Fitting parameters of atomic orbitals to reproduce optical properties of III-V systems

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The multiband $\boldsymbol{k} \cdot \boldsymbol{p}$ models in the envelope function approximation are commonly used to describe electronic and optical properties of semiconductor nanostructures [1]. However, in some applications, like the modeling of fine structure splitting [2], the precise knowledge of the wavefunction at atomic scale is needed. In consequence, it is crucial to gather some atomic-scale information on Bloch functions calculated within the $\boldsymbol{k} \cdot \boldsymbol{p}$ approach. In particular, it would be beneficial to bridge between the empirical parameters and microscopic properties of the wave functions.

In our work, we model the Bloch states around the single atoms of the crystal. We study the commonly used III-V materials of the zinc-blende structure. The zone-center Bloch states are expressed as combinations of Slater-type atomic orbitals [3], where we take into account the contributions allowed by the irreducible representation related to a given band [4]. Then, we fit the orbital-dependent coefficients and exponential decays to reproduce the optical properties of the considered materials.

The utilized theoretical framework is similar to Ref. [3]. However, we aim to fit a larger set of interband momentum matrix element parameters, which are given in the 30-band $\boldsymbol{k} \cdot \boldsymbol{p}$ Hamiltonian [5].

References

[1] *Multi-Band Effective Mass Approximations*, Vol. 94 of *Lecture Notes in Computational Science and Engineering*, edited by M. Ehrhardt and T. Koprucki (Springer International Publishing, 2014).

[2] P. T. Różański and M. Zieliński *Linear scaling approach for atomistic calculation of excitonic properties of 10-million-atom nanostructures* Phys. Rev. B 94, 045440 (2016)

[3] R. Benchamekh, F. Raouafi, J. Even, F. Ben Cheikh Larbi, P. Voisin, and J.-M. Jancu, *Microscopic electronic wave function and interactions between quasiparticles in empirical tight-binding theory*, Phys. Rev. B 91, 045118 (2015)

[4] J.-M. Jancu, R. Scholz, F. Beltram, and F. Bassani, *Empirical spds* tight-binding calculation for cubic semiconductors: General method and material parameters*, Phys. Rev. B **57**, 6493 (1998).

[5] K. Gawarecki, P. Scharoch, M. Wisniewski, J. Ziembicki, H. S. Mączko, M. Gładysiewicz, R. Kudrawiec, *Invariant expansion of the 30-band k·p model and its parameters for III-V compounds*, Phys. Rev. B 105, 045202 (2022)