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Electronic and Transport Properties of Carbon Nanotube Bundles

We present a theoretical approach to study the electronic structure of commensurate and incommensurate single-walled carbon nanotube (CNT) bundles. Basing on the technique for general two-dimensional incommensurate bilayer system, we calculate the electronic band structure of array of general CNTs with arbitrary chirality. We find that the band structures are significantly deformed by the long-range moiré interference patterns at the interface. We also demonstrate how one electron should hop from one tube to another by using the selection rule and the inter-tube hopping probability.

A CNT bundle is an array of parallel nanotubes, and it is one of the most commonly observed forms of CNT[1, 2]. It is composed of CNTs with similar diameters, while the adjacent CNTs have generally different lattice structures so that we have the lattice mismatch on the interface between CNTs. In the literature, the electronic band structures of CNT bundles were calculated mostly for commensurate bundles composed of armchair or zigzag tubes, and also several cases with relatively small unit cells [3, 4], while the general incommensurate bundles with greater diameters were not well studied. Recently, the effective continuum approach was developed for incommensurate two-dimensional superstructure such as twisted bilayer graphene[5, 6, 7], graphene-hBN bilayer [8, 9, 10], and also double-walled nanotube [11]. In this work, we further extend this effective continuum model to general CNT-bundles.

To describe the electronic interaction between adjacent CNTs, we map the two CNTs to a bilayer graphene(BLG) by unrolling them into flat planes. In this way, a commensurate tube is unrolled into non-rotated BLG with an in-plane translation, while incommensurate one is unrolled into a twisted bilayer graphene with an in-plane rotation. Here the coupling between two layers on the mapped BLG should be spatially modulated in an appropriate manner, because the interaction in the original tubes only works near the interface line at which the two cylinders are touching. We adapt the effective continuum Dirac model to describe the intra-tube Hamiltonian of each single CNT, and include the moiré interface coupling as the inter-tube matrix elements. As a result, we obtain a set of selection rules for the wave-number matching in the inter-tube coupling, which turns out to be only rigorous in axial direction of CNT, while loose along circumference.

For commensurate bundles composed metallic CNTs, we find that inter-tube coupling generally opens a gap of a few 10meV at the Fermi energy. On the other hand, the band structures of incommensurate bundles are uniquely deformed according to the additional long-range periodicity of moiré patterns. Some strong coupling cases are found in several cases including chiral CNTs (36, 1)&(36, 1) [fig 1] and (23, 20)&(20, 23), where inter-tube interaction open gaps ~20 meV. These cases are chosen by the condition that the axial component of the inter-tube matrix element exactly couples K-points of the two tubes. We also applied the analysis to the tightly-packed CNT bundles [12], where we found that the inter-tube band modulation is significantly enhanced due to the increased interface area.

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Figures

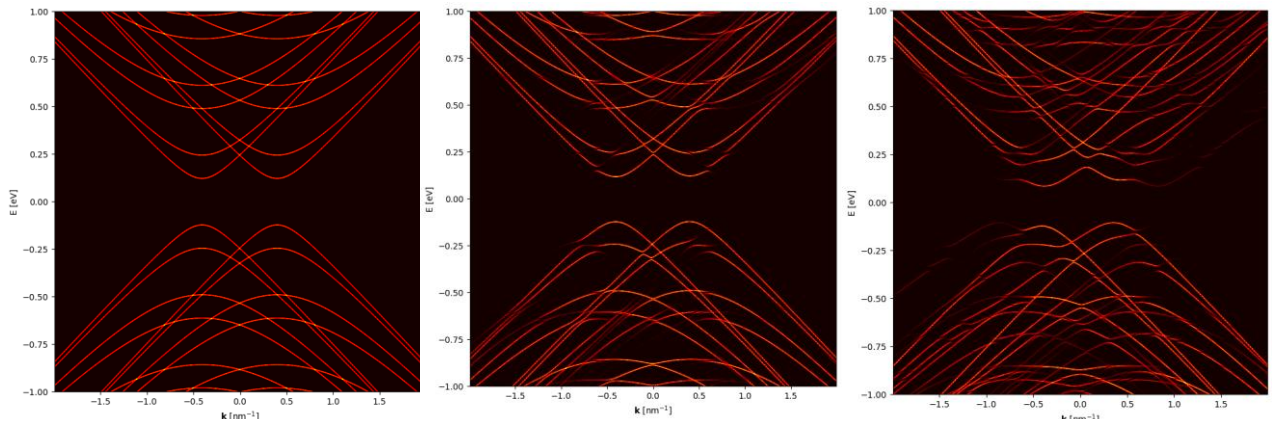

Figure 1: The band structure of (left) single (36, 1) SWNT, (middle) two neighboring (36, 1) SWNTs and (right) two neighboring deformed (36, 1) SWNT.