



# Comparing the Luttinger–Kohn–Pikus–Bir and the Empiric K·P Hamiltonians in quantum dot intermediate band solar cells manufactured in zincblende semiconductors

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## ABSTRACT

The calculation of the energy spectrum and absorption coefficients of quantum dot nanostructured intermediate band solar cells using the Empiric K·P Hamiltonian method and its agreement with experimental data are summarized. The well established Luttinger Kohn Hamiltonian modified by Pikus and Bir for strained material, such as quantum dot arrays, is presented using a simplified strain field that allows for square band offsets. The energy spectrum and absorption coefficients are calculated with this new Hamiltonian. With the approximations made the energy spectrum results to be exactly the same but the absorption coefficient fits experiments less accurately. The computer time using the latter Hamiltonian is much longer than the former one.

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## 1. Introduction

The intermediate band (IB) solar cells (SC) [1] include a band or set of levels situated in the bandgap of an ordinary semiconductor. These allow for sub-bandgap quantum efficiency using the IB as a stepping stone for electron–hole generation. IBs may be formed by the states of the conduction band electrons confined by quantum dots [2]. Much of the activity associated with this topic uses semiconductors with zincblende crystal structure.

For a sound understanding of the quantum dot (QD) IBSC operation, a model for the calculation of the light absorption mechanisms is very convenient. Simplicity of use and capacity of feedback with the device engineers is very desirable. The Empiric K·P Hamiltonian (EKPH) has been developed with this purpose [3,4].

The usual way of approaching this problem when using nanostructured zincblende materials is the use of the eight band Luttinger Kohn (LK) [5,6] Hamiltonian modified by Pikus and Bir (PB) [7,8] which accounts for the strain in the lattice. This is a variety of the K·P method introduced by Dresselhaus Kip and Kittel [9] and extensively developed by Kane [10,11] for calculations of semiconductor band structures.

However, in the used form, the EKPH method is much faster and easy to handle than the LK–PB Hamiltonian (LKPBH) method. The purpose of this paper is to compare the two methods.

Beyond this introduction, this paper is organized as follows. Section 2 summarizes the theoretical bases of the K·P methods. Section 3 describes the EKPH method leading to a 4-Band Hamiltonian matrix. Section 4 develops LKPBH in a way that makes it easily comparable with the approximations used in the EKPH method; it leads to an 8-Band Hamiltonian matrix. Section 5 evaluates the time consumed by calculations based on both methods. Finally some conclusions are drawn.

## 2. Theoretical background

K·P methods are based on developing a one-electron Hamiltonian into an orthonormal basis  $|0, \nu, \mathbf{k}\rangle = u_{0,\nu} \exp(i\mathbf{k} \cdot \mathbf{r}) / \sqrt{\Omega}$  where  $u_{0,\nu}(\mathbf{r})$  is a  $\Gamma$ -point Bloch function (GBF), which has the periodicity of the lattice,  $\nu$  is the band index,  $\mathbf{k}$  is an arbitrary wavevector of the first Brillouin zone and  $\Omega$  is the volume of calculation, which is large with respect to the nanostructure under study. The 0 index refers to the  $\Gamma$  point ( $\mathbf{k}=0$ ). In this paper, we call this basis the standard basis. For zincblende semiconductors, it is very common to use an eight band renormalized matrix where the bands are the conduction band, (cb) and three valence bands (VBs): the heavy hole (hh), the light

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hole (*lh*) and the split off (*so*) bands, each one double degenerated due to two different signs for the spin projection. This is the approach we will follow when using the LKPBH. The EKPH does not take the spin into account, and so considers only four bands.

