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Effective-mass theory of flattened carbon nanotubes as bilayer graphene with closed edges[1] TAKESHI NAKANISHI, Natl Inst of Adv Indust Sci & Tech, TSUNEYA ANDO, Tokyo Inst. Tech. — We theoretically study effects of inter-wall interaction in collapsed carbon nanotubes, first directly calculating effective inter-wall interaction within an effective-mass scheme and second regarding collapsed tubes as ribbons of bilayer graphene with closed edges described by boundary conditions explicitly derived. Within the effective-mass scheme, effects of inter-wall interactions are shown to be important in non-chiral nanotubes such as zigzag and armchair. In fact, with the increase in the width of the flattened region, the band structure approaches that of a bilayer ribbon in which the electron motion in the ribbon-width direction is discritized. In chiral nanotubes, inter-wall interaction can essentially be neglected except in the vicinity of non-chiral tubes. Inter-wall interactions diminish rapidly when chiral angle deviates from zigzag or armchair, although the decay is slower in the vicinity of the armchair tube. When the flattened region has the structure of AA and AB stacked bilayer graphene, the same results can be derived by calculating boundary conditions corresponding to the closed-edge structure in which the top and bottom layers are smoothly connected through a monolayer graphene.

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