{x^3}{r^n}dr = 0 \tag{2.9}$$

[6] Do not confuse r and $\vec{r}$ are not same $r = \sqrt{x^2+y^2+z^2}$ and $d\vec{r} = dxdydz$.

Where n is positive integer ($n = 1, 2, 3, 4, 5 \ldots$)since the integral is over entire space, preformed exact integration is not required. It is enough to know the parity of integral which does not vanish and which varnish. As we check the (2.9) function, if the integral has odd parity, the integral vanishes.

$$f(-) = \frac{-x}{r^n} = -\frac{x}{r^n} = -f(x) \tag{2.10}$$

$$f(-x) = \frac{-x^3}{r^n} = -\frac{x^3}{r^n} = -f(x) \tag{2.11}$$

So, this function and all other function that have odd parity vanish. The even functions which do not contain potential term are the following.

$$\int_{-\infty}^{-\infty} \frac{x^2}{r^n} dr = \int_{-\infty}^{-\infty} \frac{x^4}{r^n} dr \neq 0 \tag{2.12}$$

The function of this integral is

$$f(-) = \frac{x^2}{r^n} = \frac{x^2}{r^n} = f(x) \tag{2.13}$$
$$f(-x) = \frac{x^4}{r^n} = \frac{x^4}{r^n} = f(x)$$

The functions (2.12) have even parity so it does not vanish. All above function are x direction the argument of y and z are same.

The second section of typical integral including potential term$\left(\frac{\partial V}{\partial x}\right)$, the integral functions of (2.9) and (1.12) multiplied by$\left(\frac{\partial V}{\partial x}\right)$ proved the following forms. With odd function:

$$\int_{-\infty}^{\infty} \frac{\partial V}{\partial x} \frac{x}{r^n} d\vec{r} \neq 0 \neq \int_{-\infty}^{\infty} \frac{\partial V}{\partial x} \frac{x^3}{r^n} d\vec{r} \tag{2.14}$$

We assuming that potential term $\left(\frac{\partial V}{\partial x}\right)$ is spherical symmetry depend on only r and it is an even, i.e. $V(r) = V(-r)$.

$$\frac{\partial V}{\partial x} = \frac{dV}{dx}\frac{\partial r}{\partial x} = \frac{dV}{dx}\frac{\partial}{\partial x}\sqrt{x^2+y^2+z^2} = \frac{dV}{dx}\frac{x}{\sqrt{x^2+y^2+z^2}} = \frac{dV}{dx}\frac{x}{r} \tag{2. 15}$$

Appling (2.15) on one of the integrals[7] in EQ (2.14) the result can be written as:

$$\int_{-\infty}^{\infty} \frac{\partial V}{\partial x} \frac{x}{r^3} d\vec{r} = \int_{-\infty}^{\infty} \frac{dV(r)}{dr}\frac{x}{r} \frac{x}{r^3} d\vec{r} = \frac{dV(r)}{dr}\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} \frac{x^2}{r^4} dx \neq 0 \tag{2.16}$$

Here it is clear that the potential term $\frac{\partial V}{\partial x}$ is influence parity of the function. This addition term changes odd faction $\left(\frac{x}{r^n}\right)$into even function$\left(\frac{x^2}{r^n}\right)$. As shown above the integral of even function over the space does not vanish. Also integral of even function with potential term convert to:

$$\int_{-\infty}^{\infty} \frac{\partial V}{\partial x} \frac{x^2}{r^3} d\vec{r} = \int_{-\infty}^{\infty} \frac{dV(r)}{dr}\frac{x}{r} \frac{x^2}{r^3} d\vec{r} = \frac{dV(r)}{dr}\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} \frac{x^3}{r^4} dx = 0 \tag{2.17}$$

The potential term $\frac{\partial V}{\partial x}$ can changes the integral of x direction, is influence y and z direction.

$$\int_{-\infty}^{\infty} \frac{\partial V}{\partial x} \frac{y}{r^3} d\vec{r} = \int_{-\infty}^{\infty} \frac{dV(r)}{dr}\frac{x}{r} \frac{y}{r^3} d\vec{r} = \frac{dV(r)}{dr}\int_{-\infty}^{\infty} ydy \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} \frac{x}{r^4} dx = 0 \tag{2.18}$$

[7] The other give same result

Here it obvious that the integrals don not interact with each other so using the property of (2.9) directly, then then the integral EQ (2.18) disappear.

There are two vanished terms and two none vanished terms in equation (2.8) and

(2.19)

$$\left\langle -iS\left|\frac{\hbar}{4m_0^2c^2}\left(\frac{\partial V}{\partial z}p_x-\frac{\partial V}{\partial x}p_z\right)\right|\frac{Y}{\sqrt{2}}\right\rangle_y = C\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial z}\frac{-xy}{r^3}-\frac{\partial V}{\partial x}\frac{-yz}{r^3}\right)d\vec{r}=0$$

$$\left\langle -iS\left|\frac{\hbar}{4m_0^2c^2}\left(\frac{\partial V}{\partial y}p_z-\frac{\partial V}{\partial z}p_y\right)\right|\frac{X}{\sqrt{2}}\right\rangle_x = C\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial y}\frac{-xz}{r^3}-\frac{\partial V}{\partial z}\frac{-xy}{r^3}\right)d\vec{r}=0$$

we can write the following form:

The two none vanished terms in EQ (2.8) are:

(2.20)

$$\left\langle -S\left|\frac{\hbar}{4m_0^2c^2}\left(\frac{\partial V}{\partial z}p_x-\frac{\partial V}{\partial x}p_z\right)\right|\frac{X}{\sqrt{2}}\right\rangle_y = C\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial z}\frac{y^2+z^2}{r^3}-\frac{\partial V}{\partial x}\frac{-xz}{r^3}\right)d\vec{r}=\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial z}\frac{y^2}{r^3}\right)d\vec{r}$$

For simplicity all constants are denoted as C. Since cubic crystals are symmetry

(2.21)

$$\left\langle -S\left|\frac{\hbar}{4m_0^2c^2}\left(\frac{\partial V}{\partial y}p_z-\frac{\partial V}{\partial z}p_y\right)\right|\frac{Y}{\sqrt{2}}\right\rangle_x = C\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial y}\frac{-yz}{r^3}-\frac{\partial V}{\partial z}\frac{x^2+z^2}{r^3}\right)d\vec{r}=\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial z}\frac{x^2}{r^3}\right)d\vec{r}$$

(x, y and z in cubic crystal are equivalent), the last none vanished terms (2.20) and (2.21) are equal each other and they have opposite signs. Therefore, they are cancelling each other.

2.1.3 Matrix element H_{13}

(2.22)

$$\langle 1|H|3\rangle = \langle -iS\downarrow|H|Z\downarrow\rangle = KP$$

This matrix element is defined below, along with its value

Now let us evaluate each term of Hamiltonian separately

$$\langle -iS|H_0|Z\rangle = \langle -iS|E_P|Z\rangle = \frac{\sqrt{3}}{4}E_P\int_0^{2\pi} cos\theta\, d\theta = \frac{\sqrt{3}}{4}E_P.sin\theta|_0^{2\pi} = 0 \tag{2.23}$$

The only non-vanished term is

$$\langle -iS\downarrow|H_1|Z\downarrow\rangle = \left\langle -iS\left|\frac{\hbar k}{m_0}p_z\right|Z\right\rangle = -i\frac{\hbar k}{m_0}\langle S|p_z|Z\rangle = KP \tag{2.24}$$

The most H_2 terms are vanished due to the spin relation (1.5) only remain term is

$$\langle -iS\downarrow|H_2|Z\downarrow\rangle = \left\langle -iS\left|\frac{\hbar}{4m_0^2c^2}\left(\frac{\partial V}{\partial x}p_y - \frac{\partial V}{\partial y}p_x\right)\right|Z\right\rangle_z = C\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial x}\frac{-yz}{r^3} - \frac{\partial V}{\partial y}\frac{-xz}{r^3}\right)d\vec{r} = 0 \tag{2.25}$$

All constants are denoted as C for convenience the property of (2.18) is used

1.2.4 Matrix element H_{22}

Below the value of second diagonal matrix element is discussed.

$$\langle 2|H|2\rangle = \left\langle \frac{X+iY}{\sqrt{2}} \uparrow \middle| H \middle| \frac{X-iY}{\sqrt{2}} \uparrow \right\rangle = E_p - \frac{\nabla}{3} \tag{2.26}$$

Here the Hamiltonian of each term is evaluated separately.

$$\begin{aligned} \left\langle \frac{X+iY}{\sqrt{2}} \uparrow \middle| H_0 \middle| \frac{X-iY}{\sqrt{2}} \uparrow \right\rangle &= \frac{1}{2}\langle X|H_0|X\rangle + \frac{1}{2}\langle Y|H_0|Y\rangle - \frac{1}{2}\langle X|H_0|iY\rangle + \frac{1}{2}\langle iY|H_0|X\rangle \\ &= \frac{1}{2}E_p + \frac{1}{2}E_p - \frac{1}{2}i\langle X|H_0|Y\rangle + \frac{1}{2}i\langle Y|H_0|X\rangle = E_p \end{aligned} \tag{2.27}$$

Since E_p is constant we can interchange 'bra'-term Y into 'ket'-term X of the last term EQ (2.27), and last two terms of this equation are cancelled each other. Appling the property of (2.9) and (2.12) evaluation H_1 part of Hamiltonian is:

$$\begin{aligned} \left\langle \frac{X+iY}{\sqrt{2}} \uparrow \middle| H_1 \middle| \frac{X-iY}{\sqrt{2}} \uparrow \right\rangle &= \left\langle \frac{X+iY}{\sqrt{2}} \uparrow \middle| \frac{\hbar k}{m_o} p_z \middle| \frac{X-iY}{\sqrt{2}} \uparrow \right\rangle \\ &= kC. \int_{-\infty}^{\infty} \left(\frac{x}{r}.\frac{-zx}{r^3} + \frac{y}{r}.\frac{-zy}{r^3} - \frac{x}{r}.\frac{-zy}{r^3} + \frac{y}{r}.\frac{-zx}{r^3} \right) dr = 0 \end{aligned} \tag{2.28}$$