The introduction of a nanostructure of a new material embedded in the host material induces an offset of the CB and VB edges. These usually form confining potentials for the CB and VB states. This offset is the potential to be used in the so called effective mass equations

$$-\frac{\hbar^2}{2m^*}\nabla^2\Phi + E_{v,0}(\mathbf{r})\Phi = E\Phi \quad (1)$$

where  $m^*$  is the effective mass and  $E_{v,0}(\mathbf{r})$  is the band edge variable with the position because of the band offset introduced by the nanostructure. The hole effective masses are negative and different for the different bands (*hh*, *lh*, and *so*). Due to the negative effective mass, a pedestal offset potential in the VBs has the same confining properties of a well in the CB. These equations are widely used by device physicists.

In this paper, the conduction band states are divided into two groups, those in the bandgap of the host material, which form the IB (the IB is formed of *cb* states) and those within the conduction band of the host material which are the properly-speaking conduction band (CB) states.

The utilization of the effective mass equations requires the use of the integral factorization rule, which states that [12]

$$\int_{\Omega} f(\mathbf{r})g(\mathbf{r})d^3r \cong \left( \int_{\Omega} f(\mathbf{r})d^3r \right) \left( \int_{\Omega_{cell}} g(\mathbf{r})\frac{d^3r}{\Omega_{cell}} \right) \quad (2)$$

where  $f$  is a slowly varying function with negligible variation within a crystal unit cell, and  $g$  is a function with the translational periodicity of the lattice.  $\Omega_{cell}$  is the unit cell volume. If this is fulfilled for the so-called envelope functions  $\Psi_v$  and GBFs  $u_{0,v}$  respectively, both used in the next equation, the one-electron eigenfunctions are

$$\Xi(\mathbf{r}) \cong \sum_v u_{0,v}(\mathbf{r})\Psi_v(\mathbf{r}) \quad (3)$$

For the case that at least one of the wavefunctions is confined, the photon absorption coefficient by QDs is given by [13]

$$\alpha_{\Xi \rightarrow \Xi'}^{max} = \alpha'_{\Xi \rightarrow \Xi'} E\delta(E_{line} - E) \quad \text{with} \quad \alpha'_{\Xi \rightarrow \Xi'} = \frac{2\pi^2 e^2}{n_{ref} c \hbar \epsilon_0} \frac{|\langle \Xi | \mathbf{r} \cdot \boldsymbol{\epsilon} | \Xi' \rangle|^2}{4ab} F_s N_l \quad (4)$$

where  $n_{ref}$  is the index of refraction of the material involved,  $2a$  and  $2b$  are the dimensions of the QD base,  $F_s$  is the coverage factor of each QD layer and  $N_l$  is the number of layers per unit length in the growth direction.  $E_{line}$  is the photon energy and  $\boldsymbol{\epsilon}$  is the polarization vector. The super index max means that the state in the upper level is empty of electrons and the state in the lower level is full of them. The fraction of full and empty states will be factors in the calculation of the absorptions. In some cases, an additional factor of 2 will appear if transitions between spin up states and spin down states are to be added.

If the integral factorization rule is fulfilled, the dipole element of matrix for photon induced transitions depends only on the envelopes, as follows [3]:

$$\langle \Xi | \mathbf{r} \cdot \boldsymbol{\epsilon} | \Xi' \rangle \cong \sum_v \langle \Psi_v | \mathbf{r} \cdot \boldsymbol{\epsilon} | \Psi_{v'} \rangle \quad (5)$$

It is to be stressed that this expression is only valid if, at least, one of the envelopes is bound and fades at the infinite. In this paper the wavefunctions corresponding to the initial and the final states are both bound.

