Floquet engineering of carbon nanotubes

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Abstract. The Floquet theory for electrons in carbon nanotubes (CNTs) irradiated by a circularly polarized electromagnetic wave propagating along the CNT axis is developed. It is demonstrated, particularly, that the irradiation opens the gap between the conduction and valence bands of CNTs of metal type and lifts the degeneracy of electron states with mutually opposite angular momenta along the CNT axis. As a consequence, the optically-induced metal-insulator transition and the optical Zeeman effect appear in the CNTs. It follows from the theory that these light-induced phenomena can be observed in the modern experiments.

1. Introduction
The control of electronic parameters of condensed-matter structures by an electromagnetic field (the “Floquet engineering” based on the Floquet theory for periodically driven quantum systems) became the important and established research area during last decades. If the field is off-resonant, it cannot be absorbed by electrons and only “dresses” them (the dressing field), changing the band structure of irradiated solids. Particularly, many works dedicated to the Floquet engineering of electron bands were published recently for various nanostructures, including quantum rings, quantum wells, topological insulators, graphene and related 2D materials [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. As to such actively studied nanostructures as carbon nanotubes (CNTs) [13], the Floquet theory of them still waits for detailed analysis. The present study is aimed to fill partially this gap in modern physics at the border between the Floquet theory and the theory of CNTs.

2. Model
Let us consider the interaction between electrons in a carbon nanotube (CNT) and a circularly polarized electromagnetic wave propagating along the CNT axis with the frequency $\omega_0$ which differs from the frequencies corresponding to optical transitions in the electron subsystem (off-resonant dressing field). Assuming that the wave length $\lambda = 2\pi c/\omega_0$ much exceeds the CNT length, the energy of electron-field interaction can be written within the dipole approximation as $-DE$, where $D = e r$ is the electric dipole, $e$ is the electron charge, $r$ is the electron radius vector, and $E$ is the electric field of the wave. Considering the problem within the conventional quantum-field approach, the classical field, $E$, should be replaced with the field operator, $E = i\sqrt{2\pi\hbar\omega_0/V}(e_+ \hat{a} - e_- \hat{a}^\dagger)$, where $\hat{a}$ and $\hat{a}^\dagger$ are the operators of photon annihilation and creation, respectively, written in the Schrödinger representation (the representation of occupation numbers), $e_{\pm} = (e_x \pm ie_y)/\sqrt{2}$ are the polarization vectors, $e_{x,y,z}$ are the unit vectors...
directed along the $x, y, z$-axes of the Cartesian coordinate system with the $z$-axis directed along the CNT axis, and $V$ is the quantization volume. Then the total Hamiltonian of the electron-photon system reads $\hat{H} = \hat{H}_f + \hat{H}_e + \hat{H}_{\text{int}}$, where $\hat{H}_f = \hbar \omega_0 \hat{a} \hat{a}^\dagger$ is the field energy operator, $\hat{H}_e$ is the electron Hamiltonian of CNT, and $\hat{H}_{\text{int}} = -i e \sqrt{2 \pi \hbar \omega_0 / V} r \left( e_+ \hat{a} - e_- \hat{a}^\dagger \right)$ is the Hamiltonian of electron-field interaction.

In the absence of the irradiation, the electron energy spectrum, $\varepsilon_\mu(j)(k)$, and the electron wave function, $\psi_\mu(j)(k)$, satisfy the conventional Schrödinger equation, $\hat{H}_e \psi_\mu(j)(k) = \varepsilon_\mu(j)(k) \psi_\mu(j)(k)$, where $\mu$ is the quantum number labeling different electron subbands in the CNT, $j = c(v)$ is the index marking electron states in the conduction (valence) band of the CNT, and $k$ is the electron wave vector along the CNT axis [13]. To solve the Schrödinger problem for the irradiated CNT with the Hamiltonian $\hat{H}$, we will apply the methodology [2, 3] which was developed before for various nanostructures interacting with a quantized electromagnetic field. To find the energy of the interacting electron-photon system, $\varepsilon$, one has to solve the secular equation,

