



## INCLUSION OF SPIN-ORBIT COUPLING INTO TIGHT BINDING BANDSTRUCTURE CALCULATIONS FOR BULK AND SUPERLATTICE SEMICONDUCTORS

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Recent interest in superlattice based semiconductor devices has led to the need for the ability to make accurate superlattice bandstructure calculations. The tight binding model formalism has already been applied to this problem. In this paper, a technique is presented for the inclusion of spin-orbit coupling into the tight binding formalism. The most attractive feature of the technique presented is that it does not increase the size of the basis which may already be very large for superlattices. This allows a more accurate calculation of the superlattice bandstructure at no additional cost.

Recent advances in epitaxial growth techniques such as molecular beam epitaxy (MBE) and metal organic chemical vapor deposition (MOCVD) have made fabrication of thin period semiconductor superlattices possible. A number of electronic and optical devices have been proposed using the superlattice concept. Critical to the understanding of these devices is the bandstructure of the superlattices.

The tight binding method has been widely used to model superlattice bandstructure.<sup>1-3</sup> However, the results reported in literature do not incorporate spin-orbit coupling into the bandstructure calculations. Although, since the tight binding model is a fitting scheme, one can fit the band gaps and high symmetry points to obtain general trends due to superlattice effects, several important features are lost. The most important among these is that the hole states are incorrectly represented. The hole masses, (light and heavy) and the degeneracy of the states at the Brillouin zone center can not be modeled correctly without the inclusion of spin-orbit coupling into the bandstructure calculation. These effects become important when calculating optical transitions into the hole bands.

In this paper, we discuss the inclusion of spin-orbit coupling in the tight binding bandstructure formalism. An advantage of the technique presented is that it allows the spin-orbit effect to be included without increasing the size of the basis. This is particularly significant in superlattice calculations where the basis is quite large to begin with.

The tight binding method for calculating energy band structure, as it was originally formalised by Slater and Koster in 1954, expands the energy bands into a linear combination of atomic orbitals<sup>4</sup>. The tight binding method, in its usual formulation, does not include spin-orbit interactions. For group IV or III-V semiconductors, the basis for the Eigen solution to the energy band equations is normally made up of the s state and the three p states for each atom in the unit cell. These four states are said to be of the same spin. Thus, all interactions are theorized to be between states of the same spin.

For lattice structures where there are two or more atoms per unit cell the basis will be bigger than the basis for crystals with one atom per unit cell as each atom contains s and p orbitals. Spin-orbit energies are generally not considered to couple orbitals of different atoms. Because of this, we need only look at how the spin-orbit interaction couples the orbitals of one atom. We can then apply this technique to each atom within the minimal cell.

When adding spin-orbit interactions to this band structure model, one must increase the basis to include spin up and spin down states. That is from an original basis of:

$$(s, p_x, p_y, p_z)$$

for each atom in the unit cell, we go to a basis of:

$$(s\uparrow, p_x\uparrow, p_y\uparrow, p_z\uparrow, s\downarrow, p_x\downarrow, p_y\downarrow, p_z\downarrow)$$

The tight binding Hamiltonian should only yield non-zero interactions between states of the same spin. For these, it will yield the same expressions as used in the original calculation. Thus in our matrix representation of the Hamiltonian, we will have two blocks of terms each of which is a copy of the matrix used in the smaller basis. These two blocks will go along the matrix diagonal.

To the tight binding Hamiltonian we add the spin-orbit interaction energy. Thus our total Hamiltonian becomes:

$$H = H_{tb} + H_{so}$$

The matrix elements arising from the spin-orbit component of the Hamiltonian have the potential to be between states of different spin. To calculate these terms, we write the spin orbit interaction as<sup>5</sup>:

$$H_{so} = \lambda L \cdot S$$

We can write the addition of the spin and orbital angular momentum as:

$$J^2 = (L + S)^2 = L^2 + S^2 + 2L \cdot S$$

thus

$$\begin{aligned} \langle L \cdot S \rangle &= \frac{1}{2} \langle J^2 - L^2 - S^2 \rangle \\ &= \frac{\hbar^2}{2} \{ j(j+1) - l(l+1) - s(s+1) \} \end{aligned}$$

We therefore have a way of evaluating the spin-orbit interaction energy, but it is only applicable to pure angular momentum states. States like  $p_x \uparrow$  are mixed states, that is they are made up of a combination of pure states. To determine the spin-orbit interaction energy, we must first decompose our basis into states of pure angular momentum.

