Chirality Effects on an Electron Transport in Single-walled Carbon Nanotube Coupling to a Quantum Dot

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Chirality Effects on an Electron Transport in Single-walled Carbon Nanotube Coupling to a Quantum Dot

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Abstract. We investigated the effects of asymmetric velocities of Dirac particles, calculated by inducing curvature-induced σ-π mixing and Slater-Koster type projection for π-π and σ-π hopping integrals, on the transfer energy between the quantum dot (QD) and electron in a carbon nanotube. We also showed that probability for finding the electron on the left-side is more than the right-side of carbon nanotube. This result corresponds with the asymmetric velocities of Dirac particles, such a study may prove a useful for charge transport of QD-solar cell.

1. Introduction

Carbon Nanotube (CNT) photonics with fascinating properties [1] is an emerging field. It offers a challenge to both fundamental and applied sciences. Many properties of CNT are tied to its lattice structure, allowing for tuning of charge carrier dynamics through the curvature of the nanotube surface, physical scenarios in condensed matter setting: narrow-linewidth blackbody emission [2], curvature effect on polarization of light emitted from chiral carbon nanotubes [3], effect of curvature-induced superlattice structures on energy band structures of helically coiled carbon nanotubes [4], etc. The efficiency of absorption and emission of light depends on different chirality of the individualized nanotubes [5]. The photoluminescence (PL) intensity of a single-wall carbon nanotube (SWCNT) is calculated by multiplying the photon-absorption, relaxation and photon-emission matrix elements [6]. In 2012, W. Izumida *et al*. showed the velocities of Dirac particle are asymmetric due to a second order perturbation technique of curvature-induced σ - π mixing with Slater-Koster type projection for π - π and σ - π hopping integrals on the curved surface of nanotubes [7]. Concerning to the hexagonal lattice and graphene, the current-current correlation function method is used [8]. The correlation function can be decomposed into parallel and perpendicular contributions.

The present paper is organized as follows: we define the continuum model and derive the current local operator of this model (Sec. II), we further show the calculation of probability amplitude which decays the excitation state and has the electron at either right-side or left-side of the carbon nanotube. In Sec. III, we analyze the numerical results and discussion of the scattering of electron, depending on the asymmetric velocities of Dirac particles. A summary, along with some concluding remarks, is given in Sec. IV.

2. Time evolution of the right-going and left-going electrons

We investigate the scattering of a single electron in chirality single-walled carbon nanotube (C-SWCNT) interacting with a V-type three-level quantum dot (V-QD), coupled to 1D electron transport which is a metal nanowire and we consider an electron in near Dirac point region, respectively.

First of all, we study the scattering of electron interaction with V-QD as shown in Fig. 1. In our model, the composite system is considered as an electron transport-quantum dot interaction, and the Hamiltonian system is given by

$$\hat{H} = \hat{H}_{ele} + \hat{H}_{qd} + \hat{H}_{\text{int}} \ . \tag{1}$$

where $\hat{H}_{ele} = \sum_{\gamma=R,L} \int dz\ \hbar(-iv_F^{(\gamma)} c_\gamma^\dagger(z) \frac{\partial}{\partial z} c_\gamma(z) + H.c.)$ is both right-going and left-going Hamiltonian of carbon nanotube, $c_R^\dagger(z)$ and [$c_L^\dagger(z)$] are creation operator of electron a right- [left-] going at z , $C_R(z)$ and [C_L (z)] are annihilates a right-[left-] going at z, $v_F^{(\gamma)}$ is the group velocity of an electron transport in C-SWCNT for the right-going $v_F^{(R)}$ and left-going $v_F^{(L)}$ describing the creation operation. The Hamiltonian describes the Λ-type three-level structure:

$$\hat{H}_{qd} = \hbar(\omega_{10} - i\Gamma_1)|1\rangle\langle 1| + \hbar(\omega_{20} - i\Gamma_2)|2\rangle\langle 2| + \hbar\omega_{00}|0\rangle\langle 0| . \tag{2}$$

where $|0\rangle$ is ground state of quantum dot and $\Gamma_1[\Gamma_2]$ is constant of decay of electron in quantum dot at excited 1[2] state. The electron transport-quantum dot coupling Hamiltonian is given by:

$$\hat{H}_{\text{int}} = \sum_{\gamma=R,L} \sum_{\eta=1,2} V_\gamma^{(\eta)} \hbar \int dz\, \delta(z)(c_\gamma^\dagger(z)\hat{\sigma}_\eta^{(-)} + H.c.) \tag{3}$$

where $V_\gamma^{(\eta)} \alpha\ v_F^{(\gamma)} |\vec{d}_{\eta 0}|$ is coupling constants, which is proportional to the transition dipole moment $|\vec{d}_{\eta 0}|$ and $v_F^{(\gamma)}$ the group velocity of an electron transport, $V_\gamma^{(1)}$ is time independent but $V_\gamma^{(2)}$ is time dependent. Effects of the group velocity on photon emission of the dark ($|2\rangle$) and the bright ($|1\rangle$) exciton states have been investigated.

