Zero-energy Boundary States and an Induced Localized Magnetic Moment at Edges of Carbon Nanotubes

Shinsei Ryu and Yasuhiro Hatsugai

Department of Applied Physics, University of Tokyo, 7-3-1 Hongo Bunkyo-ku, Tokyo 113-8656, Japan

When a two-dimensional graphite sheet is truncated with a certain type of edges, boundary states localized near the edges are known to appear. [1] The appearance of such states is also known for other systems like $d_{x^2-y^2}$-wave superconductors, and is a reflection of the rich electronic (quasi particle) band structure. Their origin can be understood by geometrical and topological arguments in a unified manner. [2]

A natural question is then what physical consequences they lead in the presence of electron-electron or electron-phonon interactions. As the boundary states form a flat band (Fig. 1), giving rise to a sharp peak in density of states at the fermi energy, they might trigger an magnetic instability, or a distortion of the lattice. We investigate electron correlation effects on the boundary states for a wrapped quasi one-dimensional geometry, i.e., carbon nanotubes (CNTs) with edges. We consider (N, $-N$) CNTs with zigzag and bearded edges, for which boundary states appear at the fermi level for some values of the wave number along the edges. (Fig. 1) We focus on (i) whether the localized charge and spin degree of freedom carried by the edge modes can escape through the coupling between the bulk conduction electrons. This can be thought as a variant of the problem of quantum dissipation, examples of which include the Caldeira-Legget model, the X-ray edge problem, the Kondo effect, etc. We are also interested in (ii) whether the total spin at the boundary is polarized. If the answer is positive, we have a chance to see a new magnetic material made of exclusively light elements, without *d*- or *f*- electrons. [4]

Starting from lattice models with the Coulomb or the Hubbard interaction, we first establish low-energy effective theories that describe correlation effects at boundaries. We then focus on a thin metallic CNT, where one ($N=6$) or two ($N=9$) boundary states interact with the collective bulk excitations. By the renormalization group (RG) analyses combined with the open boundary bosonization, we show that (i') the repulsive bulk interactions suppress the charge fluctuations at boundaries. In the infra-red limit in RG analyses, Kondo-like couplings between conduction electrons and boundary states are vanishing, and the bulk conduction electrons and boundary states are completely decoupled. Doubly occupying a boundary state becomes unfavorable in the infra-red near half filling since the strong repulsive bulk interactions renormalizes the interactions at the edge.

Furthermore, (ii') the couplings between bulk and boundary states turn out to assist the spin polarization. Ferromagnetic couplings between the boundary states are enhanced by the interactions between conduction electrons and the boundary states, which leads to the ground state at the boundary with a highest spin $S=1/2$ for the case of one boundary state, and $S=1$ for two boundary states. Then, the boundary states, as a whole, behave as a localized moment which gives rise to a Curie-Weiss-like contribution to the magnetic susceptibility, apart from the bulk conduction electrons. The result obtained here is consistent with spin polarization found in a density matrix renormalization group study for a thin semi-conducting CNT [5], and the mean-field theory [1] or an *ab initio* local spin density functional calculation (LSDA) [6] for a two-dimensional sheet geometry.

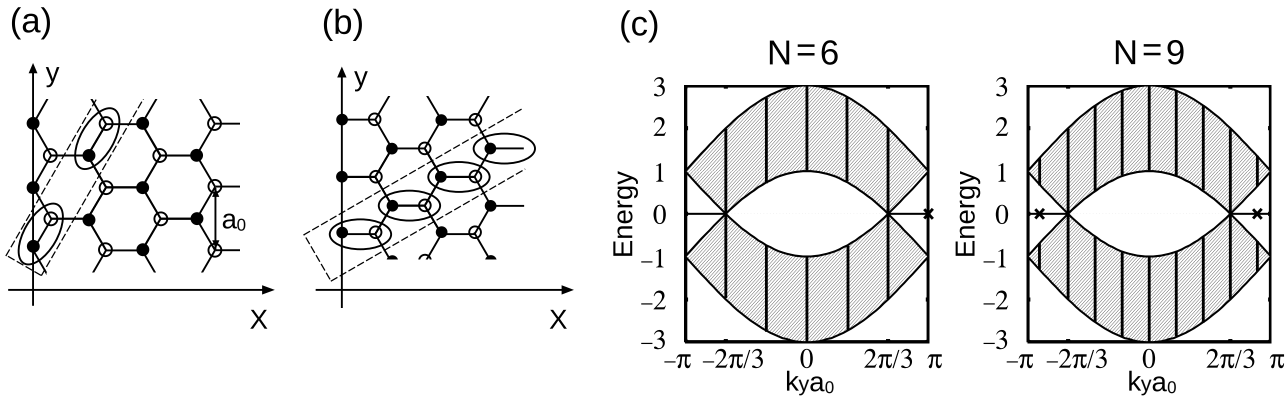

Figure 1: A (N,-N) CNT with (a) zigzag and (b) bearded edges. Two-dimensional graphite sheets are wrapped around the x-axis. Dotted squares show a choice of unit cell for each types of edges. (c) Energy spectra for a (N,-N) CNT with zigzag edges for N=6, 9. (t=1) Shaded regions represent bulk energy spectra for $N \to \infty$. Allowed wave numbers along the boundaries for N=6, 9 are shown by vertical lines. Boundary states are denoted by $\times$.

We also include discussions on coupling between lattice distortions [7], in terms of a Jahn-Teller like argument. It is based on the above topological argument and the special symmetry, so-called chiral symmetry, which ''protects'' the existence of the zero-energy edge states. The same line of the discussion was applied to the induced coexistence of time-reversal symmetry breaking order parameters near the edges of $d_{x^2-y^2}$-wave superconductors. [2]

References

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