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MAGNETICALLY CONTROLLED TERAHERTZ ABSORPTION AND EMISSION IN CARBON NANOTUBES

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We show that an experimentally attainable magnetic field applied along the axis of a metallic carbon nanotube not only opens the gap in the nanotube energy spectrum but also allows optical transitions, which are forbidden in the absence of the field. Possible terahertz applications of this effect are discussed.

Keywords: Carbon nanotubes; Aharonov-Bohm effect; terahertz radiation.

1. Introduction

Creating reliable coherent sources and sensitive detectors of terahertz (THz) radiation is one of the most formidable tasks of modern device physics.[1] Potential applications of THz spectroscopy range from medical imaging and security to astrophysics and cosmology. The unique position of the THz range in the gap between the parts of electromagnetic spectrum, which are accessible by either electronic or optical devices, leads to an unprecedented diversity in approaches to bridging this gap.[2] One of the latest trends in THz technology[3] is to use carbon nanotubes — cylindrical molecules with nanometer diameter and micrometer length[4,5] — as building blocks of high-frequency devices. There is a growing number of proposals using carbon nanotubes for THz applications including several schemes[6] put

forward by the authors of the present work. Below we discuss how the electronic properties of carbon nanotubes subjected to a strong magnetic field could be utilized for detection and generation of THz radiation.

2. Magnetically Induced Gap and Tuneable Terahertz Absorption and Emission

The Aharonov-Bohm effect[7] (also known as Ehrenberg-Siday-Aharonov-Bohm effect[8]) was one of the first phenomena discussed in relation to single-wall carbon nanotubes (SWNTs).[9] However, a field of the order of 10^4 tesla applied along the nanotube axis is needed to observe a single period in magnetically induced oscillations of a bandgap for a typical SWNT. In experimentally-attainable fields, more subtle effects, such as the magnetic brightening of "dark" excitons in semiconducting SWNTs[10] and the modulation of the magnetoconductance in field-effect transistors based on quasi-metallic SWNTs[11] have been observed. The most dramatic effect occurs when a realistic magnetic field is applied to a truly gapless highly-symmetric armchair[5] nanotube. In armchair SWNTs a longitudinal magnetic field (field applied along the nanotube axis) opens an energy gap near the Fermi level. This gap can be easily calculated in the nearest-neighbor tight binding approximation,[4] in which the influence of a magnetic field is accounted for by adding the number $f = \Phi/\Phi_0 = eBR^2/(2\hbar)$ (here Φ is a magnetic flux through the nanotube, $\Phi_0 = h/e$ is the flux quantum and R is a nanotube radius) to the angular momentum quantum number l, characterizing the lowest conduction and highest valence band branches of the SWNT energy spectrum.[5] A similar procedure was justified for an arbitrary periodic potential by Luttinger[12] almost six decades ago. For an armchair (n, n) nanotube (see Refs. 4, 5 for classification of SWNTs) the gap opened by the longitudinal magnetic field is given by

$$\varepsilon_g = 2\gamma_0 \left| \sin\left(\frac{f}{n}\pi\right) \right|, \tag{1}$$

where $\gamma_0 \approx 3$ eV is the commonly used tight-binding matrix element for graphene.[4,5] For a $(10, 10)$ SWNT this gap corresponds to 1 THz when the nanotube is subjected to a field of approximately 6 T. For attainable magnetic fields, the gap grows linearly with increasing both the magnetic field and the nanotube radius. Whereas the field dependence of the band gap is well-understood,[9] the drastic change in the probability of optical transitions caused by the magnetic field has been completely overlooked. In the absence of a magnetic field, optical transitions between the top valence subband and the lowest conduction subband in armchair SWNTs are strictly forbidden by symmetry.[13] However, the same longitudinal magnetic field, which opens the gap in the armchair SWNT spectrum, allows the dipole optical transitions. In Fig. 1 we show how the energy spectrum and matrix elements of the dipole optical transitions polarized along the nanotube axis are modified in the presence of a longitudinal magnetic field.