The evaluation of the last term of Hamiltonian H_2 is below:

$$\begin{aligned} \left\langle \frac{X+iY}{\sqrt{2}} \middle| H_2 \middle| \frac{X-iY}{\sqrt{2}} \right\rangle &= C \left\langle X \middle| \frac{\partial V}{\partial x} p_y - \frac{\partial V}{\partial y} p_x \middle| X \right\rangle - \left\langle X \middle| \frac{\partial V}{\partial x} p_y - \frac{\partial V}{\partial y} p_x \middle| iY \right\rangle \\ &+ \left\langle iY \middle| \frac{\partial V}{\partial x} p_y - \frac{\partial V}{\partial y} p_x \middle| X \right\rangle - \left\langle iY \middle| \frac{\partial V}{\partial x} p_y - \frac{\partial V}{\partial y} p_x \middle| iY \right\rangle \end{aligned} \tag{2.29}$$

To simplify EQ (2.28) we have of evaluate each term separately and take account integral property of (2.9) and (2.18):

$$\begin{aligned} \langle X| \dots |X\rangle &= \int_{-\infty}^{\infty} \frac{x}{r} \left(\frac{\partial V}{\partial x} \frac{-xy}{r^3} - \frac{\partial V}{\partial y} \frac{y^2+z^2}{r^3} \right) d\vec{r} = 0 \\ \langle Y| \dots |Y\rangle &= \int_{-\infty}^{\infty} \frac{y}{r} \left(\frac{\partial V}{\partial x} \frac{x^2+z^2}{r^3} - \frac{\partial V}{\partial y} \frac{-xy}{r^3} \right) d\vec{r} = 0 \end{aligned} \tag{2.30}$$

$$\langle iY|\ldots|X\rangle = C\int_{-\infty}^{\infty}\frac{y}{r}\left(\frac{\partial V}{\partial x}\frac{-xy}{r^3}-\frac{\partial V}{\partial y}\frac{y^2+z^2}{r^3}\right)d\vec{r} = C\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial x}\frac{-xy^2}{r^3}-\frac{\partial V}{\partial y}\frac{y^3+yz^2}{r^3}\right)d\vec{r} \quad (2.31)$$

$$-\langle X|\ldots|iY\rangle = C\int_{-\infty}^{\infty}\frac{x}{r}\left(\frac{\partial V}{\partial x}\frac{x^2+z^2}{r^3}-\frac{\partial V}{\partial y}\frac{-xy}{r^3}\right)d\vec{r} = C\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial x}\frac{x^3+xz^2}{r^3}-\frac{\partial V}{\partial y}\frac{-x^2y}{r^3}\right)d\vec{r}$$

There are many constants in our equations but they are denoted C for convenience. Here in (2.31) we write all constants explicitly instead of C and using the property of equivalent axes in cube we interchange y to x and the result will be 2 appears in front of integral. Then combine equations (2.27) and (2.31) which are non-vanished terms.

$$E_p - \frac{\hbar^2 i}{4m_0^2c^2}\cdot\frac{3}{8\pi}\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial x}\frac{-xy^2}{r^3}-\frac{\partial V}{\partial y}\frac{y^3+yz^2}{r^3}\right)-\left(\frac{\partial V}{\partial x}\frac{x^3+xz^2}{r^3}-\frac{\partial V}{\partial y}\frac{-x^2y}{r^3}\right)d\vec{r} \quad (2.32)$$
$$= E_p - \frac{\hbar^2 i}{4m_0^2c^2}\cdot\frac{3.2}{8\pi}\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial x}\frac{x^3+xz^2}{r^3}-\frac{\partial V}{\partial y}\frac{-x^2y}{r^3}\right)d\vec{r} = E_p - \frac{\nabla}{3}$$

To prove expression (2.32) let us use the definition of ∇ and expand it as integral form.

$$\nabla = i\frac{3\hbar}{4m_0^2c^2}\left\langle X\left|\frac{\partial V}{\partial x}p_y-\frac{\partial V}{\partial y}p_x\right|Y\right\rangle = \frac{3\hbar^2 i}{4m_0^2c^2}\cdot\frac{3.2}{8\pi}\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial x}\frac{x^3+xz^2}{r^3}-\frac{\partial V}{\partial y}\frac{-x^2y}{r^3}\right)d\vec{r} \quad (2.33)$$

2.1.5. Matrix element H_{23}

The off-diagonal matrix element.

$$\langle 2|H|3\rangle = \left\langle\frac{X-iY}{\sqrt{2}}\uparrow\left|H\right|Z\downarrow\right\rangle = \frac{\sqrt{2}}{3}\nabla \quad (2.34)$$

Because of spin property (1.5) some of the terms in question (2.34) are vanished, the Hamiltonian of non-zero terms are shown blow:

$$\left\langle\frac{X+iY}{\sqrt{2}}\left|H_2\right|Z\right\rangle = \left\langle\frac{X-iY}{\sqrt{2}}\left|H_2\right|Z\right\rangle_x - i\left\langle\frac{X+iY}{\sqrt{2}}\left|H_2\right|Z\right\rangle_y \quad (2.35)$$

Where

$$\left\langle \frac{X+iY}{\sqrt{2}} \middle| H_2 \middle| Z \right\rangle_x = \left\langle \frac{X}{\sqrt{2}} \middle| H_2 \middle| Z \right\rangle_x + \left\langle \frac{iY}{\sqrt{2}} \middle| H_2 \middle| Z \right\rangle_x \tag{2.36}$$

$$-i\left\langle \frac{X+iY}{\sqrt{2}} \middle| H_2 \middle| Z \right\rangle_y = -\left\langle \frac{X}{\sqrt{2}} \middle| H_2 \middle| Z \right\rangle_y + \left\langle \frac{iY}{\sqrt{2}} \middle| H_2 \middle| Z \right\rangle_y \tag{2.37}$$

The terms in (2.36) and (2.37) are separated each other below for convenient and (2.16), (2.17) and (2.18) are applied.

$$\langle X| \dots |Z\rangle_x = C\int_{-\infty}^{\infty} \frac{x}{r}\left(\frac{\partial V}{\partial y}\frac{x^2+y^2}{r^3} - \frac{\partial V}{\partial z}\frac{-zy}{r^3}\right)d\vec{r} = 0 \tag{2.38}$$

$$\begin{aligned}\langle iY| \dots |Z\rangle_x &= iC\int_{-\infty}^{\infty} \frac{y}{r}\left(\frac{\partial V}{\partial y}\frac{x^2+y^2}{r^3} - \frac{\partial V}{\partial z}\frac{-zy}{r^3}\right)d\vec{r} \\ &= ic\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial y}\frac{yx^2+y^3}{r^4} - \frac{\partial V}{\partial z}\frac{-zy^2}{r^4}\right)d\vec{r}\end{aligned} \tag{2.39}$$

$$\begin{aligned}\langle iX| \dots |Z\rangle_y &= -iC\int_{-\infty}^{\infty} \frac{x}{r}\left(\frac{\partial V}{\partial z}\frac{-xz}{r^3} - \frac{\partial V}{\partial x}\frac{x^2+y^2}{r^3}\right)d\vec{r} \\ &= iC\int^{\infty}\left(\frac{\partial V}{\partial z}\frac{-x^2z}{r^4} - \frac{\partial V}{\partial x}\frac{x^3+xy^2}{r^4}\right)d\vec{r}\end{aligned} \tag{2.40}$$

$$-\langle Y| \dots |Z\rangle_y = C\int_{-\infty}^{\infty} \frac{y}{r}\left(\frac{\partial V}{\partial z}\frac{-xz}{r^3} - \frac{\partial V}{\partial x}\frac{x^2+y^2}{r^3}\right)d\vec{r} = 0 \tag{2.41}$$

Where all constants are denoted as C for convenience. The only remaining terms are (2.39) and (2.40) (expand C as explicitly and use cube symmetry to exchange x and y)

$$\frac{\hbar^2 i}{4m_0^2c^2}\cdot\frac{3}{4\sqrt{2}\pi}\left[\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial y}\frac{x^2y+y^3}{r^4}-\frac{\partial V}{\partial z}\frac{-y^2z}{r^4}\right)+\left(\frac{\partial V}{\partial x}\frac{-x^2z}{r^3}-\frac{\partial V}{\partial y}\frac{x^3+xy^2}{r^4}\right)d\vec{r}\ \right] \tag{2.42}$$

$$=\frac{\hbar^2 i}{4m_0^2c^2}\cdot\frac{3.2}{4\sqrt{2}\pi}\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial x}\frac{x^3+xz^2}{r^4}-\frac{\partial V}{\partial y}\frac{-x^2y}{r^4}\right)d\vec{r}\ =\frac{\sqrt{2}}{3}\nabla$$

This term from ∇ expression which we have seen (2.33) in preceded section.

