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Effective kp Hamiltonians calculated from ab initio data

Abstract

In this talk we will present a new code, called QE2KP, which calculates the effective kp Hamiltonian using the ab initio wave-functions as basis functions to calculate the matrix elements of the kp theory within the Löwdin perturbation approach. The kp method is widely used to obtain effective Hamiltonians to describe a chosen set of bands of crystalline materials. The derivation of these Hamiltonians start by identifying the symmetry group of the crystal, and irreducible representations of the bands at the central k point for the perturbative expansion. Then, combining the kp method with fundamentals of group theory [1] (theory of invariants), one is able to obtain the functional form of the Hamiltonian. For instance, for graphene, and up to linear powers in k, one obtains H = $\hbar$vF σ.k, which leads to the cone Dirac. However, the kp and group theory approaches can only tell us that the coefficient $\hbar$vF is finite (selection rules), but it cannot give it a numerical value. Currently, the python packages IrRep [2] and Qsymm [3] are quite useful to help us obtain these functional forms of H. Therefore, the goal of our new code QE2KP is to take a step further and calculate the numerical values of these parameters (e.g. $\hbar$vF, Kane and Luttinger parameters). In this talk, we'll show preliminary results (see Fig. 1) of our code and describe the methodology we are using to combine the QE data with the python packages IrRep and Qsymm to fully describe both the functional form and the numerical values for the effective Hamiltonians of any crystal.

References

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