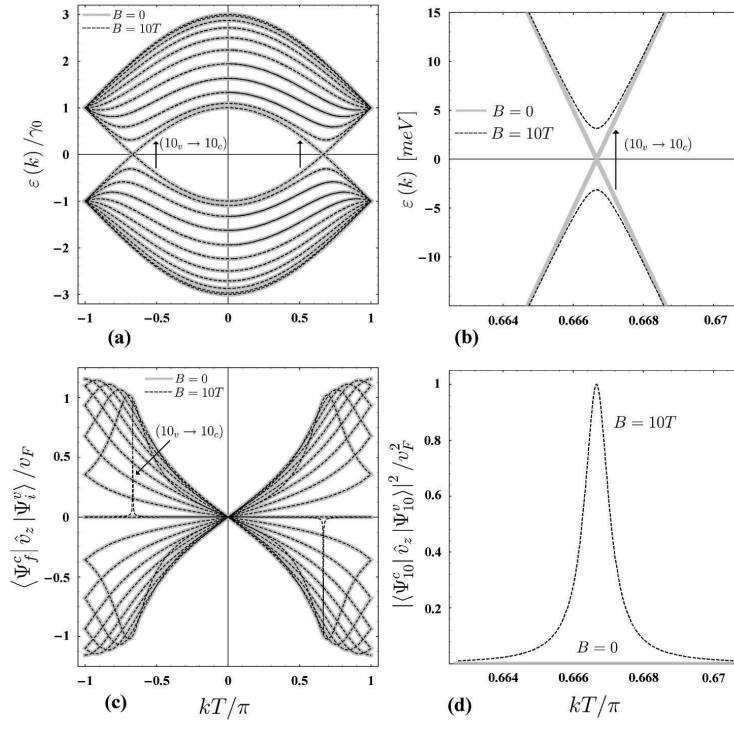

Fig. 1. (a) Band structure of a $(10, 10)$ SWNT within the first Brillouin zone, with and without an external magnetic field along the nanotube axis. (b) Detailed view of the gap, which is opened between the top valence subband (10_v) and the lowest conduction subband (10_c) in an external field $B = 10$ T. (c) The change in the dipole optical transitions matrix elements, for the light polarized along the SWNT axis, due to the introduction of the external magnetic field. The only appreciable change is in the appearance of a high narrow peak associated with the transition $(10v \rightarrow 10c)$, which is not allowed in the absence of the magnetic field. Here T is a crystal period along the nanotube axis and the subband numeration scheme is adopted from Ref. 4. (d) Dependence of the squared dipole matrix element for the transition $(10v \rightarrow 10c)$ on the 1D wave vector k, with and without an external magnetic field.

In the frame of the nearest-neighbor tight binding model, one can show that for a (n, n) armchair nanotube the squared matrix element of the velocity operator between the states at the edge of the gap opened by the magnetic field is given by a simple analytic expression:

$$\left|\left\langle \Psi_n^v \left| \hat{v}_z \right| \Psi_i^c \right\rangle\right|^2 = \frac{4}{3}\left[1 - \frac{1}{4}\cos^2\left(\frac{f}{n}\pi\right)\right] v_F^2, \tag{2}$$

where $v_F = 3\gamma_0 a_{\text{C-C}}/(2\hbar) \approx 9.8 \times 10^5$ m/s is the Fermi velocity of graphene (here $a_{\text{C-C}} = 1.42$ Å is the nearest-neighbor distance between carbon atoms in graphene). For experimentally attainable magnetic fields, when the magnetic flux through the SWNT is much smaller than the flux quantum, the absolute value of the velocity operator is close to v_F. Equation (2) is relevant to the transitions between the highest valence subband and the the lowest conduction subband only for $f \leq 1/2$,

