

MAR11-2010-008572

Abstract for an Invited Paper  
for the MAR11 Meeting of  
the American Physical Society

### **Cohesive Properties of Graphitics and the Random Phase Approximation<sup>1</sup>**

JOHN DOBSON, Micro and Nano Technology Centre, Griffith University, Australia

The van der Waals-dominated cohesive energetics of graphitic systems is important in the assembly of many graphene-based nanostructures of current technological interest. In 2006 an unusual power law  $E = -cD^{-3}$  was predicted [1] for the van der Waals (vdW, dispersion) interaction energy between parallel graphene sheets at large separations  $D$ . By contrast, a conventional sum of pairwise  $R^{-6}$  contributions yields  $E = -kD^{-4}$ . The unexpected  $D^{-3}$  result came from the electronic correlation energy within the Random Phase Approximation (RPA), which can be solved analytically in the distant regime  $D \rightarrow \infty$ . In keeping with other unusual properties of graphene, in this distant non-overlapping regime the relevant response function of a graphene sheet is dominated by the gapless electronic transitions near the Dirac points in the Brillouin Zone where the  $\pi_z$  and  $\pi_z$  Bloch bands touch. The  $D^{-3}$  result corresponds to a severe failure of pairwise additivity of the vdW interaction between local spatial regions of the sheets, and so could have implications for the most-used nanoscale energy functionals (e.g. [2,3]); these embody pairwise additivity at various levels. It has remained unclear what this result might imply for the interaction between graphene sheets at smaller spacings near to the equilibrium separation, where the response is sampled at shorter wavelengths so that analytic results cannot be obtained. Very recently, numerically well-converged exact-exchange and RPA correlation energies have been obtained for stretched graphite at a wide range of inter-layer spacings down to the equilibrium distance. These results and their implications will be discussed.

<sup>1</sup>Support is acknowledged from FAST, Egide and the Australian Research Council.