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Band crossing driven by electron phonon coupling MIRKO MOELLER, GEORGE SAWATZKY, MONA BERCIU, Univ British Columbia —
The coupling of charge carriers (electrons or holes) to phonons can lead to the formation of a polaron, a coherent quasi-particle consisting of the charge carrier and the cloud of phonons surrounding it and moving coherently with it. Polarons have been studied extensively in the Holstein model and to a lesser extent in the SSH model, both of which are single band models. However, for many of the materials in which polarons are the low-energy excitations a description with multi-band models is more appropriate. Here we present results obtained with the highly accurate momentum average approximation for the single polaron properties of a two dimensional, three-band model. The model is inspired by the perovskite $BaBiO_3$ and the coupling to phonons modifies the hopping integrals. We find that the electron phonon coupling changes the ground state momentum from $\mathbf{k} = (\pi, \pi)$ to $\mathbf{k} = (\pi, \mathbf{0})$. Furthermore it can lead to the formation of a tilted band crossing point (BCP) and/or shift the location of existing BCPs in the Brillouin zone. These findings are of interest in the light of Dirac or Weyl materials in which BCPs play an important role.

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