

## Dimer-covering RVB treatment of single-walled zigzag carbon nanotubes

M.A. Garcia-Bach

Departament de Física Fonamental, Facultat de Física  
and Institut de Química Teòrica i computacional,  
Universitat de Barcelona,  
Diagonal 647, 08028-Barcelona, Catalonia, Spain.  
[m.angels.garcia\\_bach@ub.edu](mailto:m.angels.garcia_bach@ub.edu)

Single-walled zigzag carbon nanotubes (CNTs) with  $h$  hexagons around the carbon nanotube,  $h$  ranging from 3 to 19, have been investigated from a resonating-valence-bond point of view. These values of  $h$  include realistic CNTs with diameters ranging from 0.5 to 1.5 nm, which correspond to  $h \sim 6$  and  $h \sim 19$ , respectively.

Long-range spin-pairing order (LRSP) [1,2,3] allows to separate the set of VB configurations in  $h+1$  different subsets or phases. The parameter associated with the LRSP,  $p$ , can take the relevant values  $p = 0, 1, \dots, h$ .

We have obtained the Heisenberg energy, in units of  $J$  per carbon atom,  $\mathcal{E}_p(h)$ , and also per polyene ring for zigzag single-walled CNTs with  $h = 3, 4, \dots, 19$  and  $p = 0, 1, 2, \dots, h$ , within a dimer-covering counting approximation [4,5,6]. First, the ground-state energy per carbon atom is obtained when the phase, which we design as  $p_0$ , is the integer closest to  $h/3$ . See, for instance, Figure 1.

From the difference in energy per polyene ring,  $\Delta(h)$ , in units of  $J$ , between the two lowest-lying phases,  $p_0$  and  $p_1$  it is noted that degeneracy between the two lowest-lying phases occurs when  $(h+1)/3$  is an integer. Therefore, de-confined low-energy topological spin defects would occur, and these carbon nanotubes should be conductors, in analogy to polyacetylene. See, for instance, Figure 2, where  $\Delta(h)$  is represented as a function of  $h$  for  $h = 3n-1, 3n, 3n+1$ . In clear contrast, no such degeneracy is observed for either,  $h = 3n+1$  or  $h = 3n$ , so bound pairs of topological spin defects are expected to occur in these cases.

### References:

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### Figures:

