Conduction Band Effective Mass Equation for a Nanostructure

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In this contribution we revisit the derivation of the effective Hamiltonian for the conduction band states of a quantum dot (QD) from the 8-band $\boldsymbol{k} \cdot \boldsymbol{p}$ model. We perform rigorous decoupling of valence bands and aim at obtaining an effective mass 2-band Hamiltonian which qualitatively reproduces the results of the well established 8-band $\boldsymbol{k} \cdot \boldsymbol{p}$ method. In order to examine the achievable accuracy of such an approach we perform numerical simulations of strained single and double QD structures.

We begin with the energy spectrum of the system. Because in many cases s-like (ground) and p-like (excited) states are of interest, we compare values of the ΔE_{s-p} distance in various effective mass approximations with 8 $\boldsymbol{k} \cdot \boldsymbol{p}$ results. We also analyze Landé factors, responsible for the spin behavior in the external magnetic field. Another problem we address is the spin-mixing induced by structure inhomogeneity. We study the mixing of two spin orientations by calculating the width of the tunnel spin-flip anticrossing in the double QD system.

Modeling of realistic nanostructures, based on numerical calculations, is an important tool of semiconductor physics. The $\boldsymbol{k} \cdot \boldsymbol{p}$ method has been very successful in modeling carrier dynamics, influence of strain, response to an external field, etc. [1]. However, multi-band models require large computational power for modeling large systems. Calculations for coupled nanostructures with different dimensionality [2] are particularly problematic, since one needs to combine a big computational box with a small mesh constant. When electronic states are under consideration, the Hamiltonian can be approximated by one- or two-band model. Although based on certain approximations, their numerical efficiency makes them highly valued. Moreover, in such models it is possible to introduce effective quantities (like the effective mass) which establishes analogy to well-know quantum-mechanical effects and makes physical problems much more transparent.

Our results show that an appropriately constructed, self-consistent effective mass equation with non-parabolicity corrections can provide quantitatively accurate description of the system spectrum, including the Zeeman splitting. On the other hand, we demonstrate the limitation of the effective mass approach when more sophisticated features are to be modeled, like the spin-flip admixture due to inhomogeneity and symmetry breaking. We believe that our findings shed some new light on the long-standing problem, in particular in the context of current problems in numerical modeling of nanostructures.

[1] P.-L. Ardelt, K. Gawarecki, K. Müller, A. A. Waeber, A. Bechtold, K. Oberhofer, J. J. Daniels, F. Klotz, M. Bichler, T. Kuhn, H. H. Krenner, P. Machnikowski, and J. J. Finley, *Phys. Rev. Lett.* **116**, 077401 (2016).

[2] A. Mielnik-Pyszczorski, K. Gawarecki, P. Machnikowski, *Phys. Rev. B* **91**, 195421 (2015).