2.1.6. Matrix element H_{33}

The third diagonal matrix element is defined below

$$\langle 3|H|3\rangle=\langle Z\downarrow|H|Z\downarrow\rangle=E_p \tag{2.43}$$

Below each term of Hamiltonian is evaluated separately

$$=\langle Z\downarrow|H|Z\downarrow\rangle=\langle Z|E|Z\rangle=E_p \tag{2.44}$$

Using property of (2.9) the flowing expressions are obtained

$$\langle Z\downarrow|H_1|Z\downarrow\rangle=\left\langle Z\left|\frac{\hbar k}{m_0}p_z\right|Z\right\rangle=C\int_{-\infty}^{\infty}\frac{z}{r}\left(\frac{x^2+y^2}{r^3}\right)d\vec{r}=C\int_{-\infty}^{\infty}\frac{z}{r^4}.(x^2+y^2)d\vec{r}=0 \tag{2.45}$$

Finally due to the spin relation (1.5) the Hamiltonians of H_2 mostly are vanished, the only non-vanished term is below (using the property (2.18)):

$$\langle Z\downarrow|H_2|Z\downarrow\rangle=\left\langle Z\left|\frac{\hbar}{4m_0^2c^2}\left(\frac{\partial V}{\partial x}p_y-\frac{\partial V}{\partial y}p_x\right)\right|Z\right\rangle=C\int_{-\infty}^{\infty}\frac{z}{r}\left(\frac{\partial V}{\partial x}\frac{-yz}{r^3}-\frac{\partial V}{\partial y}\frac{-xz}{r^3}\right)d\vec{r}=0 \tag{2.46}$$

Because simplicity, all constant are combined and denoted as C.

2.2. Explicit Of Kane's Matrix Hamiltonian

Section 2.1 all matrix elements are evaluated. In this section we will write complete upper matrix Hamiltonian for state (1.10) as explicit form:

$$\begin{bmatrix} E_s & 0 & kP & 0 \\ 0 & E_p - \frac{\nabla}{3} & \frac{\sqrt{2}}{3}\nabla & 0 \\ kP & \frac{\sqrt{2}}{3}\nabla & E_p & 0 \\ 0 & 0 & 0 & E_p - \frac{\nabla}{3} \end{bmatrix} \tag{2.47}$$

This is only upper part of matrix Hamiltonian, the lower part for state (1.11) is identical

2.3 Correction To Basis Functions

To convert 4×4 matrix (2.47) into 3×3 matrix for simplicity, the energy of the top of the valence band defined to be zero and we define reference energy to be $E_p = -\frac{\nabla}{3}$ so the conduction minimum is $E_s = E_g$, where $E_g$energy band gap is as it is shown of fig. The Hamiltonian (2.47) become:

$$\begin{bmatrix} E_g & 0 & kP & 0 \\ 0 & \frac{2\nabla}{3} & \frac{\sqrt{2}}{3}\nabla & 0 \\ kP & \frac{\sqrt{2}}{3}\nabla & -\frac{\nabla}{3} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{2.48}$$

The detrimental equation$[H - E'I] = 0$ provided four eigenvalues for E':

$$E' = 0 \tag{2.49}$$

(2.50)

$$E'\left(E'-E_g\right)(eE'+\nabla)-k^2P^2\left(E'+\frac{2\nabla}{3}\right)=0$$

Since k^2 is very small comparing atomic momentum, the equation (2.50) reduced as below:

(2.51)

$$E'\left(E'-E_g\right)(E'+\nabla)=0$$

Solving the above equation, it's clear that roots of this equation are given to us very close three band edges$E'=E_g$, $E'=0$ and $E'=-\nabla$ .Now let go back the original equation (2.47) and add small k^2 dependent ε, where $\varepsilon \ll \nabla$ and E_g, which give us the following three possible solutions.

1. $E'=E_g+\varepsilon(k^2)$
2. $E'=0+\varepsilon(k^2)$
3. $E'=-\nabla+\varepsilon(k^2)$

To obtain the explicit from a ε for each above cases, lest us substitute the relations into the equation (2.50).

1. $$\varepsilon E_g\left(E_g+\nabla\right)-k^2P^2\left(E_g+\frac{2}{3}\nabla\right)=0$$

$$\varepsilon=\frac{k^2P^2\left(E'+\frac{2}{3}\nabla\right)}{E_g\left(E_g+\nabla\right)}$$

2. $$\varepsilon E_g\nabla-k^2P^2\frac{2}{3}\nabla=0$$

$$\varepsilon=\frac{2k^2P^2}{3E_g}$$

3. $$\varepsilon\nabla\left(-E_g-\nabla\right)-k^2P^2\left(-\frac{1}{3}\nabla\right)=0$$

$$\varepsilon=-\frac{k^2P^2}{3\left(\nabla+E_g\right)}$$

Not it is easy to get eigenvalue using the expression of (1.8):

(2.52)

$$E' = E_n(\vec{k}) - \frac{\hbar^2 k^2}{2m_0}$$

$$E_n(\vec{k}) = E' + \frac{\hbar^2 k^2}{2m_0}$$

The following expressions are provided when we substitute the value of E' into energy of conduction and valance band.

(2.53)

$$E_C(\vec{k}) = E_g + \frac{\hbar^2 k^2}{2m_0} + \frac{k^2 P^2 \left(E_g + \frac{2}{3}\nabla\right)}{E_g(E_g + \nabla)}$$

$$E_{hh}(\vec{k}) = \frac{\hbar^2 k^2}{2m_0}$$

$$E_{lh}(\vec{k}) = \frac{\hbar^2 k^2}{2m_0} - \frac{2k^2 P^2}{3E_g}$$

$$E_{so}(\vec{k}) = -\nabla + \frac{\hbar^2 k^2}{2m_0} - \frac{k^2 P^2}{3(\nabla + E_g)}$$

The above expressions give us incorrect effective mass for heavy hole band ($E_{hh}(\vec{k})$). To obtain eigenfunctions which are useful for LKM, it is eccentrical to develop Kane's basis function for upper matrix in equation (2.47) (in this point $n = c, lh$, so, and $\alpha,\ \beta$ are used for upper and lower basis respectively).

(2.54)

$$\emptyset_{hh\alpha} = \left| \frac{-X + iY}{\sqrt{2}} \uparrow \right\rangle$$

$$\emptyset_{n,\alpha} = a_n |iS \downarrow\rangle + b_n \left| \frac{X - iY}{\sqrt{2}} \uparrow \right\rangle + c_{n|Z \downarrow\rangle}$$

The lower matrices are

(2.55)

$$\emptyset_{hh\beta} = |\frac{X - iY}{\sqrt{2}} \downarrow\rangle$$

$$\emptyset_{n,\alpha} = a_n|iS \uparrow\rangle + b_n\,|-\frac{X + iY}{\sqrt{2}} \downarrow\rangle + c_{n|Z\uparrow\rangle}$$

By solving Eigen equation:

(2.56)

$$\begin{bmatrix} E_g - E_n' & 0 & kP \\ 0 & \frac{2}{3}\Delta - E_n' & \frac{\sqrt{2}}{3}\nabla \\ kP & \frac{\sqrt{2}}{3}\nabla & -\frac{\nabla}{3} - E_n' \end{bmatrix} \begin{bmatrix} a_n \\ b_n \\ c_n \end{bmatrix} = 0$$

To obtain values for eigenvector Column $[a_n b_n, c_n]$ we have substituted each eigenvalue into the eigen equation, and we assume limit $k^2 \rightarrow 0$:

(2.57)

$$n = c \qquad \begin{bmatrix} 0 & 0 & 0 \\ 0 & -\frac{2}{3}\Delta - E_n' & \frac{\sqrt{2}}{3}\nabla \\ 0 & \frac{\sqrt{2}}{3}\nabla & -\frac{\nabla}{3} - E_n' \end{bmatrix} \begin{bmatrix} a_n \\ b_n \\ c_n \end{bmatrix} = 0$$

It is clear that a_c has finite solutions where b_c and c_c are only zero. To find the value $a_c$we normalize this term $(a_n^2 + b_n^2 + c_n^2)^{1/2} = 1$ and as you can see $a_c = 1$ since b_c and c_c are zero. Then the value will change as below.

$$n = c \quad a_c \simeq 1 \;\; b_c \simeq 0 \quad c_c \simeq 0$$

$$\begin{bmatrix} E_g & 0 & 0 \\ 0 & -\frac{2}{3}\Delta & \frac{\sqrt{2}}{3}\nabla \\ 0 & \frac{\sqrt{2}}{3}\nabla & -\frac{\nabla}{3} \end{bmatrix} \begin{bmatrix} a_{lh} \\ b_{lh} \\ c_{lh} \end{bmatrix} = 0 \tag{2.58}$$

Up to here we can see clearly that $a_{lh} = 0$ and$c_{lh} = \sqrt{2b_{lh}}$. This c_{lh} and b_{lh}have finite number of solutions. Using the same normalization as before we obtain$(b_{so}^2 + c_{so}^2)^{1/2} = 1$. Which gives us:

$$\frac{3b_{so}^2}{2} = 1, \quad b_{so}^2 = \frac{2}{3}, \qquad b_{so} = \sqrt{\frac{2}{3}}, \qquad c_{so} = -\frac{1}{\sqrt{3}}$$

Therefore, the values are:

$$n = so \qquad a_{so} \simeq 0, \qquad b_{so} = \sqrt{\frac{2}{3}}, \qquad c_{so} = -\frac{1}{\sqrt{3}}$$

Now we can obtain well developed basis functions which LKM can be used:

$$\begin{aligned}
&\emptyset_{c\alpha} = |iS \downarrow\rangle \\
&\emptyset_{c\beta} = |iS \uparrow\rangle \\
&\emptyset_{hh\alpha} = -\frac{1}{\sqrt{2}}|(X + iY) \uparrow\rangle && = |\tfrac{2}{3}\ \tfrac{3}{2}\rangle \\
&\emptyset_{hh\beta} = \frac{1}{\sqrt{2}}|(X - iY) \downarrow\rangle && = |\tfrac{2}{3}\ \ \tfrac{-3}{2}\rangle \\
&\emptyset_{lh\alpha} = \frac{1}{\sqrt{6}}|(X - iY) \uparrow\rangle + \sqrt{\frac{2}{3}}|Z \downarrow\rangle && = |\tfrac{2}{3}\ \ \tfrac{-1}{2}\rangle \\
&\emptyset_{lh\beta} = \frac{-1}{\sqrt{6}}|(X + iY) \downarrow\rangle + \sqrt{\frac{2}{3}}|Z \uparrow\rangle && = |\tfrac{2}{3}\ \ \tfrac{1}{2}\rangle \\
&\emptyset_{so,\alpha} = \frac{1}{\sqrt{3}}|(X - iY) \uparrow\rangle - \frac{1}{\sqrt{3}}|Z \downarrow\rangle && = |\tfrac{1}{2}\ \ \tfrac{-1}{2}\rangle \\
&\emptyset_{so,\beta} = \frac{-1}{\sqrt{3}}|(X + iY) \downarrow\rangle + \frac{1}{\sqrt{3}}|Z \uparrow\rangle && = |\tfrac{1}{2}\ \ \tfrac{1}{2}\rangle
\end{aligned} \tag{2.59}$$

