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Eigenstate Fitting in the k • p Method

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The $\mathbf{k}\cdot\mathbf{p}$ method [1] is widely used in computational electronics for its ability to yield accurate band structures in the region of relevance for device operation. Several models can be constructed, based on the number of bands that are explicitly treated. Thus, it is common to talk about a single band (or two-band, with spin) model when only the conduction band (CB) is of interest, a four-band model describing heavy and light holes (HH, LH), or an eight-band for equal treatment of the CB, HH, LH and split-off (SO) bands. If nonparabolicity effects farther from the zone center need to be included, or the device operates under the action of a magnetic field, it may become necessary to venture into fourteen- [2] or even sixteen-band models [3], [4]. Of course, if the parametrization of these models is appropriately obtained, the obtained value for, say, the conduction band effective mass should be independent from the model choice. Thus, we can say that these $\mathbf{k}\cdot\mathbf{p}$ models provide good fitting of the *eigenvalues* to experiment.

Then, the natural question arises to whether $\mathbf{k}\cdot\mathbf{p}$ models can also provide good fittings to experimental *eigenstates*. The correct computation of these eigenstates is of great importance for optical transitions [5] or in interband tunneling [6], whose magnitude is given by the amount of coupling and, ultimately, by the overlap between different eigenstate components. These components also play a determinant role in some aspects of spin dynamics, such as the Elliot-Yafet [7], [8] spin relaxation mechanism. By eigenstate components we mean the coefficients $c^{m,n}(\mathbf{k}) = \langle u^m_{\mathbf{k}_0} | u^n_{\mathbf{k}} \rangle$, where $u^n_{\mathbf{k}}(\mathbf{r})$ is the periodic part of the wavefunction of band n at a general $\mathbf{k}$ point in the Brillouin zone, and $u^m_{\mathbf{k}_0}(\mathbf{r})$ is the wavefunction for the preferred $\mathbf{k}_0$ about which the $\mathbf{k}\cdot\mathbf{p}$ development is made—the set of $|u^m_{\mathbf{k}_0}\rangle$ for all m form a basis.

For some cases, the answer to the question in the preceding paragraph is obviously not. Take, for example, a single band model. Far from the zone center, this model would be unaware that the true eigenstate acquires some hole component (and split-off, remote conduction band... components as well). Thus, we are interested in studying how big a model must be taken in order to ensure that the eigenstates have the correct mixing behavior.

Here we will present a systematic study with several $\mathbf{k}\cdot\mathbf{p}$ models with increasing number of bands to determine the minimum number required to obtain realistic descriptions of the eigenstate behavior close to the Brillouin zone center for zincblende semiconductors. Because of the difficulty of finding experimental values for the eigenstate components, we will fit to eigenstates computed by more atomistic methods, such as a 40-band empirical tight binding model [9] and Quasiparticle self-consistent GW (QPscGW) [10], [11] calculations.

We will also show how the eigenstate fitting procedure can remove some of the uncertainties that the determination of $\mathbf{k}\cdot\mathbf{p}$ parameters from the effective masses only has.

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