Calculation of complex band structure for low symmetry lattices[1]

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— Complex band structure calculation is an integral part of a first-principles plane-wave based quantum transport method. [1] The direction of decay for the complex wave vectors is also the transport direction. The existing algorithm [1] has the limitation that it only allows the transport direction along a lattice vector perpendicular to the basal plane formed by two other lattice vectors, e.g., the c-axis of a tetragonal lattice. We generalize this algorithm to nonorthogonal lattices with transport direction not aligned with any lattice vector. We show that this generalization leads to changes in the boundary conditions and the Schrodinger's equation projected to the transport direction. We present, as an example, the calculation of the complex band structure of fcc Cu along a direction perpendicular to the (111) basal plane. [1] Hyoung Joon Choi and Jisoon Ihm, Phys. Rev. B 59, 2267 (1999).

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