Remember α and β represent the upper and the lower matrix in (1.17) respectively and for convenience Dirac's notation of wave equation is used:

$$|j, m\rangle$$

Where j is total angular momentum $j = l + s$, and l is just angular momentum but s is the spin, and m is magnetic quantum number of z component of j. for electron spin always is ½ but for p-state $l = 1$, thus $j = l + s$ and $j = l - s$ which implies 3/2 or ½ . $m = 2j + 1$Therefore, m has the following values: $j, j-1, -j \ldots \ldots + 1, -j$. For the case where m 3/2 the value of j will be $\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$. For $j = \frac{1}{2}$ there are only two values ½ and -1/2. Between $j = \frac{1}{2}$ and $j = \frac{3}{2}$ states, the spin orbit interaction is not responsible for spin-orbit split-off ∇. Here the spin-orbit interaction is mostly constant for all materials.

The quantum numbers which related states (2.59) are labeled as a below:

$\emptyset_{hh\alpha} = Y_{11} \uparrow$

Here $\uparrow$ represent spin up when$s = \frac{1}{2}$, thus the above explanation proved us the following information $j = 1 + \frac{1}{2} = \frac{3}{2}\ and\ m = \frac{3}{2}$which is spin up condition and for spin down$m = -\frac{3}{2}$.

CHAPTER THREE: CONSTRUCTION OF K.P HAMILTONIAN WITH USING LKM MODEL

In chapter two we discussed Kane's model which has two problems first it neglected the distance between bands and explain only four bands. The second weakness is: it provided incorrect result of heavy hole. Luttinger Kohn Model solved those challenges. This model classified bands into two categories, the main interest band name class A which LKM considered exactly and influence of other bands labelled class B treated as perturbation. In this case we will use Lowdin's perturbation method [9] and treated valence bands are our main interest class A state and all others treated as class B state. (fig. 1.1.b)

3.1. Zinc Blende Structure

3.1.1. Hamiltonian of zinc blende structure

Let us go back the total Hamiltonian (1.7) which works with $u_{\vec{k}}(r)$.

$$H = H_0 + \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar}{4m_0^2 c^2}\left[\vec{\nabla} V \times p\right].\vec{\sigma} + H' \tag{3.1}$$

Where

$$H_0 = \frac{P^2}{2m_0} + V(\vec{r}) \tag{3.2}$$

$$H' = \frac{\hbar}{m_0}\vec{k}.\overrightarrow{\prod} \tag{3.3}$$

Here

$$\overrightarrow{\prod} = \vec{p} + \frac{\hbar}{4m_0^2 c^2}\vec{\sigma} \times \vec{\nabla} \tag{3.4}$$

The last term of equation (3.4) is negligible because k dependent crystal momentum is very small comparing the p dependent atomic momentum ($\hbar k \ll p$). Therefore equation (3.3) is reduced as a below.

$$H' \cong \frac{\hbar}{m_0}\vec{k}.\vec{p} \tag{3.5}$$

This equation (3.5) is the term which is responsible for coupling class A to class B state. Eigen function of Schrödinger equation with Hamiltonian is expanded using L*ö*wdin's perturbation method.

$$u_{\vec{k}}(r) = \sum_{j}^{A} a_j\,(k) u_{j0}(\vec{r}) + \sum_{\gamma}^{B} a_\gamma\,(k) u_{\gamma 0}(\vec{r}) \tag{3.6}$$

First summation represent class A where the subscript index j is $1,\ 2, \ldots \ldots 6$ and second summation with γ represent state of class B. To improve Kane's mode (2.57) we take basis function in class A, for heavy hole ($u_{10,}\ u_{40}$), light hole ($u_{20,}\ u_{30}$) and spin split-off ($u_{50,}\ u_{60}$) bands:

$$u_{10}(\vec{r}) = \left|\frac{3}{2}, \frac{3}{2}\right\rangle = \frac{-1}{\sqrt{2}}\left|(X + iY)\uparrow\right\rangle$$

$$u_{20}(\vec{r}) = \left|\frac{3}{2}, \frac{1}{2}\right\rangle = \frac{-1}{\sqrt{6}}\left|(X + iY)\downarrow\right\rangle + \sqrt{\frac{2}{3}}\left|Z\uparrow\right\rangle$$

$$
\begin{aligned}
u_{30}(\vec{r}) &= \left|\frac{3}{2},\frac{-1}{2}\right\rangle = \frac{-1}{\sqrt{6}}|(X-iY)\uparrow\rangle + \sqrt{\frac{2}{3}}|Z\downarrow\rangle \\
u_{40}(\vec{r}) &= \left|\frac{3}{2},\frac{-3}{2}\right\rangle = \frac{1}{\sqrt{2}}|(X-iY)\downarrow\rangle \\
u_{50}(\vec{r}) &= \left|\frac{1}{2},\frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}|(X+iY)\downarrow\rangle + \frac{1}{\sqrt{3}}|Z\uparrow\rangle \\
u_{60}(\vec{r}) &= \left|\frac{1}{2},\frac{-1}{2}\right\rangle = \frac{1}{\sqrt{3}}|(X-iY)\uparrow\rangle - \frac{1}{\sqrt{3}}|Z\downarrow\rangle
\end{aligned}
\tag{3.7}
$$

At k =0 these basis function which represent band edges satisfy:

$$H(O)u_{j0}(\vec{r}) = E_j(0)u_{J0}(\vec{r})$$

Where

$E_j(0) = 0$ For $j = 1,2,3,4.$

$E_j(0) = -\nabla$ For $j = 5,6.$

As we assume $E_p = -\frac{\nabla}{3}$.

Matrix element of Luttinger-Kohn Hamiltonian (LKH) are obtained using the perturbation theory of Lowdin's method [9]. Here we solve Eigen equation H_{jj}^{LK} which is associate class A states.

$$\sum_{\boldsymbol{j,}}^{\boldsymbol{A}} \left(H_{jj}^{LK} - E\delta_{jj,}\right)a_j(\vec{k}) \tag{3.9}$$

Where

$$H_{jj}^{LK} = H_{jj} + \sum_{\boldsymbol{\gamma,}}^{\boldsymbol{B}} \frac{H_{j\gamma}H_{\gamma j}}{E_0 - E_j} \tag{3.10}$$

Here $\gamma \neq jj,$ the first term of equation (3.10) is unperturbed term which corresponding coupling between states of class A and the second term is perturbed term which also correspond coupling between states class A and class B. the coupling between states in class B is neglected.

$$H_{jj,} = \langle u_{j0}|H|u_{j'0}\rangle = \left[E_j(0) + \frac{\hbar^2k^2}{2m_0}\right]\delta_{jj} \tag{3.11}$$

$$H'_{j\gamma} = \left\langle u_{j0} \middle| \frac{\hbar}{m_0} k.p \middle| u_{\gamma 0} \right\rangle = \sum_{\alpha} \frac{\hbar k_\alpha}{m_0} p^{\alpha}_{j\gamma} \tag{3.12}$$

Where $\alpha = x, y, z, p_{jj} = 0\ for\ j, j' \in A$.The perturbed part does not have any influence on class A state and $p^{\alpha}_{j\gamma} \neq 0\ for\ \gamma \notin A$ and the following notation is used.

$$p^{\alpha}_{j\gamma} = \langle u_{j0} | p_\alpha | u_{\gamma 0} \rangle \tag{3.13}$$

These equations (3.12) represent perturbed part where equation (3.13) shows us unperturbed part. Here the operator $p_\alpha = -i\hbar \frac{\partial}{\partial \alpha}$. If we substitute equations (3.12) and (3.11) into equation (3.10), we obtain:

$$H^{LK}_{jj} = \left[E_j(0) + \frac{\hbar^2 k^2}{2m_0} \right] \delta_{jj} + \frac{\hbar^2}{m_0} \sum_{\gamma,}^{\boldsymbol{B}} \sum_{\alpha,\beta} \frac{k_\alpha k_\beta p^{\alpha}_{j\gamma} p^{\beta}_{\gamma j,}}{E_0 - E_j} \tag{3.14}$$

Where $\alpha, \beta == x, y, z$ and δ_{jj} is Kronecker symbol. To simplify the complicated expression in equation (3.14) we can write as a below:

$$H^{LK}_{jj} = E_j(0)\delta_{jj} + \sum_{\alpha,\beta} D^{\alpha,\beta}_{jj,} k_\alpha k_\beta \tag{3.15}$$

Here the term

$$D^{\alpha,\beta}_{jj,} = \frac{\hbar^2}{2m_0} \left\{ \delta_{jj}\delta_{\alpha,\beta} + \sum_{\gamma}^{B} \frac{p^{\alpha}_{j\gamma} p^{\beta}_{\gamma j,} + p^{\beta}_{j\gamma} p^{\alpha}_{\gamma j,}}{m_0 (E_0 - E_j)} \right\} \tag{3.16}$$

