Data-driven electronic structure calculations in semiconductor nanostructures — beyond the eight-band $\mathbf{k}\cdot\mathbf{p}$ formalism

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***Abstract*—In this work, we present a scheme to extract electronic structure parameters for multi-band $\mathbf{k}\cdot\mathbf{p}$ models beyond the well-established eight-band approach using up-to-date *ab initio* band structures. Our scheme allows us to identify parameters for $\mathbf{k}\cdot\mathbf{p}$ models with Hamiltonian matrices of arbitrary complexity and level of sophistication. The computational effort of our approach is very small and increases only slightly with the number of parameters that need to be fitted. We can furthermore apply priorities to specific bands or high-symmetry points of the Brillouin zone and can incorporate routines that help to increase the numerical stability of electronic structure simulations of semiconductor nanostructures using the obtained parameter sets.**

I. Introduction

The development of novel electronic devices and light sources requires efficient techniques to model the optoelectronic properties of semiconductor nanostructures. For about two decades now, the six- and eight-band $\mathbf{k}\cdot\mathbf{p}$ formalisms represent the back bone of semiconductor device modelling and were employed to study semiconductor nanostructures of a wide range of shapes, dimensions, and material compositions [1–3]. These approaches describe the bulk electronic band structure of a material perturbatively such that it is accurate in the vicinity of a high-symmetry point within the Brillouin zone (commonly the zone centre Γ) and becomes inaccurate for wave vectors away from the selected high-symmetry point. An accurate description of the electronic properties of semiconductor nanostructures can thus be achieved only if these properties are governed by the band structure around the high-symmetry point selected for the $\mathbf{k}\cdot\mathbf{p}$ model employed. Within the eight-band $\mathbf{k}\cdot\mathbf{p}$ model, where one conduction and three valence bands with each $|\uparrow\rangle$ and $|\downarrow\rangle$ components act as basis functions, an accurate description of the band structure reproduced from the $\mathbf{k}\cdot\mathbf{p}$ model is possible only for direct gap semiconductors as additional band extrema at other high-symmetry points, such as e.g. occur in Si/Ge nanostructures, cannot be resolved. Additionally, the well-established eight-band approach becomes unsuitable in cases where additional bands add a crucial contribution to the physical phenomena to be addressed, as e.g. in GaAs crystal-phase heterostructures where two energetically close conduction bands dominate the electronic properties [4]. This problem can be overcome by taking more bands into account, which allows not only to consider these bands directly for simulations of the electronic properties of the system under consideration but also to describe more complex features of the overall band structure, such as additional extrema at different high-symmetry points.

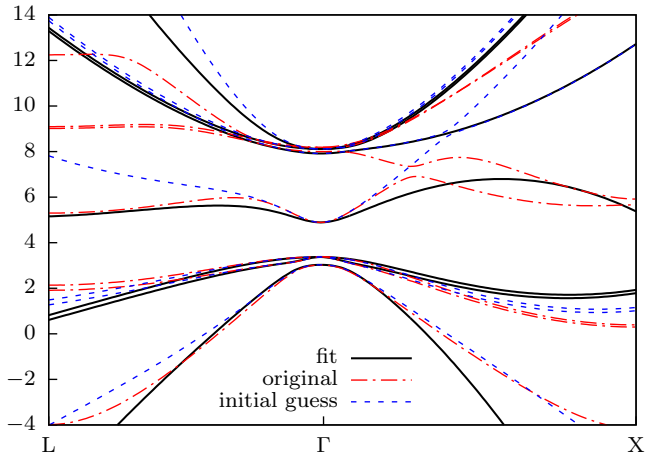

Fig. 1. Band structure of zincblende GaAs obtained from density functional theory (red dash-dotted), from literature parameters for a 14-band $\mathbf{k}\cdot\mathbf{p}$ model (dashed blue), and from parameters obtained from our fitting scheme with priority to the L valley of the bottom conduction band (solid black).

Moreover, the band structure reproduced from an eight-band $\mathbf{k}\cdot\mathbf{p}$ model differs dramatically from the actual band structure in the outer regions of the Brillouin zone. In fact, this behaviour can induce artificial, false conduction band minima

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or valence band maxima which are an origin of spurious solutions in the electronic structure [5].