### 3. The Empiric K · P Hamiltonian

Let us start with the case in which the spin is neglected (spin and strain effects will be considered later). The Hamiltonian development in the standard basis is [12]

$$\begin{aligned} \forall v = v'; \quad (H_0)_{v,v,\mathbf{k}} &\equiv \langle 0, v, \mathbf{k} | H | 0, v, \mathbf{k} \rangle = E_{v,0} + \frac{\hbar^2 k^2}{2m_0} \\ \forall v \neq v'; \quad (H_0)_{v,v',\mathbf{k}} &\equiv \langle 0, v, \mathbf{k} | H | 0, v', \mathbf{k} \rangle = \frac{\hbar \mathbf{k} \cdot \mathbf{P}_{v,v'}}{m_0} \\ P_{v,v'} &\equiv -i\hbar \langle u_{v,0} | \nabla u_{v',0} \rangle \end{aligned} \quad (6)$$

( $\equiv$  is used for the definition of a new symbol), with  $m_0$  being the electron mass in vacuo. Different values of  $\mathbf{k}$  could have been considered for the initial and final states, but these matrix elements are all zero. Therefore,  $(H_0)$  is a four dimensional matrix whose terms are functions of  $\mathbf{k}$ .

Let us assume for a moment a homogeneous material with a zincblende lattice. The zincblende lattice belongs to the  $T_d$  symmetry group. The *cb* GBF is called  $|S\rangle$  and has a spherical symmetry (it is an *s* function). At  $\mathbf{k}=0$ , the three VBs are degenerate and are linear combinations of the three GBFs called  $|X\rangle$ ,  $|Y\rangle$  and  $|Z\rangle$  with the symmetry of *x*, *y* and *z* (see, e.g. [12]) respectively (they are *p*-functions). These functions fulfill the following:

$$\langle S | -i\hbar \frac{\partial}{\partial x} | X \rangle = \langle S | -i\hbar \frac{\partial}{\partial y} | Y \rangle = \langle S | -i\hbar \frac{\partial}{\partial z} | Z \rangle \equiv P_0 \quad (7)$$

The rest of the  $P_{v,v'}$  are zero.  $P_0$  is often called the Kane matrix element. This, with the knowledge of the bandgap ( $E_{cv,0}=E_g$  and  $E_{hh,0}=E_{lh,0}=E_{so,0}=0$ ), allows the matrix  $(H_0)$  to be written in full (round brackets represent a matrix). All the elements are analytical functions of  $\mathbf{k}$  and the eigenvectors and eigenvalues can also be written (using Mathematica©) as analytical functions of  $\mathbf{k}$  (see [4]). The  $\mathbf{k}$ -function eigenvalues are the so-called dispersion functions.

The analytical value of the CB eigenvalue (the dispersion function) allows for an analytical expression of the CB effective mass. By equating it with the experimental effective mass, the value of  $P_0$  can be obtained. It is given by the following expression:

$$P_0 = \sqrt{\frac{E_g}{2} m_0 \left( \frac{m_0}{m_{cb}^*} - 1 \right)} \quad (8)$$

Unfortunately, two of the three VB eigenvalue  $\mathbf{k}$ -functions (dispersion functions) are not acceptable because they present positive effective masses. The main reason for it is that the spin-orbit coupling has been neglected. The EKPH approximation is based on building a new Hamiltonian matrix ( $H_{EKPH}$ ) in which the VB eigenvalues are parabolic dispersion functions obtained from setting the experimental values of the effective masses and their position at  $\mathbf{k}=0$  ( $E_{cv,0} \equiv E_g$ ,  $E_{hh,0} = E_{lh,0} = 0$ ,  $E_{so,0} \equiv -\Delta$ ). That is,

$$\begin{aligned} E_{cb}(k) &= E_g + \frac{\hbar^2 k^2}{2m_{cb}} \\ E_{hh}(k) &= -\frac{\hbar^2 k^2}{2m_{hh}} \\ E_{lh}(k) &= -\frac{\hbar^2 k^2}{2m_{lh}} \\ E_{so}(k) &= -\Delta - \frac{\hbar^2 k^2}{2m_{so}} \end{aligned} \quad (9)$$

By their experimental origin, the Hamiltonian so formed includes a number of effects that are neglected in  $(H_0)$ . In particular, it neglects the spin-orbit coupling and the strain effects caused by the insertion of the QDs.

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