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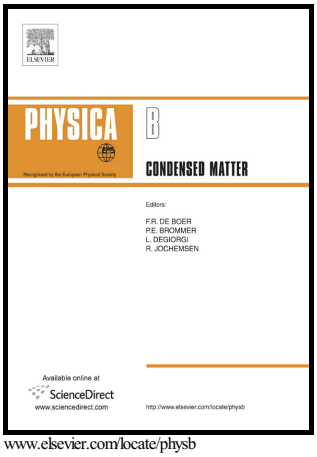

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Band warping, band non-parabolicity, and Dirac points in electronic and lattice structures

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Abstract

We illustrate at a fundamental level the physical and mathematical origins of band warping and band non-parabolicity in electronic and vibrational structures. We point out a robust presence of pairs of topologically induced Dirac points in a primitive-rectangular lattice using a *p*-type tight-binding approximation. We analyze two-dimensional primitive-rectangular and square Bravais lattices with implications that are expected to generalize to more complex structures. Band warping is shown to arise at the onset of a singular transition to a crystal lattice with a larger symmetry group, which allows the possibility of irreducible representations of higher dimensions, hence band degeneracy, at special symmetry points in reciprocal space. Band warping is incompatible with a multi-dimensional Taylor series expansion, whereas band non-parabolicities are associated with multi-dimensional Taylor series expansions to all orders. Still band non-parabolicities may merge into band warping at the onset of a larger symmetry group. Remarkably, while still maintaining a clear connection with that merging, band non-parabolicities may produce pairs of conical intersections at relatively low-symmetry points. Apparently, such conical intersections are robustly maintained by global topology requirements, rather than any local symmetry protection. For two *p*-type tight-binding bands, we find such pairs of conical intersections drifting along the edges of restricted Brillouin zones of primitive-rectangular Bravais lattices as lattice constants vary relatively to each other, until these conical intersections merge into degenerate warped bands at high-symmetry points at the onset of a square lattice. The conical intersections that we found appear to have similar topological characteristics as Dirac points extensively studied in graphene and other topological insulators, even though our conical intersections have none of the symmetry complexity and protection afforded by the latter more complex structures.

Keywords: Band Warping, Non-parabolicity, Dirac Points, Electronic Band Structure, Tight Binding, Nearly Free Electron Model

1. Introduction

In this paper we analyze the physical and mathematical origin of band warping using two fundamental and complementary approaches to calculate electronic band structures, namely, the tight-binding (TB) method and the nearly-free-electron (NFE) model. More generally, we demonstrate that for the majority of non-degenerate bands one should not expect band warping at energy extrema, irrespective of whether band non-parabolicity may or may not be prominent. Band non-parabolicity should not be confused with band warping. Band non-parabolicity derives from terms of order higher than quadratic in a multi-dimensional Taylor series expansion. By contrast, in the case of band warping, there is no possibility of performing a multi-dimensional Taylor series approximation at the quadratic order already. Now, band non-parabolicity becomes more and more evident when greater and greater coefficients of higher-order terms develop in its Taylor series expansion, possibly as a result of stronger and stronger interactions with other bands approaching in energy the non-parabolic band. Nevertheless, insofar as a non-parabolic band remains non-degenerate

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