To clarify the above equivalence, we substitute equations (3.15) and (3.16) and we get the following terms:

$$H^{LK}_{jj} = E_j(0)\delta_{jj} + \frac{\hbar^2}{2m_0} \sum_{\alpha,\beta} k_\alpha k_\beta \left\{ \delta_{jj}\delta_{\alpha\beta} + \sum_{\gamma}^{B} \frac{p^{\alpha}_{j\gamma} p^{\beta}_{\gamma j,} + p^{\beta}_{j\gamma} p^{\alpha}_{\gamma j,}}{m_0 (E_0 - E_j)} \right\}$$

$$= \left[E_j(0) + \frac{\hbar^2 k^2}{2m_0}\right]\delta_{jj} + \frac{\hbar^2}{m_0}\sum_{\boldsymbol{\gamma},}^{\boldsymbol{B}}\sum_{\alpha,\beta} k_\alpha k_\beta \frac{p^\alpha_{j\gamma}p^\beta_{\gamma j,} + p^\beta_{j\gamma}p^\alpha_{\gamma j,}}{m_0(E_0 - E_j)}$$

$$= \left[E_j(0) + \frac{\hbar^2 k^2}{m_0}\right]\delta_{jj} + \frac{\hbar^2}{m_0}\sum_{\boldsymbol{\gamma},}^{\boldsymbol{B}}\sum_{\alpha,\beta} \frac{k_\alpha k_\beta p^\alpha_{j\gamma}p^\beta_{\gamma j,}}{m_0(E_0 - E_j)}$$

The last is obtained from the following relations:

$$p^\alpha_{j\gamma}p^\beta_{\gamma j,} + p^\beta_{j\gamma}p^\alpha_{\gamma j,} = \langle u_{j0}|p_\alpha|u_{\gamma 0}\rangle\langle u_{\gamma 0}|p_\beta|u_{j,0}\rangle + \langle u_{j0}|p_\beta|u_{\gamma 0}\rangle\langle u_{\gamma 0}|p_\alpha|u_{j,0}\rangle = 2p^\alpha_{j\gamma}p^\beta_{\gamma j,}$$

Since α and β represent x, y and z we can interchange each other. Now we need to introduce short notation which based on the fact that each basis function contains with$|X\rangle$, $|Y\rangle$ and $|Z\rangle$ then we break all matrix element into the part that consist of one of these basis function. According the explanation above the following short notation is used:

$$\begin{aligned} A &= \frac{\hbar^2}{2m_0} + \frac{\hbar^2}{m_0}\sum_{\boldsymbol{\gamma}}^{\boldsymbol{B}} \frac{p^x_{X\gamma}p^x_{\gamma X}}{E_0 - E_\gamma} \\ B &= \frac{\hbar^2}{2m_0} + \frac{\hbar^2}{m_0}\sum_{\boldsymbol{\gamma}}^{\boldsymbol{B}} \frac{p^y_{X\gamma}p^y_{\gamma X}}{E_0 - E_\gamma} \\ C &= \frac{\hbar^2}{2m_0} + \frac{\hbar^2}{m_0}\sum_{\boldsymbol{\gamma}}^{\boldsymbol{B}} \frac{p^X_{X\gamma}p^y_{\gamma Y} + p^y_{X\gamma}p^X_{\gamma Y}}{E_0 - E_\gamma} \end{aligned} \tag{3.17}$$

Where A and B explain the coupling of class A state to the all-other states but C is anisotropy which related the band structure around the extremum point (Γ point). for cubic crystal, the notions above can be used as an experimental band structure or Luttinger parameter γ_i and defined as below:

$$\begin{aligned} -\frac{\hbar^2}{2m_0}\gamma_1 &= \frac{1}{3}(A + 2B) \\ -\frac{\hbar^2}{2m_0}\gamma_2 &= \frac{1}{6}(A - B) \\ -\frac{\hbar^2}{2m_0}\gamma_3 &= \frac{C}{6} \end{aligned} \tag{3.18}$$

Here the definitions we made in the right-hand side in equation (3.18) are invariant under operation of cubic group and we labeled by Luttinger parameter γ_i.

3.2. Matrix In $|X\rangle$, $|Y\rangle$ And $|Z\rangle$ Basis

To obtain the matrix element of u_{j0} which we constructed section 3.1.1, the evaluation of Hamiltonian matrix element of$|X\rangle$, $|Y\rangle$ and $|Z\rangle$ basis functions are required**.** In this section we will use to indices which are $a, b = |X\rangle, |Y\rangle, |Z\rangle$ the other indices are $\alpha, \beta = x, y, z$.

For matrix element below the notations are used similarly as (3.17) and (3.13) the only change made is that we use $|X\rangle, |Y\rangle, |Z\rangle$ instead of u_j.

$$\langle X|p_y|\gamma\rangle = p_{X\gamma}^{y} \qquad (3.19)$$
$$\left|\langle X|p_y|\gamma\rangle\right|^2 = p_{X\gamma}^{y} p_{\gamma X}^{y}$$

Here X represent X, Y or Z states, and γ is for class B state and also p_y is momentum operator with values$-i\hbar\frac{\partial}{\partial y}$. The flowing relation should be Hermitian[8]. This property of Hamiltonian following relations are required.

$$p_{X\gamma}^{y} = \left(p_{\gamma X}^{y}\right)^* \qquad (3.20)$$
$$\left(D_{ab}^{\alpha\beta}\right)^* = D_{ba}^{\alpha\beta}$$

Where * sign represent complex conjugated and for cubic symmetry can be write as following:

$$p_{X\gamma}^{y} p_{\gamma X}^{y} = p_{X\gamma}^{z} p_{\gamma X}^{z} \neq p_{X\gamma}^{x} p_{\gamma X}^{x} \qquad (3.21)$$

[8]Hermitian conjugation means complex conjugation and transpose, which is shown as eq. (3.20).

Which mean the property of material along all axis of cubic symmetry its sides are equal each other. To simplify our calculation the following notation required:

$$A = D_{XX}^{xx} \tag{3.22}$$
$$B = D_{XX}^{yy}$$
$$C = D_{XY}^{xy} + D_{YX}^{yx}$$

Where A, B, C are defined (3.17) and $D_{ab}^{\alpha,\beta}$ are calculated by (3.16) we use indices of a , b instead of j, j' the expression can be written as:

$$A = \frac{\hbar^2}{2m_0}\left\{\delta_{XX}\delta_{xx} + \sum_{\gamma}^{B}\frac{p_{X\gamma}^{x}p_{\gamma X}^{x} + p_{X\gamma}^{x}p_{\gamma X}^{x}}{m_0(E_0 - E_\gamma)}\right\} = \frac{\hbar^2}{2m_0}\left\{1 + 2\sum_{\gamma}^{B}\frac{p_{X\gamma}^{x}p_{\gamma X}^{x}}{m_0(E_0 - E_\gamma)}\right\}$$
$$= \left\{\frac{\hbar^2}{2m_0} + \frac{\hbar^2}{m_0}\sum_{\gamma}^{B}\frac{p_{X\gamma}^{x}p_{\gamma X}^{x}}{m_0(E_0 - E_\gamma)}\right\}$$

The other term B and C we can find the same way as A. We also defined as:

$$\langle X|H|Y\rangle = D_{XY} \tag{3.23}$$

Here D_{ab} has the following value:

$$D_{ab} = \sum_{\alpha\beta} D_{ab}^{\alpha\beta} k_\alpha k_\beta \tag{3.24}$$

If we write D_{ab} as matrix from we obtain same expression like the following structure:

$$D = \begin{bmatrix} D_{XX} & D_{XY} & D_{XZ} \\ D_{YX} & D_{YY} & D_{YZ} \\ D_{ZX} & D_{ZY} & D_{ZZ} \end{bmatrix} \tag{3.25}$$

The explicitly of equation (3.24) the following expression are obtained if we write the as a summation:

$$D_{XX} = \sum_{\alpha\beta} D_{XX}^{\alpha\beta} k_\alpha k_\beta = D_{XX}^{xx} k_x^2 + 2\, D_{XX}^{xy} k_x k_y + D_{XX}^{yy} k_y^2 + 2D_{XX}^{xz} k_x k_z + D_{XX}^{zz} k_z^2$$

$$+ 2D_{XX}^{yz} k_y k_z = D_{XX}^{xx} k_x^2 + D_{XX}^{yy} k_y^2 + D_{XX}^{zz} k_z^2 = Ak_x^2 + B\left(k_y^2 + k_z^2\right)$$

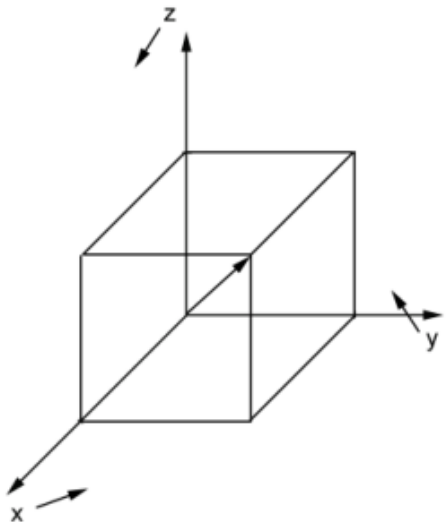


Figure 3.1. Symmetry group

Figure 3.1.: T_d^2Symmetry group has main symmetry axis, which is a diagonal of cube, and rotation of coordinate system around this axis for each 120° degree causes the axis to convert as such: x→y, y→z, z→x.