$$\det|\hat{H}_{nm} - \varepsilon I| = 0,$$

where $\hat{H}_{nm}$ is the matrix Hamiltonian of the system, and $I$ is the unity matrix. The solution results in the energy $\varepsilon = N_0 \hbar \omega_0 + \varepsilon_\mu^0(j)(k)$, where $N_0$ is the photon occupation number of the dressing field. Correspondingly, the first term is the dressing field energy, whereas the second term, $\varepsilon_\mu^0(j)(k)$, should be treated as the electron energy spectrum of CNT modified by the field. In the following, we will assume the field to be classically intensive ($N_0 \gg 1$) and, therefore, the classical field amplitude, $E_0 = \sqrt{4\pi N_0 \hbar \omega_0 / V}$, can be introduced. Certainly, the energy spectrum of CNT, $\varepsilon_\mu^0(j)(k)$, for a classically intensive quantized field exactly coincides with the Floquet (quasi)energy which can be found as a solution of the conventional Floquet problem for the CNT driven by a classical field.

3. Results and discussion

![Figure 1](image)  

**Figure 1.** (a) The electron energy spectrum of CNT with the armchair crystal structure (5,5). The Fermi energy of the electron system is $\varepsilon_F = 0$, the threshold of interband optical absorption is $\Delta_0$ and the Dirac point wave vector is $k_0 = 2\pi/3a$; (b) The structure of electron energy spectrum of the armchair CNT near the Dirac point: in the absence of the dressing field (the dashed lines) and in the presence of the dressing field (the solid lines), where $\varepsilon_g$ is the field-induced band gap.

For definiteness, let us apply the developed theory to CNTs with the armchair crystal structure $(n, n)$ and the electron energy spectrum $\varepsilon_\mu^{(2)}(k) = \pm t \left[ 1 + 4\cos(\mu \pi / n) \cos(ka/2) + 4 \cos^2(ka/2) \right]^{1/2}$, where $t = 3.033$ eV is the energy of interatomic electron interaction in the
graphene crystal lattice, \( a = 2.46 \) Å is the lattice constant of graphene, \( \mu = 0, 1, 2, ..., n - 1 \), and the signs “+” and “−” correspond to electron subbands of the conduction and valence bands, respectively [13]. This energy spectrum is plotted for the \((5,5)\) CNT within the first Brillouin zone \((-\pi/a < k < \pi/a)\) in Fig. 1a, where the bold blue lines mark the doubly degenerate subbands corresponding to mutually opposite directions of the averaged electron momentum along the CNT axis, the thin lines (red and green) mark the nondegenerate subbands with the zero momentum, and the thin red lines correspond to the band edge subbands with \( \mu = 5 \). It follows from the plots that the electron energy structure of the CNT is of metal type and the Dirac (linear) electron dispersion takes place near the band edge with the Dirac point at the electron wave vectors \( k_0 = \pm 2\pi/3a \). Since the selection rules forbid the optical transitions between the two band edge subbands, the threshold of optical absorption by valence electrons is \( \Delta_0 = |\varepsilon_{n\pm 1}(k_0)| = 2t \sin(\pi/2n) \) (see Fig. 1a). To avoid the field absorption by the electrons, we will assume the off-resonant condition, \( \hbar\omega_0 < \Delta_0 \), to be satisfied. To describe the electron energy spectrum of the irradiated CNT near the Dirac point, one can apply the conventional perturbation theory to the matrix Hamiltonian \( H_{nm} \), considering its off-diagonal matrix elements coupling the doubly degenerate electron state at the Dirac point with other states as a perturbation. Then the electron energy spectrum near the Dirac point has the structure pictured schematically in Fig. 1b, where

