Terahertz Transitions and Excitons in Narrow-Gap Carbon Nanotubes

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We calculate the exciton binding energy in narrow band gap single-walled carbon nanotubes, accounting for the quasi-relativistic dispersion of electrons and holes. Exact analytical solutions of the quantum relativistic two-body problem are obtained for several limiting cases. We show that the binding energy scales with the band gap and conclude on the basis of the data available for semiconductor nanotubes that there is no transition to an excitonic insulator in quasi-metallic nanotubes and that their proposed THz applications [1] are feasible.

Depending on the presence of a metallic gate and the carrier density, excitons can be either described by a short-range electron-hole interaction potential [2] or by an unscreened cusp potential, similar to that considered by Loudon in the 1950s [3]. Our analysis shows that the Loudon potential is a good fit for the quasi-one-dimensional Coulomb potential, obtained by averaging the three-dimensional Coulomb potential with the envelope functions. We report exact analytic solutions for the quasi-relativistic Loudon problem for an exciton with a zero total momentum along the nanotube axis. The complex four-component structure of the electron-hole relative motion wavefunction, which is obtained when two graphene sublattices and two types of particles are taken into account, results in a counterintuitive dip in the shape of the particle density distribution within the exciton, shown in Figure 1.

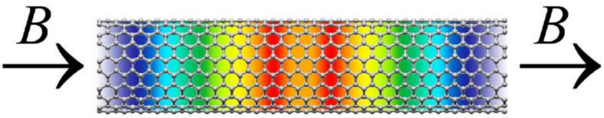

Figure 1. Distribution of the electron density in a 1s exciton assuming that the hole is in the center of the picture. Red and blue colors correspond to the highest and lowest values of density, respectively.

The vanishing exciton binding energy with decreasing of the energy gap removes for narrow-gap nanotubes the undesirable effect of strongly-bound dark excitons, which is known to suppress optical emission in semiconductor nanotubes [4]. However, the Coulomb interaction remains important as it smears the van Hove singularity in the one-dimensional density of states [5]. We report the resulting shape of the terahertz emission from narrow-gap carbon nanotubes with the Coulomb effects taken into account, for both the long-range and short-range interaction models.

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