FRIEDEL OSCILLATIONS IN CARBON NANOTUBE QUANTUM DOTS

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Recently, important advances in the controlled synthesis of carbon nanotube intramolecular junctions during growth have been reported [1]. This may open the possibility to control the production of carbon nanotube quantum dots (QDs) and superlattices (SLs).

We have studied the interface states of all-metallic carbon nanotube quantum dots and superlattices using a tight-binding approach and a Green function matching technique. We have focused on systems made by connecting (n,n) and (2n,0) tubes, in which the interface states appear due to n pairs of pentagon/heptagon topological defects [2,3,4]. The M(2n,0) quantum dots are formed by sandwiching M unit cells of (2n,0) tube between two semi-infinite (n,n) leads, whereas the N(n,n) dots consist of N unit cells of the (n,n) tube between two (2n,0) leads. The superlattices are made by a periodic sequence of N(n,n) and M(2n,0) tubes.

When the armchair length N is increased in both, QD and SL, the energy of the interface states oscillates with N. However, when the size of the zigzag part M is increased, the energy of interface states shows a monotonic behavior with M. We attribute this effect to a Friedel-like oscillation. We have successfully fitted the interface energies to the expression

$$f(d) \propto \frac{\sin(2k_F(d+\delta_0))}{d^{\alpha}} \quad , \qquad (1)$$

where d is the length of QD, δ_0 is the surface shift, and α is the exponent decay. All the cases studied have an unusual decay (>1). For zigzag NTs, $k_F = 0$, so the dependence is monotonic (Fig. 1), and for armchair tubes, with nonzero k_F, oscillations appear (Fig. 2).
In order to see this oscillating behavior more clearly, we have plotted and fitted the second derivative of the energy with respect to the system size, as shown in Fig. 3 [5].

The reported oscillatory changes of the separation energy between the interface states should be seen in optical experiments. We also expect this interaction to be important for the understanding of other physical processes, such as selective dot growth and magnetic interaction of transition metal contacts through carbon nanotubes.

References:

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[5] A. Ayuela, W. Jaskólski, M. Pelc, H. Santos, and L. Chico 'Friedel Oscillations in Carbon nanotube Quantum Dots, (submitted 2008).

Figures:

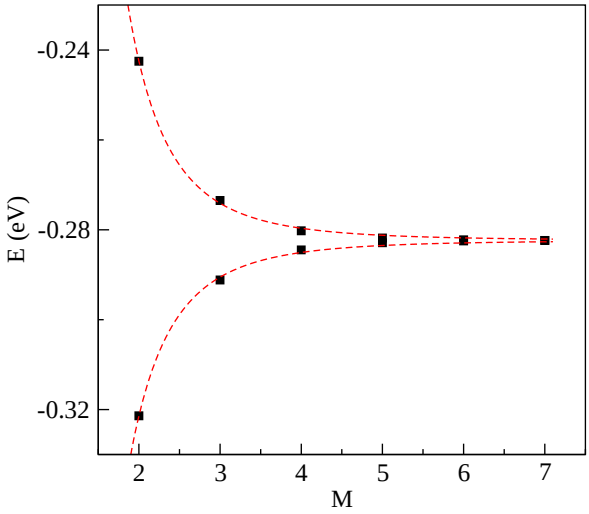

Fig. 1. Interface states energies for the M(18,0) quantum dot vs dot size M corresponding to the series which converges to E = -0.2824 eV. The dashed line shows the fits to $\propto 1/d^{\alpha}$.

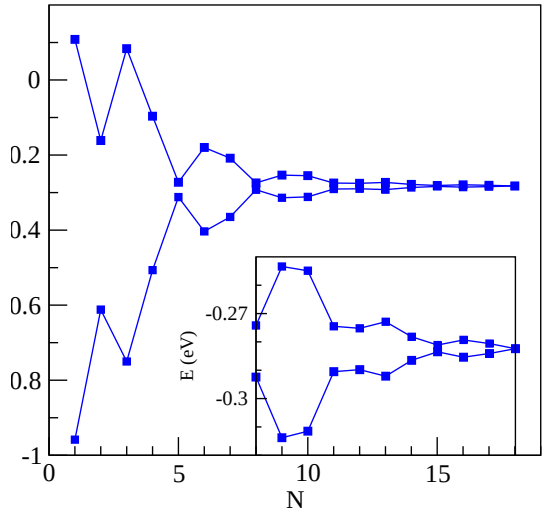

Fig. 2. Interface states energies for the N(9,9) quantum dot as a function of dot size N corresponding to the series which converging to E = -0.2824 eV. Lower inset: zoom in the region of large N.

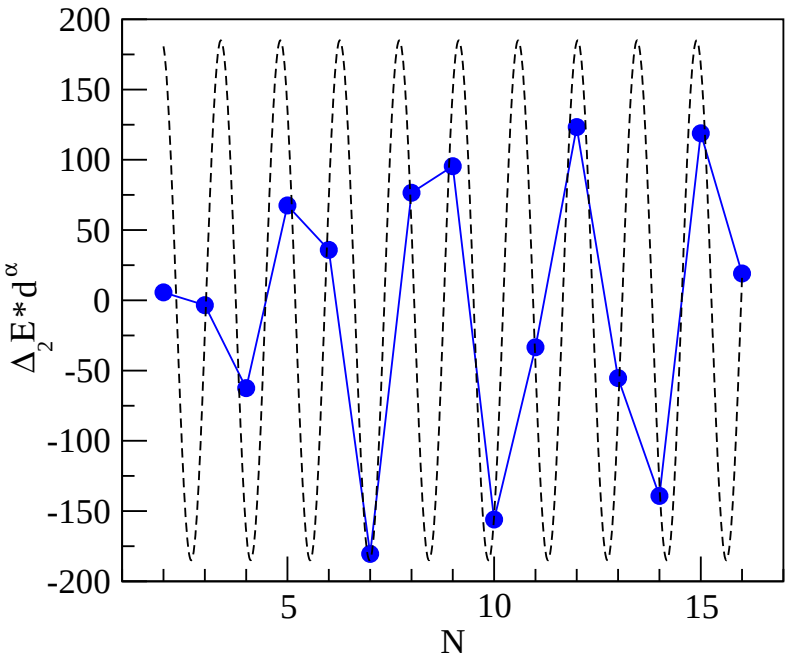

Fig 3. Second derivative of the lowest interface state energy series (shown in Fig. 2) with respect to the system size N. The dashed line is the fit to the function given by Eq. (1).