$$D_{YY} = D_{YY}^{xx} k_x^2 + D_{YY}^{yy} k_y^2 + + D_{YY}^{zz} k_z^2 + == Ak_y^2 + B(k_x^2 + k_z^2)$$

$$D_{ZZ} = D_{ZZ}^{xx} k_x^2 + D_{ZZ}^{yy} k_y^2 + + D_{ZZ}^{zz} k_z^2 + = Ak_z^2 + B\left(k_x^2 + k_y^2\right)$$

$$D_{XY} = \sum_{\alpha\beta} D_{XY}^{\alpha\beta} k_\alpha k_\beta$$

$$= D_{XY}^{xx} k_x^2 + D_{XY}^{xy} k_x k_y + D_{YX}^{yx} k_y k_x + D_{XY}^{yy} k_y^2 + 2D_{XY}^{xz} k_x k_z + D_{XY}^{zz} k_z^2$$

$$+ 2D_{XY}^{yz} k_y k_z = D_{XY}^{xy} k_x k_y + D_{XY}^{xz} k_y k_x = Ck_x k_y$$

$$D_{XZ} = D_{XZ}^{xy} k_x k_z + D_{XY}^{xz} k_z k_x = Ck_x k_z$$

$$D_{YZ} = D_{YZ}^{xy} k_y k_z + D_{YZ}^{xz} k_z k_y = Ck_y$$

The property of the figure 3.1 allows us by $T_d$group symmetry are be used.

$$D_{Xx}^{xx} = D_{YY}^{yy} = D_{ZZ}^{zz}$$

$$D_{XX}^{yy} = D_{XX}^{zz} = D_{YY}^{xx} = D_{YY}^{zz} = D_{ZZ}^{xx} = D_{ZZ}^{yy}$$

$$D_{XY}^{xy} = D_{YX}^{yx} = D_{XZ}^{xz} = D_{ZX}^{zx} = D_{YZ}^{yz} = D_{ZY}^{zy}$$

$$D_{YX}^{yx} = D_{XY}^{xy} = D_{XZ}^{zx} = D_{ZX}^{xz} = D_{YZ}^{zy} = D_{ZY}^{yz}$$

According these expressions to figure 3.1 if we exchange the axis with each other the result will not change the form. Matrix element with different power and lower indices are given below

$$D_{YX}^{zx} = D_{XX}^{zx} = D_{ZZ}^{xy} = 0$$

This form [10] (p.74) for example: The matrix element of $p_{XZ}^{y} = \langle X|p_y|Y\rangle$ has two parts, the first part which has this form $\langle X|p_y$ has odd parity with respect x and y therefore it is not contribute our matrix element. The second part which contributes our matrix element is the function with odd parity with respect x or y but not both. Also, the function $|Z\rangle$ has odd parity with respect all axis (x, y, and z) so the matrix element of the form p_{XZ}^{y} is vanish. ($p_{XZ}^{y} = 0$)

The explicitly form of matrix Hamiltonian in $|X\rangle, |Y\rangle, |Z\rangle$ basis is the following

$$D = \begin{bmatrix} Ak_x^2 + B(k_y^2 + k_z^2) & Ck_xk_y & Ck_xk_z \\ Ck_xk_y & Ak_y^2 + B(k_y^2 + k_z^2) & Ck_yk_z \\ Ck_xk_z & Ck_yk_z & Ak_z^2 + B(k_y^2 + k_z^2) \end{bmatrix} \begin{bmatrix} |X\rangle \\ |Y\rangle \\ |Z\rangle \end{bmatrix} \tag{3.26}$$

3.3. **Matrix In $u_{no}(\vec{r})$ Basis**

Now Hamiltonian in the basis u_{jo} in equation (3.7) are necessary to be written. This Hamiltonians are combination of matrix element $|X\rangle\ |Y\rangle\ |Z\rangle$ basis equation (3.26). In this section the following new notation for matrix elements is introduce.

$$P_k = \frac{\hbar^2}{2m_0}\gamma_1\left(k_x^2 + k_y^2 + k_z^2\right) \tag{3.27}$$

$$Q_k = \frac{\hbar^2}{2m_0}\gamma_2(k_x^2 + k_y^2 + k_z^2)$$

$$R_k = \frac{\hbar^2}{2m_0}[-\sqrt{3}\gamma_2(k_x^2 - k_y^2) + i2\sqrt{3}\gamma_3 k_x k_y]$$

$$S_k = \frac{\hbar}{m_0}\gamma_3\sqrt{3}(k_x - ik_y)k_z$$

The subscript k means "kinetic", the matrix elements below are find using the result of section 3.2 in equation (3.26). Hamiltonian H is given by equation (3.1). $H_{jj}^{LK} = \langle u_{10}|H|u_{10}\rangle$ With $j, j = 1, \ldots \ldots \ldots 6$. Which are indices of the base function (3.7).

$$H_{jj}^{LK} = \langle u_{10}|H|u_{10}\rangle \frac{1}{2}\langle (X - iY)\uparrow |H|(X + iY)\uparrow\rangle$$

$$\frac{1}{2}[\langle X|H|X\rangle + i\langle X|H|Y\rangle - i\langle Y|H|X\rangle + \langle Y|H|Y\rangle] = \frac{1}{2}[D_{XX} + iD_{XY} - iD_{YX} + D_{YY}]$$

$$\frac{1}{2}\left[A(k_x^2 + k_y^2) + B(k_x^2 + k_y^2 + k_z^2)\right] = -(P_x + P_y)$$

Here we apply the definitions of (3.22) -(3.24) then the explicitly of above relation is:

$$-(P_k + Q_k) = -\frac{\hbar^2}{2m_0}\gamma_1(k_x^2 + k_y^2 + k_z^2) - \frac{\hbar^2}{2m_0}\gamma_2(k_x^2 + k_y^2 + k_z^2)$$

$$\frac{1}{3}(A + 2B)(k_x^2 + k_y^2 + k_z^2) + \frac{1}{6}(A - B)(k_x^2 + k_y^2 - 2k_z^2)$$

$$\frac{2Ak_x^2 + 2Ak_y^2 + 2Ak_z^2 + 4Bk_x^2 + 4Bk_y^2 + 4Bk_z^2 + Ak_x^2 + Ak_y^2 - 2Ak_z^2 - Bk_x^2 - Bk_y^2 + 2Bk_z^2}{6}$$

$$\frac{3Ak_x^2 + 3Ak_y^2 + 3Bk_x^2 + 3Bk_y^2 + 2Bk_z^2}{6} = \frac{A(k_x^2 + k_y^2) + B(k_x^2 + k_y^2 + \frac{2}{3}k_z^2)}{2}$$

According spin relation (1.5) interaction with opposite spin the expression below will vanish:

$$H_{41}^{LK} = H_{14}^{LK} = \langle u_{10}|H|u_{40}\rangle = \frac{1}{2}\langle (X - iY)\uparrow |H|(X + iY)\downarrow\rangle = 0$$

We do other terms similar way

$$H_{12}^{LK} = \langle u_{10}|H|u_{20}\rangle = \frac{1}{\sqrt{3}}\langle (X - iY)\uparrow |H|Z\uparrow\rangle = \frac{1}{\sqrt{3}}(D_{XZ} - iD_{YZ})$$

$$-\frac{1}{\sqrt{3}}[C(k_x k_z) - iC(k_Y k_z)] = -\frac{C}{\sqrt{3}}[k_x - k_Y]k_z = S_k$$

$$H_{21}^{LK} = \langle u_{20}|H|u_{10}\rangle = \frac{1}{\sqrt{3}}\langle Z\uparrow|H|(X+iY)\uparrow\rangle = \frac{1}{\sqrt{3}}(D_{ZX} + iD_{ZY})$$

$$-\frac{1}{\sqrt{3}}[C(k_x k_z) - iC(k_Y k_z)] = -\frac{C}{\sqrt{3}}[k_x - k_Y]k_z = S_k$$

$$H_{13}^{LK} = \langle u_{10}|H|u_{30}\rangle = \frac{1}{\sqrt{12}}\langle (X+iY)\uparrow|H|(X+iY)\uparrow\rangle$$

$$= -\frac{1}{\sqrt{12}}(D_{XX} - iD_{XY} - iD_{YX} - D_{YY}) = -\frac{1}{\sqrt{12}}(A-B)\left(k_x^2 + k_y^2\right) - 2iCk_x k_Y = -R_k$$

$$H_{31}^{LK} = \langle u_{30}|H|u_{10}\rangle = \frac{1}{\sqrt{12}}\langle (X+iY)\uparrow|H|(X+iY)\uparrow\rangle$$

$$= -\frac{1}{\sqrt{12}}(D_{XX} - iD_{XY} - iD_{YX} - D_{YY}) = -\frac{1}{\sqrt{12}}(A-B)\left(k_x^2 + k_y^2\right) + 2iCk_x k_Y = -R_k^+$$

Where the "+" superscript on some result of the matrix element represent Hermitian conjugations.

Below we will summarize the full explicitly of (4×4) Luttinger Kohn Hamiltonian denoted as H^{LK}

$$H^{LK} = -\begin{bmatrix} P_k + Q_k & -S_k & R_k & 0 \\ -S_k^+ & P_k - Q_k & 0 & R_k \\ R_k^+ & 0 & P_k - Q_k & S_k \\ 0 & R_k^+ & S_k & P_k + Q_k \end{bmatrix} \tag{3.28}$$

To get above notation the relation of equation (3.27) is used.

