The electron- acoustic phonon interaction in monolayer graphene

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The electron- acoustic phonon interaction in monolayer graphene is studied in this paper. The interaction Hamiltonian of the electron and acoustic phonon in monolayer graphene is derived. The self-trapping transition of the acoustic polaron in monolayer graphene is investigated by using the variation of the ground-state energy of the acoustic polaron based on the electron-acoustic phonon coupling constant. It is shown that the electron near the Dirac point can not form normal polaron and the self-trapping transition of the acoustic polaron can not realized in this point of the monolayer graphene. The results show that outside the Dirac point, the self-trapping of acoustic polaron is consistent with the theory in ideal two-dimensional systems.

(Received July 24, 2019; accepted February 17, 2020)

Keywords: Two dimensional materials, Acoustic polaron, Self-trapping, Graphene

1. Introduction

As the simplest model of the interaction between particles and fields, polarons play many important roles in many aspects, such as solid quantum systems, polar semiconductors, and even high temperature superconductors (HTS). As the basic carriers in crystals, there is great significance for polarons in explaining the optical transitions and transport phenomena in ionic crystals and polar semiconductors. The idea of polaronic dressing has been by now extended far beyond electron-phonon systems and has become an important paradigm in physics [1-6]. It is known that the migration effects, such as effective mass, migration rate and ground state energy, varied with the electron-phonon interaction when electrons move in crystals with phonon clouds. For acoustic polaron, there is a self-trapping state based on abrupt change of energy and effective mass in transportation. Superconductivity is a special transport phenomenon, the microscopic mechanism at low temperature is also the electron-phonon interaction. Cooper pair in BCS theory of cryogenic superconductivity is also the polaron effect caused by interaction between electrons and phonons. There are many models can explain the microscopic mechanism of high temperature superconducting material, and the polaron-bipolaron model is just the natural extension of BCS theory [7-8]. Therefore, studying the properties of polarons is beneficial to the development and perfection of HTS model.

Many new physics phenomena and application prospects has been found due to the discovering of graphene. As a new two-dimensional material, graphene has shown its characteristics in various aspects and brought new vitality to condensed matter physics [9-12]. Recent research has shown that the two layer graphene twisted together at 1.1 degree will present high temperature superconducting effect [13-14]. Although there are many studies on graphene, the problem of polaron self-trapping is still imperfect and needs to be explored.

In this work, the Hamiltonian of the special structure of the graphene material is introduced firstly. The ground state energy of acoustic polaron near the Dirac cones and far away from it are derived by using Huybrechts variational method. By introducing the electron-acoustic phonon coupling constant, the self-trapping transition of the polaron will be discussed.

2. Graphene and Electron-Phonon Interaction

Graphene is a two-dimensional material consisting of a layer of carbon atoms arranged in honeycomb-like crystal lattice. The band structure of the graphene is obtained according to the tight-binding approximation. It is found that the valence band of graphene is connected with the conduction band at six vertices of Brillouin zone. This architecture pattern forms the band-gap-free semiconductor. The energy spectrum near the vertices is linear dispersion relation, these vertices are called Dirac points. According to the effective mass theory in the crystal, the effective mass near the points is zero. Therefore, the motion of electrons in graphene will be replaced by the massless Dirac equation, that is, the Weyl equation

$$i\hbar\frac{\partial\psi}{\partial t}=\mp c\vec{\sigma}\cdot\vec{p}\psi \qquad (1)$$

where c is the kinematic velocity of massless particle, its Fermi velocity in graphene. $\vec{\sigma}$ and $\vec{p}$ are the Pauli matrix and carrier momentum in two dimensional system

respectively. The positive and negative signs correspond to different helicity. In this paper, only the positive helicity is considered, then the kinematic energy of the electron can be written as the following formula

$$c\vec{\sigma}\cdot\vec{p}=c\begin{bmatrix}0 & p_x-ip_y\\ p_x+ip_y & 0\end{bmatrix} \tag{2}$$

