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Surface States and Transport in Bismuth Nanowires with Strong Magnetic Field[1] SHIANG FANG, BERTRAND HALPERIN, EFTHIMIOS KAXIRAS, Department of Physics, Harvard University — Bismuth nanowires have attracted attention due to the enhancement of thermoelectricity in the one-dimensional geometry. Because of the large surface-bulk ratio and gapped bulk-like states, the transport in Bismuth nanowires is dominated by surface states, which may be probed by measurement in magnetic field ∼14T. However, due to the spiral motion of electrons between various nanowire facets, the electron would bounce between multiple wire surface with different crystal orientations. Shubnikov-de Haas oscillations in magneto-resistance in transport encode the convoluted information for different surface states. To study these effects and the mechanism for transport in strong magnetic field, we employ a density functional theory calculation for the band structure. Maximally-Localized Wannier Functions are used to construct an empirical tight-binding model, which provides numerically accurate results at reduced computational cost. In this way, the surface states in a semi-infinite geometry can be obtained from the efficient iteration of Greens functions. The formation of Landau levels can also be studied by Peierls substitution.

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