CHAPTER FOUR: CALCULATION RESULTS OF BAND STRUCTURE

4.1 Electronic Properties of Quantum Wells

In this chapter we will calculate band structures, then the result is compared the published papers. To calculate the band structure, the multi-band effective-mass theory is used. We assume for convenience conductions band and valence band are decoupled. This approximation is helpful for wide-band-gap semiconductors such as GaAs [11]. This wide energy band gap isotropic simple parabolic is used for conduction band while 4×4 Luttinger-Kohn Hamiltonian is used for valence band. In quantum well the envelope-function approximation of the wave function of the valence band is given by:

$$\Psi_{mk_{\parallel}} = \sum_{v=1}^{4} G_m^v(k_{\parallel}, z)\, e^{ik_{\parallel}\cdot p} U^v(r) \tag{4.1}$$

In equation (4.1) G_m^vrepresent enveloped function while $U^v(r)$is cell periodic function which is a part of Block function at zone center, $k_{\parallel} = k_x\hat{x} + k_y\hat{y}$ and $p = x\hat{x} + y\hat{y}$. Here the enveloped function $G_m^v(k_{\parallel}, z)$ satisfies the multi-band effective mass equation.

$$\sum_{v}\left[H^{LK}\left(k_{\parallel} - i\frac{\partial}{\partial z}\right) + V(z)\delta_W\right] G_m^v(k_{\parallel}, z) = E_m G_m^v(k_{\parallel}, z) \tag{4.2}$$

Where V(z) is quantum well potential with extra bias field, H^{LK} is Luttinger Kohn Hamiltonian which has the following basis:

$$\left|\frac{3}{2},\frac{3}{2}\right\rangle, \qquad \left|\frac{3}{2},\frac{1}{2}\right\rangle, \qquad \left|\frac{3}{2},\frac{-1}{2}\right\rangle, \qquad \left|\frac{3}{2},\frac{-3}{2}\right\rangle$$

These bases simply are labelled v and 4×4 Luttinger Kohn Hamiltonian is shown equation (3.28). As we have seen chapter three, the matrix element in Luttinger-Kohn Hamiltonian represent as following

$$H = \|H^{LK}\| = \begin{bmatrix} P+Q & R & -S & 0 \\ R^* & P-Q & 0 & S \\ -S^* & 0 & P-Q & R \\ 0 & S^* & R^* & P_k+Q_k \end{bmatrix} \tag{4.3}$$

$$P = \frac{\hbar^2}{2m_0}\gamma_1\left(k_x^2 + k_y^2 + k_z^2\right)$$

$$Q = \frac{\hbar^2}{2m_0}\gamma_2(k_x^2 + k_y^2 + k_z^2)$$

$$R = \frac{\hbar^2}{2m_0}\left[\frac{\sqrt{3}}{2}\tilde{\gamma}\left(k_x - ik_y\right)^2 - \frac{\sqrt{3}}{4}(\gamma_3 - \gamma_2)\left(k_x + ik_y\right)^2\right]$$

Where

$$S = \frac{\hbar}{m_0}\gamma_3\sqrt{3}\left(k_x - ik_y\right)$$

Here m_0 is mass of free electron, where $\gamma_1, \gamma_2$and γ_3 are Luttinger parameters and $\tilde{\gamma} = \frac{1}{2}(\gamma_2 + \gamma_3)$. For simplicity unitary transformation of the 4×4 matrix H is used. To do this transformation we follow the methods of Broido [12], Sham [13] and also Twardoski and Herman [14]

$$\bar{H} = UHU^+ = \begin{bmatrix} H^U & 0 \\ 0 & H^L \end{bmatrix} \tag{4.4}$$

Where the H^U and H^L are represent the upper and lower blocks ang given by

$$H^\sigma = \begin{bmatrix} P \pm Q & \tilde{R} \\ \tilde{R}^* & P \mp Q \end{bmatrix} \tag{4.5}$$

Here $\tilde{R} = |R| - i|S|$

The term σ refer to the upper or lower block. Axial approximation [15] which assumed that $\gamma_2 = \gamma_3$ in R term is used for simplicity. Thus, negligent the warping of

the bulk valence band lies only in the $(k_x,\ k_y)$ plane. This method of approximation gives us very good valence sub-band energy dispersion and correct sub-band position at $k_x,\ k_y = 0$. Under unitary transformation the upper and lower block Hamiltonians H^U and H^L are decoupled and its enveloped function is denoted as following.

$$\Psi^{\mathrm{U}}_{mk_\parallel}(r) = \sum_{1,2} g^v_m(k_\parallel, z)\, e^{ik_\parallel \cdot p}|v\rangle \tag{4.6}$$

And

$$\Psi^{L}_{mk_\parallel}(r) = \sum_{2,3} g^v_m(k_\parallel, z)\, e^{ik_\parallel \cdot p}|v\rangle \tag{4.7}$$

As we mentioned beginning of this chapter $|v\rangle$ is represent the transformation basis set. After that the block envelope function g^v_m satisfy multiband effective mass.

$$\sum_{v=1,2}\left[H^{LK}\left(k_\parallel - i\frac{\partial}{\partial z}\right) + V(z)\delta_W\right] g^v_m(k_\parallel, z) = E_m(k_\parallel) g^{v'}_m(k_\parallel, z) \tag{4.8}$$

$$\sum_{v=3,4}\left[H^{LK}\left(k_\parallel - i\frac{\partial}{\partial z}\right) + V(z)\delta_W\right] g^v_m(k_\parallel, z) = E_m(k_\parallel) g^{(v+2)}_m(k_\parallel, z) \tag{4.9}$$

4.2 FİNİTE DİFFERENCE METHOD

For v = 1,2. In our k'p approach, the multiband effective- mass equations (4.8) and (4.9) are solved numerically using the finite-difference method.The finite difference method is useful for conventional variational approach [16] because it can be easily handled a quantum-well geometry or potential shape. for numerical accuracy, the size of the matrix becomes larger in finite difference method and this a possible problem of this method. To solve sub-band energies $E_m(k_\parallel)$ we have to discrete the coupled differential equation in (4.8) and (4.9). This discretizing reduced our problem to eigenvalue problem and it discretized envelope functions.

In this section we describe only upper block of Hamiltonian H using the finite difference method and lower block follows same procedure. From equations (4.5), (4.6), and (4.6) there are two coupled differential equations for $g_m^1(k_\parallel, z)$ and $g_m^2(k_\parallel, z)$:

$$\begin{bmatrix} P+Q+V(z) & \tilde{R} \\ \tilde{R}^* & P-Q+V(z) \end{bmatrix} \begin{bmatrix} g_m^1(k_\parallel, z) \\ g_m^2(k_\parallel, z) \end{bmatrix} = E_m(k_\parallel) \begin{bmatrix} g_m^1(k_\parallel, z) \\ g_m^2(k_\parallel, z) \end{bmatrix} \tag{4.10}$$

After that we eliminate the subscript m and define $\Phi^h(z)$ and $\Phi^l(z)$ by:

$$\Phi^h(z) = \mathrm{g}^1(k_\parallel, z) \text{ and } \Phi^l(z) = \mathrm{g}^2(k_\parallel, z) \tag{4.11}$$

The coupled differential equation for $\Phi^h(z)$ and $\Phi^l(z)$ can be written as:

$$\left[\frac{1}{2}(\gamma_1+\gamma_2)k_\parallel^2 - \frac{1}{2}(\gamma_1-2\gamma_2)\frac{d^2}{dz^2} + \frac{m}{\hbar^2}V(z)\right]\Phi^h(z) + \left(\frac{\sqrt{3}}{2}\bar{\gamma}k_\parallel^2 - \sqrt{3}\gamma_3 k_\parallel \frac{d}{dz}\right)\Phi^l(z) = \frac{m}{\hbar^2}E\,\Phi^h(z) \tag{4.12}$$

$$\left(\frac{\sqrt{3}}{2}\bar{\gamma}k_\parallel^2 + \sqrt{3}\gamma_3 k_\parallel \frac{d}{dz}\right)\Phi^h(z) + \left[\frac{1}{2}(\gamma_1-\gamma_2)k_\parallel^2 - \frac{1}{2}(\gamma_1+2\gamma_2)\frac{d^2}{dz^2} + \frac{m}{\hbar^2}V(z)\right]\Phi^l(z) = \frac{m}{\hbar^2}E\,\Phi^l(z) \tag{4.13}$$

It is appropriate to normalize equations (4.12) and (4.13) by defined

$$\lambda = \frac{mL^2}{\hbar^2}E, \qquad f = \frac{mL^2}{\hbar^2}V(z)$$

$$A_1 = \frac{1}{2}(\gamma_1+\gamma_2)L^2k_\parallel^2, \qquad A_2 = \frac{1}{2}(\gamma_1-2\gamma_2)$$

$$C = \frac{\sqrt{3}}{2}\bar{\gamma}L^2k_\parallel^2, \qquad D = \sqrt{3}\gamma_3 Lk_\parallel$$

$$B_1 = \frac{1}{2}(\gamma_1-\gamma_2)L^2k_\parallel^2, \qquad B_2 = \frac{1}{2}(\gamma_1+2\gamma_2)$$

Therefore, equation (4.12) and (4.13) are reduced as following:

$$\left(A_1 - A_2 + \frac{d^2}{dz^2} + f(z)\right)\Phi^h(z) + \left(C - D\frac{d}{dz}\right)\Phi^l(z) = \lambda\Phi^h(z) \tag{4.14}$$

$$\left(C + D\frac{d}{dz}\right)\Phi^h(z) + \left(B_1 - B_2 + \frac{d^2}{dz^2} + f(z)\right)\Phi^l(z) = \lambda\Phi^l(z) \tag{4.15}$$

Then the rest of procedures follow the standard finite difference method. The only remaining is to discretize $k_{\|}$, find the ecoefficiency in equations (4.14) and (4.15) and finally evaluate eigenvalue λ numerically.

To obtain eigenvalues from equations (4.8) and (4.9) we multiplied by a negative sign, then we obtain conventionally that the hole energy is negative and the top of the valence band at the center of quantum well without electric field is chosen to be zero energy level.

In our analysis, we assume that the effective mass of electron and hole in the barrier material are same as those in quantum well. There is difference between Luttinger parameters and the electron effective mass in GaAs and AlGaAs regions. Therefore, a small correction of wave function and sub-band energy levels order of few meV is required, which can be neglected as compare band-gap energy ($E_g = 1.42\ eV$ for GaAs). We use the following value for Luttinger parameters ($\gamma_1 = 6.85,\ \gamma_2 = 2.1\ and\ \gamma_3 = 2.9$). for the band-gap offset parameter $Q_C = \frac{\Delta E_c}{\Delta E_g}$, and its value $Q_C = 0.57$ is used. The potential V(z) in equation (4.8) and (4.9) is sum of quantum well potential and the external bias.

$$V(z) = V_h(z) - |e|fz \tag{4.16}$$

Here we choose at the center of quantum well as a ($z = 0$). Where $V_h(z)$and F are the confining square well potential of the valence band and applied electric field respectively.