The studied system is modeled as shown in Fig. 1, the V-QD has been exited to the excitation state, $|1\rangle$ or $|2\rangle$. Then, the excitation state decay and has the transitions $|1\rangle \leftrightarrow |0_{qd}\rangle$ or $|2\rangle \rightarrow |0_{qd}\rangle$ with resonance frequencies (dipole transition) ω_{10} and ω_{20}, accompanying the transition dipole moment ($\vec{d}_{10}$) and ($\vec{d}_{20}$) respectively.

Energy is transferred to C-SWCNT, creating both right-going and left-going electrons in the carbon nanotube. We investigate the effects of asymmetric velocities of Dirac particles on the probability amplitude for finding at the right-side and left-side of the carbon nanotube, given by $Amp_L^{(\eta)} = \langle L|\exp(-i\hat{H}t/\hbar)|in\rangle$ | and $Amp_R^{(\eta)} = \langle R|\exp(-i\hat{H}t/\hbar)|in\rangle$, respectively.

where $|L\rangle = \theta(-x)e^{-\frac{i}{\hbar}\hat{H}_{ele}t}\hat{c}_L^{\dagger}(x)|0,0_{qd}\rangle$ and $|R\rangle = \theta(x)e^{-\frac{i}{\hbar}\hat{H}_{ele}t}\hat{c}_R^{\dagger}(x)|0,0_{qd}\rangle$ are a quantum state for finding the electron at the right-side and left-side of the carbon nanotube, respectively, $|0,0_{qd}\rangle$ is the V-QD at ground state and the electron in the carbon nanotube is in vacuum state. In Fig. 1, the initial state of system can be assumed that $|in\rangle = |0,\eta\rangle$ is the V-QD at excitation state, $|\eta\rangle;\eta = 1,2$ and the electron in carbon nanotube is in vacuum state.

For calculation of probability amplitude $\langle L|\exp(-i\hat{H}t/\hbar)|in\rangle$ and $\langle R|\exp(-i\hat{H}t/\hbar)|in\rangle$, we keep only the terms of first-order in $V_{\gamma}^{(\eta)}$ and we then obtain can be given as:

$$Amp_L^{(\eta)}(x,t) = \langle L|e^{-\frac{i}{\hbar}\hat{H}t}|in\rangle \approx \theta(-x)\langle 0_{qd}|\hat{c}_L(x)\sum_{n=0}^{\infty}\frac{(-i)^n\hbar^n}{n!\hbar!}\int_0^t dt'\cdots\int_0^{t^{(n-1)}}dt^{[n]}\left(\omega_{\eta 0}-\frac{i\Gamma_{\eta 0}}{2}\right)^n\left[\frac{V^L}{\sqrt{2}}\hat{c}_L^{\dagger}(0,t^n)+\frac{V^R}{\sqrt{2}}\hat{c}_R^{\dagger}(0,t^n)\right]|\eta\rangle \quad (4)$$

and

$$Amp_R^{(\eta)}(x,t) = \langle R|e^{-\frac{i}{\hbar}\hat{H}t}|in\rangle \approx \theta(x)\langle 0_{qd}|\hat{c}_R(x)\sum_{n=0}^{\infty}\frac{(-i)^n\hbar^n}{n!\hbar!}\int_0^t dt'\cdots\int_0^{t^{(n-1)}}dt^{[n]}\left(\omega_{\eta 0}-\frac{i\Gamma_{\eta 0}}{2}\right)^n\left[\frac{V^L}{\sqrt{2}}\hat{c}_L^{\dagger}(0,t^n)+\frac{V^R}{\sqrt{2}}\hat{c}_R^{\dagger}(0,t^n)\right]|\eta\rangle \quad (5)$$

We can calculate the probabilities for finding the electron at the right and left of the carbon nanotube by using the creation operator of the electron a right- and left-going as defined [14]:

$$\hat{c}_R^{\dagger}(0,t) = \int_0^{\infty}\frac{dk}{2\pi}e^{-i\omega_k t}\hat{b}_k^{\dagger} \text{ and } \hat{c}_L^{\dagger}(0,t) = \int_{-\infty}^{0}\frac{dk}{2\pi}e^{-i\omega_k t}\hat{b}_k^{\dagger}. \quad (6)$$

where $\hat{b}_k^{\dagger}$ is a creation operator of electron in momentum space to be the Fourier transforms of real-space operators.

