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Terahertz transitions in narrow-gap carbon nanotubes and graphene nanoribbons

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Abstract. We show that the curvature effects in quasi-metallic carbon nanotubes and edge effects in narrow-gap graphene nanoribbons not only open band gaps in the THz range but also result in giant enhancement of the transition probabilities across these gaps. This makes these nanostructures perspective candidates for sources and detectors of THz radiation.

1. Introduction

Creating reliable, portable, tunable sources and detectors of terahertz (THz) radiation is one of the most challenging tasks of contemporary applied physics. One of the recent trends in bridging the so-called THz gap is to use carbon-based nanostructures [1]. Several original schemes utilizing the unique electronic properties of carbon nanotubes (CNTs) and graphene for THz application were brought forward by our group [2-6]. These schemes include THz generation by hot electrons in quasi-metallic CNTs, frequency multiplication in chiral-nanotube-based superlattices controlled by a transverse electric field, tunable THz radiation detection and optically-pumped emission in metallic CNTs in a strong magnetic field and using graphene p-n junctions for sub-wavelength polarization-sensitive THz detection. In the current presentation, we focus on direct interband dipole transitions in narrow-gap CNTs and graphene nanoribbons (GNRs).

2. Narrow-gap carbon nanotubes and graphene nanoribbons

The main conclusions of the reported work is that the curvature effects in quasi-metallic single-walled CNTs and edge effects in gapless graphene nanoribbons not only open band gaps, which are typically in the THz range, but also result in giant enhancement of the probability of optical transitions across these gaps. Moreover, the matrix element of the velocity operator for these transitions has a universal value when the photon energy coincides with the band gap energy E_g . Namely, the absolute value of this matrix element for band-edge transitions is equal to graphene's Fermi velocity v_F . Upon increasing the excitation energy the absolute value of the transition matrix element first rapidly decreases (for photon energies remaining in the THz range but exceeding $2E_g$ it is reduced by three orders of magnitude) and thereafter it starts to increase proportionally to the photon frequency. A similar effect occurs in an armchair CNT with a band gap opened and controlled by a magnetic field applied along the nanotube axis [4-6]. As can be seen from Fig. 1, there is a direct correspondence between armchair graphene nanoribbons (AGNRs) and single-walled zigzag CNTs.

Figure 1. Energy spectra and interband transitions velocity matrix elements for CNT (9,0) (upper panel) and AGNR (8) (lower panel) as a function of momentum in the first Brillouin zone.

The described sharp photon-energy dependence of the transition matrix element together with the van Hove singularity at the band gap edge of the considered quasi-one-dimensional systems make them promising candidates for active elements of coherent THz radiation emitters. The effect of Pauli blocking of low-energy interband transitions caused by residual doping can be suppressed by creating the population inversion using high-frequency (optical) excitation. Excitonic effects, which are known to dominate the optical properties of semiconductor CNTs, are of less importance in narrow-gap CNTs and ANGRs where the exciton binding energy is proportional to the bandgap [7] and dark excitonic states become irrelevant.

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