The calculations result of valence sub-band for GaAs $Al_{0.25}$ Ga$As_{0.75}$ of quantum well which has 100Å of width are shown in the figures4.1 and 4.2. for (4.1) at $F = 0$ and (4.2) at $F = 50\ kV/cm$. At $k_{\|} = 0$, the upper block energy $E^U$and lower block energy E^L are degenerate and heavy hole and light hole are also decoupled. Therefore, it is correct to label sub-bands as “heavy hole” or “light hole” with respect the property of $k_{\|} = 0$.

For nonzero $k_{\|}$, the commixture of light-(heavy) hole functions into heavy-(light) hole states rise strong non-parabolicities in the valence band structure. Specially for light hole (LH1) has negative effective mass at the zone center. Without external electric field the upper and lower block of Hamiltonian would produce degenerate energy bands for finite $k_{\|}$, but when electric field is applied, the inversion symmetry is broken and lead to the E^U and E^L to split for a finite $k_{\|}$. This lifting of increase twice spin degeneracy which is lack of inversion symmetry and the existing of spin-orbit coupling. This results also agree new calculation by Sanders and Bajaj [17] which focusing on spin splitting of a valence band with an electric field using different methods.

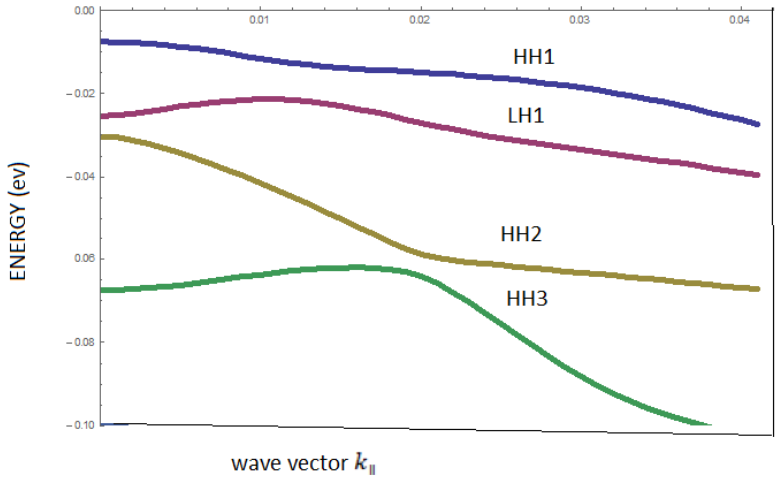


Figure 4.1 valence band for f=0

Figure 4.1. valence band structure for GaAs $Al_{0.25}$ $GaAs_{0.75}$ of quantum well which has 100Å of width without applied external electric field ($f = 0$)

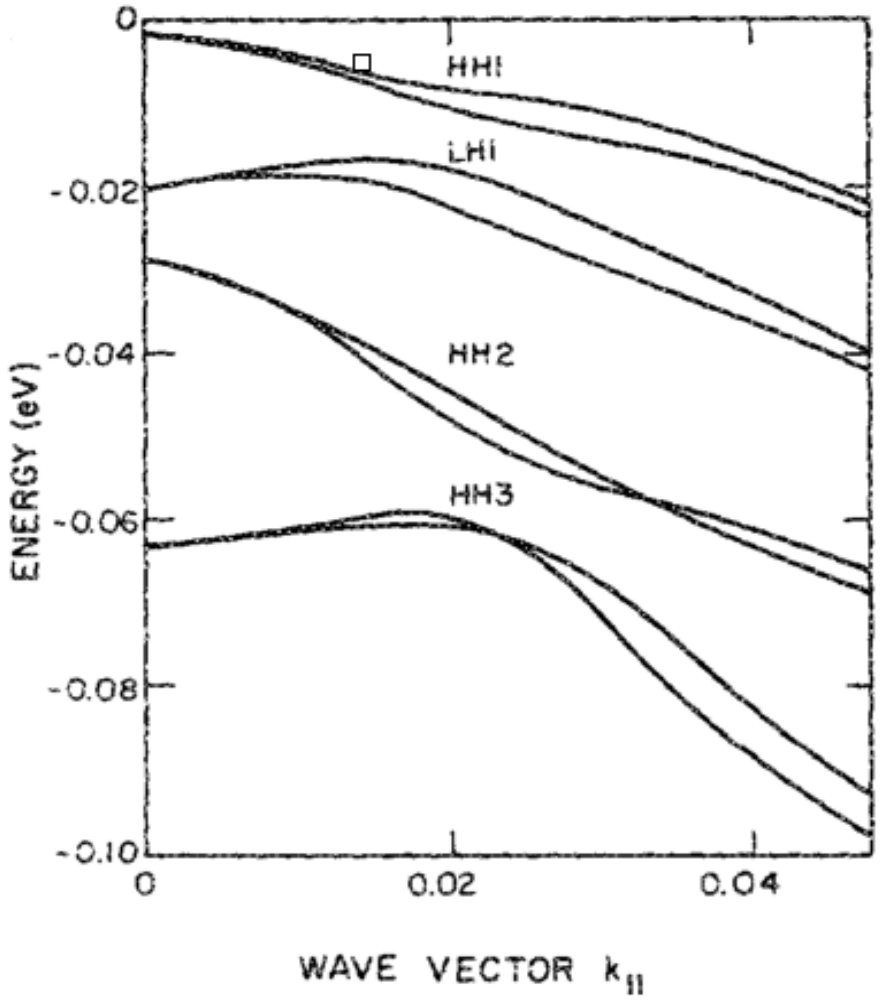
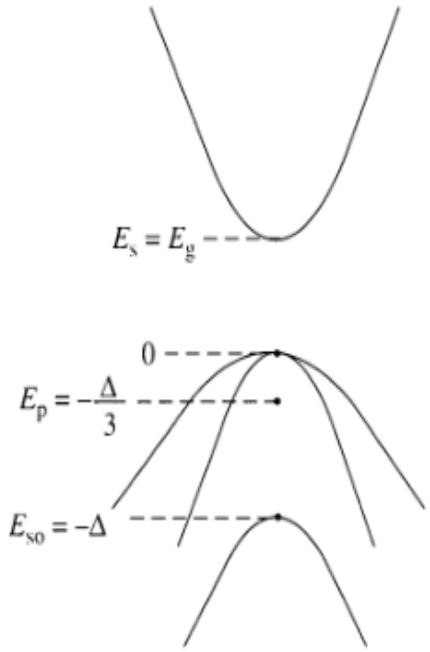


Figure 4.2. valence band structure for f=50 kV/cm

Figure 4.2 valence band structure for GaAs $Al_{0.25}$ $GaAs_{0.75}$ of quantum well which has 100Å of width with applied external electric field ($f = 50\ kV/cm$).

CHAPTER 5: CONVOLUTIONS

We conclude the goals that we have achieved during the preparation of this thesis paper: After long calculation and proves we construct 4×4 matrix element of Kane's model Hamiltonian. This model generalized k.p method which only consider; a conduction, a heavy hole, a light hole and a spin-orbit split-off bands and each band has double degeneracy. This model provides every important basis function which all other band structure models are used.



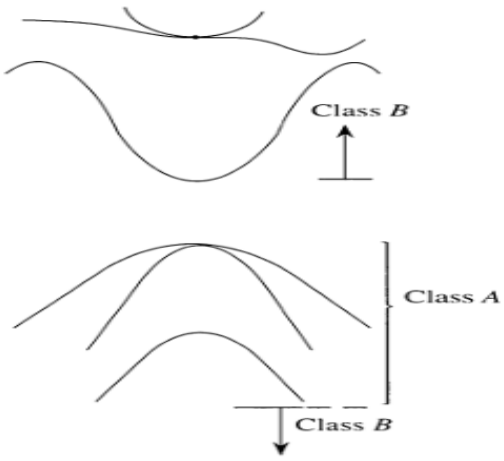
$$E_C(\vec{k}) = E_g + \frac{\hbar^2 k^2}{2m_0} + \frac{k^2 P^2\left(E_g + \frac{2}{3}\nabla\right)}{E_g\left(E_g + \nabla\right)}$$

$$E_{hh}(\vec{k}) = \frac{\hbar^2 k^2}{2m_0}$$

$$E_{lh}(\vec{k}) = \frac{\hbar^2 k^2}{2m_0} - \frac{2k^2 P^2}{3E_g}$$

$$E_{so}(\vec{k}) = -\nabla + \frac{\hbar^2 k^2}{2m_0} - \frac{k^2 P^2}{3\left(\nabla + E_g\right)}$$

Kane's model gives us incorrect effective mass for heavy bands. To obtain correct effective mass for the heavy hole bands LKM is used. This model use Kane's basis function then it dived bands into two categories: first bands which is our main interest is named class A and other bands which are influence class A is denoted class B. this model treated class B as first order of perturbed while class A is unperturbed part.



Since we are dealing wide-band-gap semiconductors such as GaAs, the multi-band effective-mass theory is used. This method assumed the conductions band and valence band are decoupled. It used isotropic simple parabolic for conduction band while 4× 4 Luttinger-Kohn Hamiltonian is used for valence band. Finally multi-band effective mass equations are solved numerically using finite difference method. The finite difference method is useful for conventional variational approach because it can be easily handled a quantum-well geometry or potential shape. discretized envelope functions. Solving sub-band energies $E_m(k_{\|})$ discretized the coupled differential equation of multi band effective-mass. This discretizing reduced our problem to Eigenvalue problem and it discretized envelope functions.

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