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Novel, discontinuous polaron transition in a two-band model[1]
MIRKO M. MOELLER, GEORGE A. SAWATZKY, MONA BERCIU, Univ British Columbia — The coupling of charge carriers (electrons or holes) to phonons leads 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. Here we present exact diagonalization and momentum average approximation results for the single polaron properties of a two-band model with phonon modulated hopping, inspired by the perovskite $BaBiO_3$. For large coupling we find that the ground state momentum changes *discontinuously* from $k = \pi$ to $k = 0$. Such sharp transitions of the polaron's ground state properties cannot occur in the well-studied models of the Holstein or Fröhlich type in which the carrier-phonon coupling modulates the on-site energies. However, they can occur in models where the carrier-phonon coupling modulates the hopping integrals such as the SSH model for which a similar yet smooth transition of the ground state momentum was recently shown to exist. We compare our findings to the SSH model and point out qualitative differences which we believe to be due to the two band nature of our model versus the single band SSH model.

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