The first step in such a decomposition is to define what we mean by states like  $p_x \uparrow$ . The original three p states,  $p_x$ ,  $p_y$  and  $p_z$ , are well known simple linear combinations of the three fundamental p states. That is:

$$p_x = \frac{1}{\sqrt{2}} [\phi_{11} + \phi_{1-1}]$$

$$p_y = \frac{-i}{\sqrt{2}} [\phi_{11} - \phi_{1-1}]$$

$$p_z = \phi_{10}$$

By using a natural extension of these equations, we make similar definitions for the spin up and spin down p states as exemplified in the following:

$$p_x \uparrow = \frac{1}{\sqrt{2}} [\phi_{11} + \phi_{1-1}] \uparrow$$

This formulation, however, is still in terms of mixed states. To decompose these mixed states into states of pure angular momentum, we must perform the addition of the spin and the orbital angular momentum to obtain the total angular momentum states. Applying standard Clebsch Gordan technique for the addition of angular momentum to the p electron states yields the following six equations<sup>6</sup>:

$$\Phi_{\frac{3}{2}, \frac{3}{2}} = \phi_{11} \uparrow$$

$$\Phi_{\frac{3}{2}, \frac{1}{2}} = \frac{1}{\sqrt{3}} \phi_{11} \downarrow + \frac{\sqrt{2}}{\sqrt{3}} \phi_{10} \uparrow$$

$$\Phi_{\frac{3}{2}, \frac{-1}{2}} = \frac{\sqrt{2}}{\sqrt{3}} \phi_{10} \downarrow + \frac{1}{\sqrt{3}} \phi_{1-1} \uparrow$$

$$\Phi_{\frac{3}{2}, \frac{-3}{2}} = \phi_{1-1} \downarrow$$

$$\Phi_{\frac{1}{2}, \frac{1}{2}} = \frac{-1}{\sqrt{3}} \phi_{10} \uparrow + \frac{\sqrt{2}}{\sqrt{3}} \phi_{11} \downarrow$$

$$\Phi_{\frac{1}{2}, \frac{-1}{2}} = \frac{-\sqrt{2}}{\sqrt{3}} \phi_{1-1} \uparrow + \frac{1}{\sqrt{3}} \phi_{10} \downarrow$$

These six equations must be inverted to find the states like  $\phi_{10} \uparrow$  in terms of the total angular momentum states. Once this is done, we can substitute back into the definitions for the states like  $p_x \uparrow$  to get them in terms of the total angular momentum states. This procedure results in the following six equations:

$$p_x \uparrow = \frac{1}{\sqrt{2}} \left\{ \Phi_{\frac{3}{2}, \frac{3}{2}} + \frac{1}{\sqrt{3}} \Phi_{\frac{3}{2}, \frac{1}{2}} - \frac{\sqrt{2}}{\sqrt{3}} \Phi_{\frac{1}{2}, \frac{1}{2}} \right\}$$

$$p_x \downarrow = \frac{1}{\sqrt{2}} \left\{ \frac{1}{\sqrt{3}} \Phi_{\frac{3}{2}, \frac{1}{2}} + \frac{\sqrt{2}}{\sqrt{3}} \Phi_{\frac{1}{2}, \frac{1}{2}} + \Phi_{\frac{3}{2}, \frac{-3}{2}} \right\}$$

$$p_y \uparrow = \frac{-i}{\sqrt{2}} \left\{ \Phi_{\frac{3}{2}, \frac{3}{2}} - \frac{1}{\sqrt{3}} \Phi_{\frac{3}{2}, \frac{1}{2}} + \frac{\sqrt{2}}{\sqrt{3}} \Phi_{\frac{1}{2}, \frac{1}{2}} \right\}$$

$$p_y \downarrow = \frac{-i}{\sqrt{2}} \left\{ \frac{1}{\sqrt{3}} \Phi_{\frac{3}{2}, \frac{1}{2}} + \frac{\sqrt{2}}{\sqrt{3}} \Phi_{\frac{1}{2}, \frac{1}{2}} - \Phi_{\frac{3}{2}, \frac{-3}{2}} \right\}$$

$$p_z \uparrow = \frac{\sqrt{2}}{\sqrt{3}} \Phi_{\frac{3}{2}, \frac{1}{2}} - \frac{1}{\sqrt{3}} \Phi_{\frac{1}{2}, \frac{1}{2}}$$

$$p_z \downarrow = \frac{\sqrt{2}}{\sqrt{3}} \Phi_{\frac{3}{2}, \frac{-1}{2}} + \frac{1}{\sqrt{3}} \Phi_{\frac{1}{2}, \frac{-1}{2}}$$