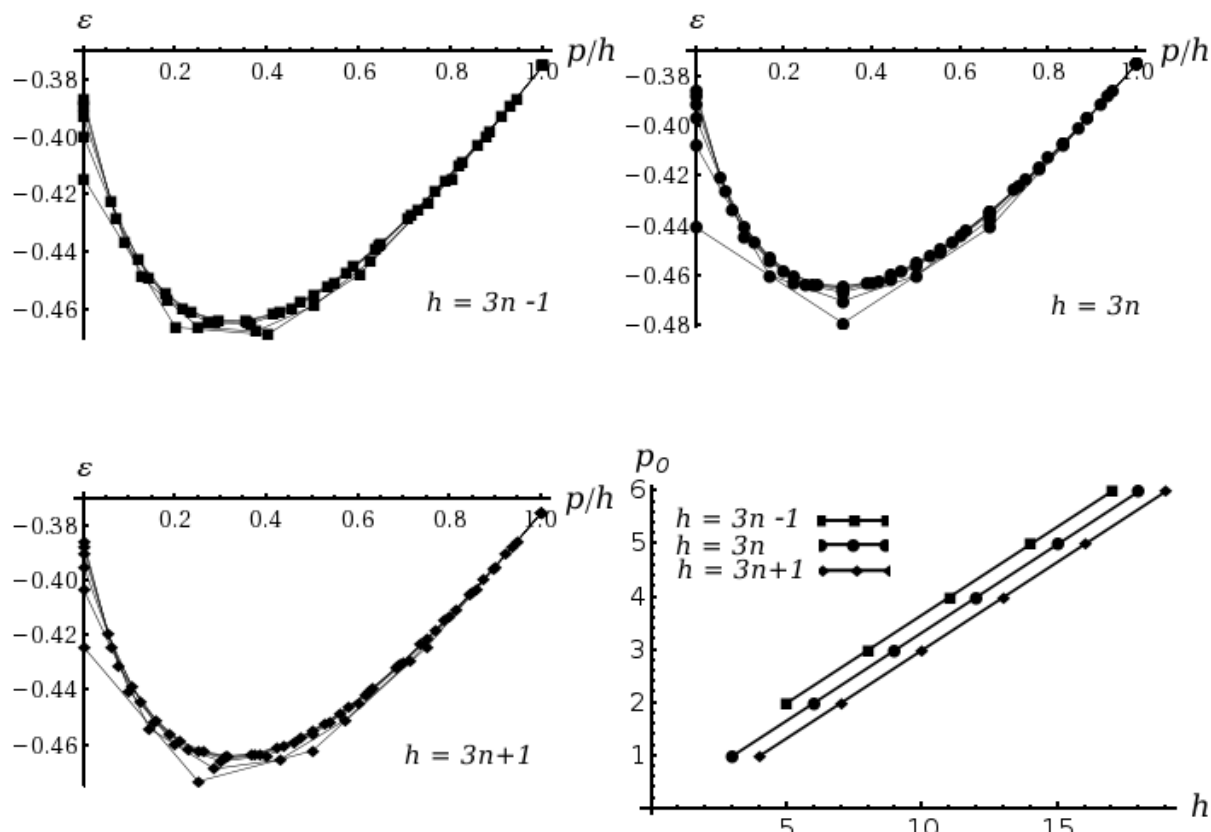


Figure 1.

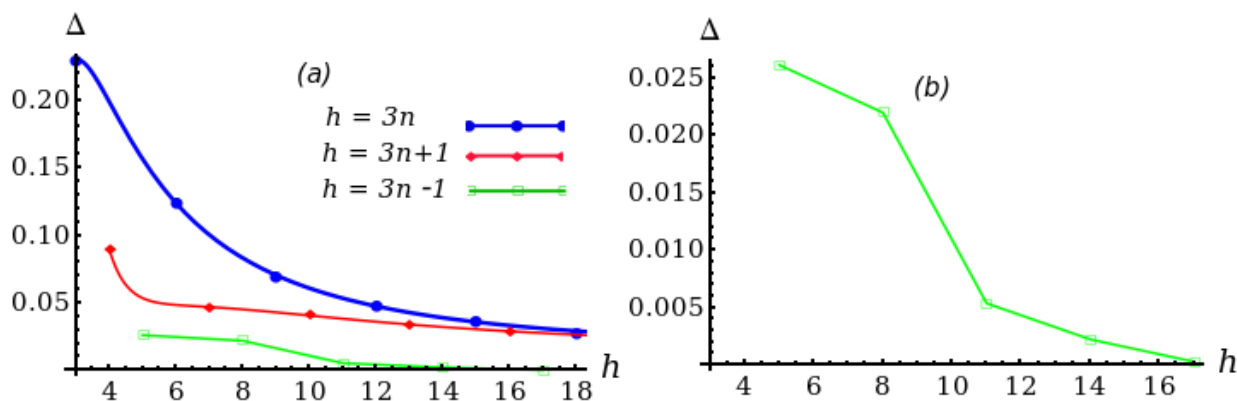


Figure 2.

Figure caption

**Figure 1.** The energy per carbon atom,  $\varepsilon_p(h)$ , as a function of  $p/h$ :  $h = 3n-1$  (■),  $h = 3n$  (●),  $h = 3n+1$  (◆), with  $n =$  integer and  $h$  decreasing from top to bottom. Bottom right: The value of the phase  $p_0$  yielding the lowest-lying energy per polyene ring, for  $h=3n$  (●),  $h=3n+1$  (◆), and  $h=3n-1$  (■).

**Figure 2.** (a) Difference in energy per polyene ring,  $\Delta(h)$ , in units of  $J$  between the two lowest-lying phases,  $p_0$  and  $p_1$ , as a function of the number of hexagons around the CNT. De continuous lines, from top to bottom, correspond to  $h = 3n$  (●),  $h = 3n+1$  (◆), and  $h = 3n-1$  (□), respectively. The top two continuous lines are obtained by fitting the  $\Delta$  values by a power series on  $1/h$ , and tend asymptotically to 0.0125907 and 0.0123187, respectively. The bottom continuous line is obtained by simply joining the calculated values of  $\Delta$ . (b)  $\Delta$  for  $h = 3n-1$ , for  $n = 2, \dots, 6$ .