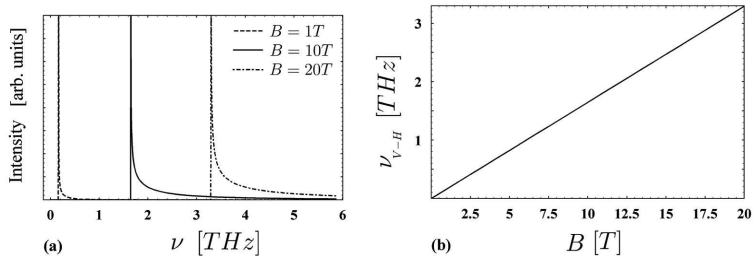

Fig. 2. (a) Calculated photon absorption spectra for a $(10, 10)$ SWNT, for three different magnetic field values. The absorption intensity is proportional to the product of $\left|\left\langle \Psi^v_{10}\right| \hat{v}_z \left|\Psi^c_{10}\right\rangle\right|^2$ and the joint density of states. (b) Dependence of the position of the peak in the absorption intensity, associated with the Van Hove singularity, on the magnetic field.

since for the higher values of f the order of the nanotube subbands is changed. Notably, the same equation can be used to obtain the maximum value of the velocity operator in any armchair SWNT for the transitions polarized along its axis: this value cannot exceed $2v_F/\sqrt{3}$ (see panel (c) in Fig. 1).

The electronic (hole) energy spectrum near the bottom (top) of the gap produced by the magnetic field is parabolic as a function of carrier momentum along the nanotube axis. This dispersion results in the van-Hove singularity in the reduced density of states, which in turn leads to a very sharp absorption maximum near the band edge and, correspondingly, to a very high sensitivity of the photocurrent to photon frequency, see Fig. 2.

3. Tuneable Terahertz Emitter

The same effect can be used for the generation of a very narrow emission line having the peak frequency tunable by the applied magnetic field. A population inversion can be achieved, for example, by optical pumping, with the exciting light polarized normally to the nanotube axis, as shown in Fig. 3.

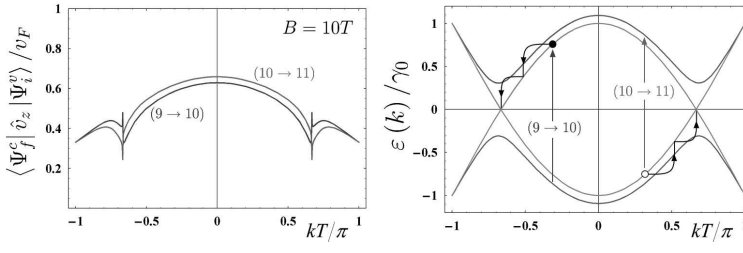

Fig. 3. A scheme for creating a population inversion between the lowest conduction subband and the top valence subband of an armchair SWNT in a magnetic field. The left plot shows the calculated matrix elements of the relevant dipole optical transitions polarized normally to the axis of a $(10, 10)$ SWNT. The right plot shows several energy subbands closest to the Fermi level and illustrates the creation of photoexcited carriers and their non-radiative thermalization.

4. Concluding Remarks

It should be noted, that a similar scheme of using SWNTs as tuneable THz detectors and emitters can be applied to quasi-metallic nanotubes, which unlike the armchair nanotubes have a small curvature-induced gap[14] even in the absence of magnetic field. The gap in the quasi-metallic nanotubes can also be controlled by the applied field,[11] though the expression for this gap is somewhat different from Eq. (1).

Finally, our recent analysis[15] shows that the many-body (excitonic) effects, which dominate optical properties of semiconducting SWNTs,[10] are also important in the narrow-gap nanotubes. However, due to the quasi-relativistic character of the free-particle dispersion near the band edge of the narrow-gap SWNTs, which results in a spectacular decrease in the exciton binding energy, these effects do not alter significantly the main results of this paper.

Acknowledgments

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