\[
\varepsilon_{\alpha} = \left( \frac{e R_n E_0}{2} \right)^2 \left[ \frac{1}{\Delta_0 - \hbar \omega_0} + \frac{1}{\Delta_0 + \hbar \omega_0} \right] \sin \left( \frac{\pi}{2n} \right) \tag{2}
\]

is the field-induced gap between the conduction and valence band and \( R_n = \sqrt{3}na/2\pi \) is the CNT radius. Thus, the irradiation turns the metallic CNT into insulator with the band gap (2) which depends on both the field amplitude \( E_0 \) and the field frequency \( \omega_0 \). It should be noted that the field-induced band gap in graphene [2] is linear in the electric field amplitude, \( E_0 \), whereas the gap (2) in CNTs is quadratic in the amplitude. To avoid the destructive dephasing influence of scattering processes on the gap (2), the field frequency, \( \omega_0 \), must meet the condition \( \omega_0 \tau \gg 1 \), where \( \tau \) is the mean free time of charge carriers in CNTs. This condition is of general character for the Floquet theory of various condensed-matter structures [2, 11] and can be satisfied for the high field frequencies starting approximately from the upper microwave range limit.

Besides the metal-insulator transition originated from the irradiation, it should be noted also the irradiation-induced splitting of the doubly generate subbands marked by the bold blue lines in Fig. 1a, which is also quadratic in the field amplitude \( E_0 \) and can be found from the numerical solving of the secular equation (1). Thus, the irradiation lifts the degeneracy of CNT electron states with respect to its angular momentum. This means, particularly, that a circularly polarized electromagnetic wave propagating along the CNT axis acts similarly to a stationary magnetic field directed along the same axis since the magnetic field also induces the gap at the Dirac point [14] and lifts the angular momentum degeneracy (the Zeeman effect). Physically, this similarity is a consequence of the broken time-reversal symmetry of the electron system, which takes place due a circularly polarized electromagnetic field as well as a stationary magnetic one. Indeed, the circularly polarized field is non-invariant with respect to the time reversal since it turns clockwise polarized photons into counterclockwise polarized ones and vice versa. Since the irradiation-induced effects discussed above follow from the broken time-reversal symmetry of the electron-photon system, they take place in CNTs with any crystal structure as well. However, CNTs with the crystal structure devoid of an inversion center (the chiral CNTs) [13] should be noted specially. It follows from the well-known Kramers theorem that the symmetric dependence of the electron energy on the electron wave vector in solids, \( \varepsilon(k) = \varepsilon(-k) \), is the direct consequence of one of two symmetries: The inversion symmetry of crystal structure and the time-reversal symmetry (see, e.g., Ref. [15]). If the both symmetries are broken, the asymmetrical energy spectrum of electrons, \( \varepsilon(k) \neq \varepsilon(-k) \), appears. Particularly,
such an asymmetrical spectrum takes place in various nanostructures without an inversion center exposed to a stationary magnetic field, including asymmetric semiconductor quantum wells in the presence of an in-plane magnetic field [16], magnetic edge states in two-dimensional electron systems [17] and chiral CNTs subjected to a magnetic field directed along the CNT axis [18, 19, 20]. As a consequence of the asymmetric electron dispersion, unusual photovoltaic effect [21, 22] and the anomalous thermal effects [16, 17, 19] induced by a magnetic field appear. Since a circularly polarized electromagnetic field acts similarly to a stationary magnetic field, the corresponding optically-induced effects are expected in the irradiated chiral CNTs as well.

4. Conclusion
It is shown that an irradiation opens band gap between conduction and valence bands and lifts the degeneracy of electron states with mutually opposite angular momenta in armchair carbon nanotubes. For the field amplitude $E_0 \sim 10^6 \text{ V/m}$ and the resonance difference $\Delta_0 - \hbar \omega_0 \sim \text{meV}$, the optically induced band gap in armchair CNTs with the radius $R_a \sim 10 \text{ nm}$ is of meV scale and, therefore, can be detected in the modern experiments with using the angle-resolved photoemission spectroscopy (APRES).

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