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Band structure fitting method for constructing effective Hamiltonians involving symmetry properties

Wanderley, A. B.[1] and Sipahi, G. M.[2]
[1] [2] *São Carlos Institute of Physics - USP, C.P. 369, 13560-970, São Carlos, SP, Brazil*
adilson.wanderley@usp.br

Abstract

Effective Hamiltonians allow a realistic description of electronic band structures by offering a low computational cost compared to models using *ab initio* calculations. [1, 2] The **k·p** method has been used successfully for some decades to construct these Hamiltonians to obtain the band structure and describe the spin-splittings and effective g-factors of III-V semiconductor. [1, 2] These Hamiltonians are constructed with the support of the symmetry of the crystalline group of the material studied, however, they have dependence on some parameters that are obtained by fitting the curves of the minimization calculations with preexisting band structures. [1] The approach in our research includes methods already used in our group adding strategies that allow to obtain effective mass parameters, Luttinger and Kane parameters and optical matrix elements. [1] The strategy involved a 14-band **k·p** model for GaAs in the Zinc Blende phase (see figure 1), with inclusion of constraints among some parameters, resulting in more realistic band structures, with fittings that remained in regions far from the Γ-point and with improved computational cost.

References

[1] Carlos M. O. Bastos, Fernando P. Sabino, Guilherme M. Sipahi, and Juarez L. F. Da Silva, Journal of Applied Physics 123 (6), 065702 (2018)
[2] Oliver Marquardt, Miguel A. Caro, Thomas Koprucki, Peter Mathé and Morten Willatzen, Physical Review B 101 (23), 235147 (2020)

Figure

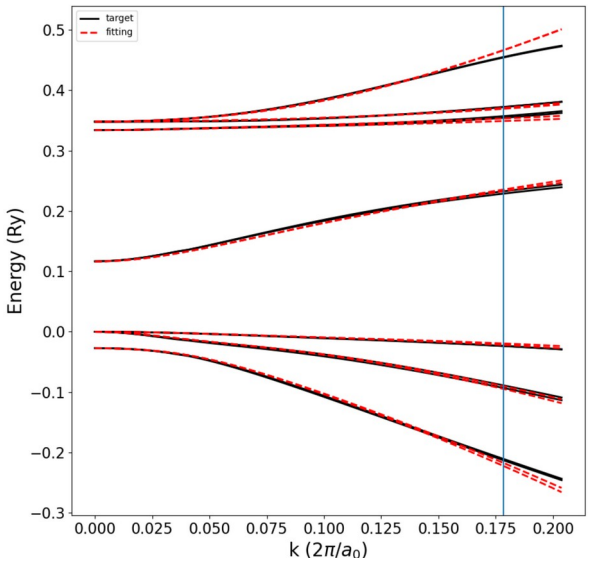

Figure 1: Band structure of GaAs evaluated with PBE functional (black filled lines) and fitted (red dashed lines). Blue vertical line represents the last calculated k-point.