Excitons and terahertz transitions in narrow gap carbon nanotubes and graphene nanoribbons

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Abstract

We calculate the exciton binding energy in narrow band gap single-walled carbon nanotubes with and graphene nanoribbons, 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, exciton can be either described by a short-range electron-hole interaction potential [2] or by an unscreened potential, similar to that considered by Loudon in the 1950s [3, 4]. 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 (Fig. 1). We report exact analytic solutions for the quasi-relativistic Loudon problem for an exciton with a zero total momentum along the nanoribbon or 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 Fig 2.

The vanishing exciton binding energy with decreasing the energy gap removes for narrow gap graphene-based nanostructures the undesirable effect of strongly-bound dark excitons, which is known to suppress optical emission in semiconducting nanotubes. However, the Coulomb interaction remains very 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 and nanoribbons with the Coulomb effect taken into account, for both the long-range and short-range interaction models [6].

References

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Fig 1. A plot of the dimensionless quasi-one dimensional Coulomb potential as a function of scaled relative coordinate x/R, with the regularized potential of Loudon denoted by a solid (red) line and the averaged potential given by the dotted (blue) line.



Fig 2. The density of a 1s-exciton for a (10,10) carbon nanotube with a magnetic field induced gap of 10 meV (2.5 THz) corresponding to a magnetic field of 15 T along the nanotube axis. The density represents the probability of finding the electron and hole comprising the exciton at the indicated relative separation. Red and blue colours correspond to the highest and lowest values of density, respectively.