3. Calculation and Discussion

In order to compute the correlation function with the diameter of SWCNTs and the chiral angle as the zigzag SWNT, (9,0) and the chiral SWNT (7,1) and the armchair SWNT, (4,4). The armchair (4,4) is gapless but the energy gap appears for the zigzag (9,0) and the chiral (7,1), the group velocity has the asymptotic velocity of the conduction and valence bands having a linear dispersion. Here the velocities are given by $v_F^L = -\partial E_L/\hbar\partial k, v_F^R = \partial E_R/\hbar\partial k$ where $E_{L(R)}$ is the energy band of the left-going (right-going) particle, which has the negative (positive) slope. The ratio of velocities to be $|v_F^R/v_F^L|$ are about 0.8, 0.94, and 0.75 for the armchair (4,4), the chiral (7,1), and the zigzag (9,0), respectively. We numerically calculate Eq. (5) by following parameters in ref. [9] as shown in Fig. 2 and Fig. 3

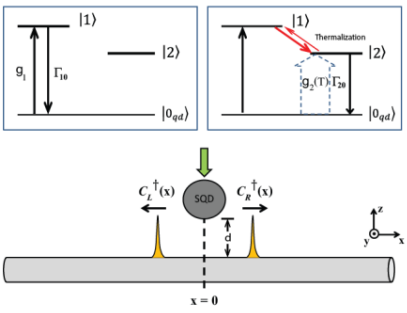

Fig. 1 Schematic diagrams of SWCNT directly coupled to the exciton state $|1\rangle$ (upper left) and virtually coupled to the exciton state $|2\rangle$, through thermalization, (upper right). (Bottom) Propagating electrons in the nanowire are created by decaying the exciton state.

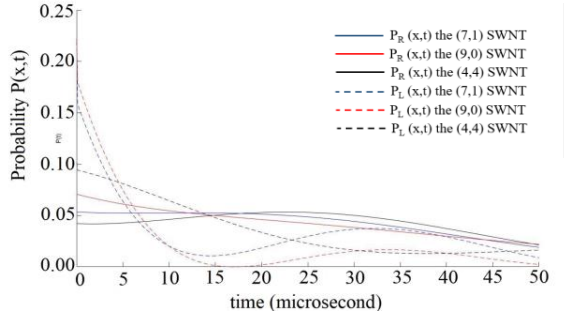

Fig. 2 Show that numerical results of probability for finding the electron at the right and left of the carbon nanotube are the function of time for the position x fixed. A probability for finding the electron at the left (Dot line) is more than the right (Solid line).

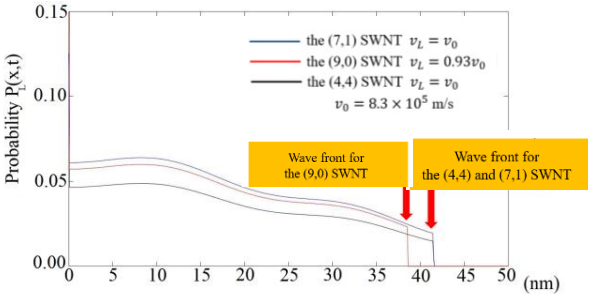

Fig. 3 Show that numerical results of probability for finding the electron at the left of the carbon nanotube is a function of position for time t fixed. A probability for finding the electron at the left of SWCNT correspond with the velocities, given by defining $v_F^L = -\partial E_L / \hbar \partial k$.

4. Conclusions

We have provided a quantum mechanical theoretical study of the stimulated electron which has right- or left-going in SWCNT. Numerical results of probability for finding the electron at the right-side and left-side of the carbon nanotube show that a probability for finding the electron at the left-side of the carbon nanotube is a function of position for time *t* fixed. Probability for finding the electron at the left-side SWCNT corresponds to the velocities, given by defining $v_F^L = -\partial E_L / \hbar \partial k$. This study provides insights into this fundamental process of nature, including the role of lattice structure on the probability of creation of the right- and left-going electrons.

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