With these decompositions, the evaluation of terms like:

$$\langle p_x \uparrow | H_{so} | p_x \downarrow \rangle$$

becomes straight forward. Because the pure states are orthogonal, many of the terms will be zero. Evaluation of all possible terms gives non-zero results only in the following cases:

$$\langle p_x \uparrow | H_{so} | p_y \uparrow \rangle = -i\lambda$$

$$\langle p_x \uparrow | H_{so} | p_z \downarrow \rangle = \lambda$$

$$\langle p_y \uparrow | H_{so} | p_z \downarrow \rangle = -i\lambda$$

$$\langle p_x \downarrow | H_{so} | p_y \downarrow \rangle = i\lambda$$

$$\langle p_x \downarrow | H_{so} | p_z \uparrow \rangle = \lambda$$

$$\langle p_y \downarrow | H_{so} | p_z \uparrow \rangle = i\lambda$$

The matrix terms which are reflections about the diagonal of these terms, are also, of course, non zero since our Hamiltonian is Hermitian. The numerical values for the constant lambda are taken from measured atomic spin-orbit splitting. These values are corrected for the fact that the splitting will be slightly different in a crystal than in an isolated atom. Values for various elements are given by Chadi<sup>7</sup>.

One final observation must be made before the band structure can be calculated. This observation concerns the original basis. The tight binding Hamiltonian must conserve angular momentum. This fact tells us that there must be something wrong with our notion of what our original basis was. We had originally postulated that our basis contained all states of the same spin. However, straight forward inspection of the makeup of our states will show us that terms like:

$$\langle p_x \uparrow | H_{tb} | p_z \uparrow \rangle$$

must be zero. That is, all of the states which make up  $p_x \uparrow$  are orthogonal to all of the states in  $p_z \uparrow$ . In the original formulation of the tight binding Hamiltonian, however, we need to have an interaction between the  $p_x$  and the  $p_z$  states to preserve symmetry. This leads to the conclusion that although we were not aware of it, our original basis was actually:

$$(s, p_x \uparrow, p_y \uparrow, p_z \downarrow)$$

If we relabel the matrix rows and columns to reflect this and then put the spin-orbit terms in their correct places, we will notice that there are no terms outside of the two diagonal blocks which were defined by the tight binding interactions. The further observation that all of the entries in the lower block are complex conjugate to the terms in the upper block ensures that all Eigen values will be doubly degenerate. That is, we need only calculate the Eigen energies for one of the two blocks, or on a basis the size of our original one, in order to see the complete spin-orbit energy band structure.

Thus, we have a revised tight binding method which yields band structures including spin-orbit interactions. The most attractive feature of this method is that it does not increase the size of the basis over the standard tight binding formalism. The application of the technique to both bulk and superlattice tight binding bandstructure calculations is identical. The only change from a standard tight binding matrix will be an additional six terms per atom in the unit cell.

Figure 1 depicts the top of the valence band for a typical diamond structure or zincblende bulk semiconductor as calculated by the tight binding model with and without spin-orbit interactions included. When spin-orbit interactions are ignored, the top of the valence band is a triply degenerate state at the center of the Brillouin zone. Moving away from the zone center, the top two valence bands retain their degeneracy. Inclusion of the spin-orbit coupling removes much of this degeneracy. The lowest of these three bands is split off, and the upper two separate everywhere but at the gamma point. Figure 1 indicates the makeup of the bands very close to the band center. Moving away from the gamma point, these states are quickly contaminated.

