Fitting method for band structures using strategies involving k·p Hamiltonians and symmetry properties

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The study of electronic band structures has enabled the development of new semiconductor electronic devices and the understanding of the magnetic properties of materials, such as Diluted Magnetic Semiconductors (DMS)[1], which in turn are associated with modern LED technologies and smaller, faster computers. Effective Hamiltonians, used in realistic calculations of band structures, offer lower computational cost compared to methods using first-principles calculations. The **k·p** method has been used for some decades in the construction of such Hamiltonians for describing spin-splittings and effective g-factor calculations by fitting curves under experimental data[2][3]. The construction of these Hamiltonians involves the symmetries of the crystal group of the material being studied and depends on parameters that are obtained by fitting the minimization calculations with pre-existing band structures. Using the **k·p** method in conjunction with Löwdin partitioning, we obtain Hamiltonians known as multiband **k·p** [3][4]. However, calculations involving parameter search with these models can still have a high computational cost when seeking a more realistic description of the effective mass and g-factor parameters[3], e.g. In this project an approach is performed that includes the methods already used in our group, with the novelty of the inclusion of strategies such as: use of energy difference and bonds guaranteed by the symmetry of the system in the minimization process, which allows the search for the effective mass parameters, Luttinger and Kane parameters and optical matrix elements, for example. These strategies lead to a more realistic description with lower computational cost. The fittings obtained were extremely good and also remained well-fitting in regions far from the Γ point in the Brillouin Zone.

References

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