Finally, while the material parameters employed within the eight-band $\mathbf{k}\cdot\mathbf{p}$ model are well known for most semiconductor materials such as e.g. GaAs or InAs, established parameter sets for more sophisticated $\mathbf{k}\cdot\mathbf{p}$ models are quite rare.

In the following, we present a parameter fitting tool for $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians of arbitrary complexity that is suited to provide material parameters based on up-to-date *ab initio* band structures, thus extending the applicability of the well-established $\mathbf{k}\cdot\mathbf{p}$ formalism to novel heterostructures as well as other crystal structures and wide temperature ranges.

II. Fitting of parameter sets for multi-band $\mathbf{k}\cdot\mathbf{p}$ models

We begin our search for electronic-structure material parameters with up-to-date *ab initio* band structures. The band structures used to fit the parameters of $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians were computed within the framework of density functional theory with the range-separated HSE hybrid functional [6]. For an accurate representation, we used an optimized screening parameter for the exact exchange [7] and included spin-orbit coupling effects. Some parameters, such as band gaps, crystal-field and spin-orbit splitting parameters can be read directly from the band structure at the centre of the Brillouin zone. Effective masses of the bands involved can be estimated from the slope at the high-symmetry points of interest but need modifications if coupling between the bands is enabled by off-diagonal elements in the corresponding $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian. As, in particular, the coupling parameters are hard to obtain directly from experiments or band structure simulations, the most direct approach is to fit the $\mathbf{k}\cdot\mathbf{p}$ band structure to an *ab initio* band structure via the parameters to be obtained. For the example of an eight-band $\mathbf{k}\cdot\mathbf{p}$ model in zincblende crystals, the parameters that cannot be read directly from the band structure are: the electron effective mass $\mathrm{m_e}$, three Luttinger parameters $\gamma_{1,2,3}$, and the optical Kane parameter, $\mathrm{E_P}$. Within a wurtzite crystal, the number of parameters required is doubled already to a total of ten and more sophisticated models require even more parameters. A gradient minimisation scheme for the fitting of multiple parameters commonly fails due to the existence of various local minima. Furthermore, realistic search intervals can be estimated for all parameters involved based on known parameters from comparable materials. What is then minimised is the difference between eigenvalues of the Hamiltonian using a certain parameter set from the search interval and the *ab initio* band structure for all $\mathbf{k}$ values. While the calculation of eigenvalues of a single matrix is a matter of milliseconds, loops over all $\mathbf{k}$ values of the band structure to be fitted ($n_\mathbf{k}$) and, in particular, over a large number of parameters can easily produce a computational effort of several years of single-processor time. The main reason for this is the discretisation of the search intervals for larger parameter sets. For a 14-band $\mathbf{k}\cdot\mathbf{p}$ model taking six more conduction bands into account, cf. Ref. [8], an equidistant discretisation in each parameter would require to solve $10^8 \times n_k$ eigenvalue problems of a 14×14 matrix. Instead we use points from an n-dimensional Sobol sequence [9,10], which is a low discrepancy point set, to overcome the curse of dimensionality in high dimensional optimisation, and to reduce the computational effort. For the above example problem, 500 Sobol points already yield a fit of similar quality solving only $500\times n_k$ eigenvalue problems. The sobol points were generated by using the MATLAB routine 'sobolset'.

Furthermore, our fitting routine allows us to apply priorities to selected bands and $\mathbf{k}$ values if specific bands or particular high-symmetry points are of pronounced importance for the electronic properties of a device. As our routine is implemented within a few, compact MATLAB scripts, other factors, such as conditions that make the occurence of spurious solutions due to erroneous band bending more unlikely [11] can also be taken into account. In this manner, our routine can also be employed to compute parameter sets for the well-established six- or eight-band $\mathbf{k}\cdot\mathbf{p}$ models that are more robust against the occurence of spurious solutions. Figure 1 shows an *ab initio* bandstructure, to which a 14-band model was fitted first with parameters from literature and then with priority to the bottom conduction band at its L valley. It can be seen that the bottom conduction band shows a reasonable agreement given the intrinsic limitations of the 14-band $\mathbf{k}\cdot\mathbf{p}$ model, whereas other bands match the *ab initio* band structure only in the vicinity of the Γ point.

We discuss the application of our fitting scheme to more sophisticated $\mathbf{k}\cdot\mathbf{p}$ models to obtain consistent parameter sets for these approaches based on most recent *ab initio* band structures.

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