When performing tight binding calculations of superlattice bandstructure, the number of atoms in the minimal cell can be large. The order of the basis vector will be four times the number of atoms in the unit cell. For superlattices composed of many mono-layers of each type of material, this could necessitate performing an Eigen value solution on matrices with up to one hundred rows and bigger. Because of this, it is very important that any attempt to include spin-orbit interactions does not increase the size of the basis. The technique presented in this paper is ideal for this purpose.

Figure two shows the calculated bandstructure, with and without spin-orbit interactions, for a  $(GaAs)_1(AlAs)_1$  superlattice. Note that the effects of spin-orbit interaction on the top of the valence band are similar in superlattices to the effects in bulk semiconductors. In a superlattice, the upper two valence bands will not be degenerate even when spin-orbit terms are neglected, that is, although their masses are similar, there already is a light and heavy hole band.

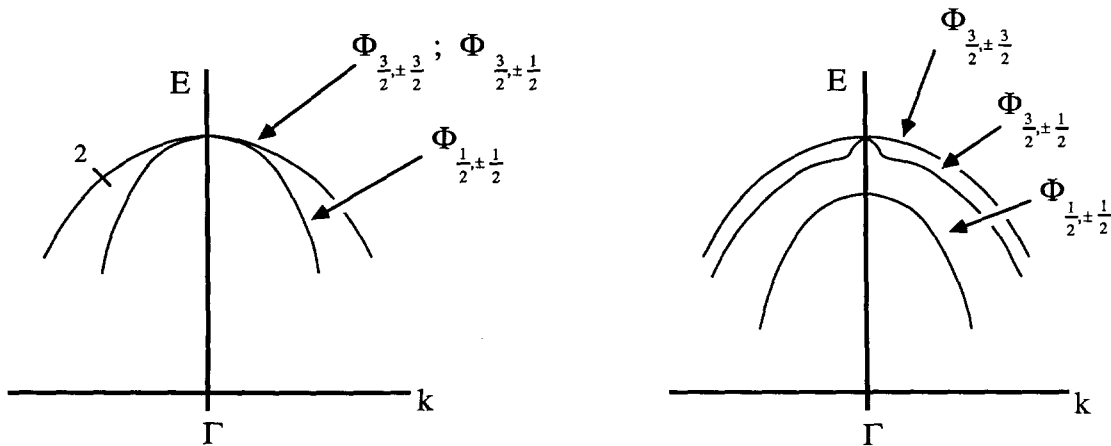


Figure 1: Typical hole bandstructures for bulk III-V semiconductors as calculated by the tight binding method with and without spin-orbit interactions. The wavefunction makeup of each of the bands is shown.

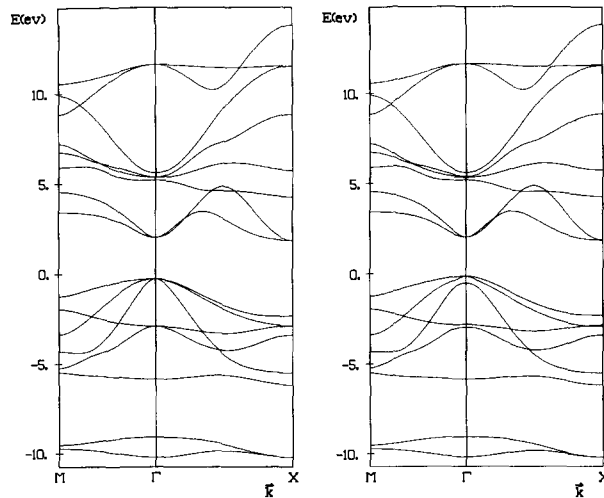


Figure 2: Energy band structure for a (GaAs)<sub>1</sub>(AlAs)<sub>1</sub> superlattice calculated by the tight binding model with and without spin-orbit interactions. "M" is the Brillouin zone edge in the (110) direction. "X" is the edge in the (100) direction. Note the loss of degeneracy at the top of the valence band.

However, as can be seen in the figures, inclusion of spin-orbit coupling increases the difference between the effective masses of the top two hole bands. Coupling also splits off the third hole band in a superlattice as it does in bulk semiconductor material. Since the tight binding model is a fitting scheme, the band gaps and effective masses can be fit to measured values with or without spin-orbit interactions included in the model. But only with the

inclusion of the spin-orbit terms can the wave functions and the degeneracies of the states at the top of the valence band be correctly modeled.

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