

This paper provides a theory of discrete energy levels in finite-length single-wall carbon nanotubes for the carbon nanotube quantum dots.

Most of studies are based on the band theory, which assumes length of nanotubes infinite. But in fact, the nanotubes have finite lengths and then the energy levels are discretized [Fig. (a)]. Observed spectra have exhibited not only degenerate levels expected in the conventional picture, in which two valleys in the energy bands are decoupled, but also unexpected large lift of degeneracy. Providing a theory beyond the conventional picture is, therefore, important.

In this paper, it is shown that valley coupling is unavoidable in the sense of symmetry because two valleys have the same angular momentum in majority (more than 80%) of nanotubes [Fig. (b)]. To provide a microscopic theory including intrinsic valley coupling, a 1D model is derived [Fig. (c)] and a variety of formations of eigenstates are analytically shown. Furthermore, a bulk-edge correspondence, which shows new property of nanotubes as topological insulators, is exactly proven [Fig. (d)], as a byproduct of the theory.

