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Theory of Resonance Raman Scattering in Carbon Nanotubes using Excitonic Intermediate States JOSE MENENDEZ, Arizona State University, ERIC CHANG, GIOVANNI BUSSI, ALICE RUINI, ELISA MOLINARI, INFM National Center on nanoStructures and bioSystems at Surfaces (S3), Universita di Modena e Reggio Emilia, Italy — Optical transition energies in carbon nanotubes can be obtained with high precision from Raman excitation profiles (REPs) measured with continuously tunable laser sources. In the case of Raman scattering by the radial breathing mode (RBM), the measured frequency of this mode makes it possible to associate the optical transition energies with a particular tube diameter, a unique feature of the Raman approach. The theoretical interpretation of REPs has been so far limited to free-electron-hole pairs. However, large excitonic binding energies are expected in quasi one-dimensional systems, and this expectation has been recently confirmed by detailed first principles calculations. Here we present an extension of the ab initio approach to the computation of REPs in semiconducting tubes. A many-body method based on the GW approximation and the Bethe-Salpeter equation is developed to compute the REP for RBMs. This approach yields REPs that take into account the electron-hole interaction and excitonic effects. The method has been applied to the (4,2) tube. The calculated REP iscompared with predictions for the case of free electron-hole pairs as well as with the theoretical optical absorption. Such a comparison makes it possible to identify the relative advantages of these two different optical techniques.

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