The interaction of electron and acoustic-phonon is

$$H_{e-p}=\begin{bmatrix}\sum_q iV_q a_q e^{i\vec{q}\cdot\vec{r}}+h.c & 0\\ 0 & \sum_q iV_q a_q e^{i\vec{q}\cdot\vec{r}}+h.c\end{bmatrix} \tag{3}$$

where $V_q=\sqrt{\frac{\hbar qD^2}{2A\rho c}}$ is the interaction coefficient [15], D is the deformation potential constant, ρ is the density of mass, A is the superficial area, q is the wave vector of phonon, a_q and $a_q^\dagger$ are annihilation and creation operators of phonon. So that the Hamiltonian of polaron near the Dirac point can be described as

$$\begin{aligned}H_1=&c\begin{bmatrix}0 & p_x-ip_y\\ p_x+ip_y & 0\end{bmatrix}+\sum_q a_q^\dagger a_q\hbar\omega\\ &+\begin{bmatrix}\sum_q iV_q a_q e^{i\vec{q}\cdot\vec{r}}+h.c & 0\\ 0 & \sum_q iV_q a_q e^{i\vec{q}\cdot\vec{r}}+h.c\end{bmatrix}\end{aligned} \tag{4}$$

3. The Ground State Energy of Polaron

In order to calculate the ground state energy of the polaron in the graphene system, Huybrechts variational method [16] had been used to make two variations to Formula (4). The first unitary transformation is

$$U_1=\exp\left(-ia\sum_q\vec{q}\cdot\vec{r}a_q^\dagger a_q\right) \tag{5}$$

Introducing the creation and annihilation operators b_j and $b_j^\dagger$ by

$$p_j=\left(\frac{\hbar\lambda}{2}\right)^{1/2}\left(b_j^\dagger+b_j\right) \tag{6a}$$

and

$$r_j=i\left(\frac{\hbar}{2\lambda}\right)^{1/2}\left(b_j-b_j^\dagger\right) \tag{6b}$$

where a and λ are variational parameters, the index j refers to the x and y directions. To calculate the energy eigenvalue, the second unitary transformation is necessary. Introducing displacement amplitude f_q to approximate the Hamiltonian to diagonalization and obtain the non-perturbative results

$$U_2=\exp\sum_q\left(f_q a_q^\dagger-f_q^* a_q\right) \tag{7}$$

For the ground state of zero phonon $|0\rangle$,

$$b_j|0\rangle=a_q|0\rangle=0$$

In Fock representation, the ground state wave function of polaron in monolayer graphene is

$$\left|1_q\right\rangle\left|\prod_q 0_q\right\rangle$$

where

$$\left|1_q\right\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}e^{-i\theta/2}\\ \pm e^{i\theta/2}\end{pmatrix} \tag{8}$$

is the electronic state function near the Dirac point in momentum space. θ is

$$\theta=\arctan\left(\frac{q_x}{q_y}\right) \tag{9}$$

then the ground state energy of the polaron is

$$\begin{aligned}E_0=&-2ac\sum_q\hbar q\left|f_q\right|^2+2\sum_q\hbar\omega\left|f_q\right|^2\\ &+2\sum_q\left[iV_q f_q\exp\left(-\frac{\hbar}{4\lambda}(1-a)^2q^2\right)+h.c\right]\end{aligned} \tag{10}$$

According to symmetry we can obtain the displacement amplitude

$$f_q=\frac{iV_q^*\exp\left(-\frac{\hbar}{4\lambda}(1-a)^2q^2\right)}{2\hbar\omega-2ac\hbar q} \tag{11}$$

Substituting (11) into (10), we can get

$$E_0^D=-\sum_q\frac{\left|V_q\right|^2}{2\hbar(\omega-acq)}\exp\left(-\frac{\hbar}{2\lambda}(1-a)^2q^2\right) \tag{12}$$

Substituting the V_q into (12), the Hamiltonian is then last written as

$$E_0^D=-\frac{D^2}{8\pi\rho}\int_0^{q_0}\frac{1}{1-a}\exp\left(\frac{-\hbar(1-a)^2q^2}{2\lambda}\right)dq \tag{13}$$

For the electron which far from the Dirac point, the Hamiltonian of electron-acoustical phonon interaction due to the deformation potential can be written as [15]

$$H_{DA} = \frac{1}{\sqrt{A}} \sum_q V_q e^{i\vec{q}\cdot\vec{r}} a_q + c.c \qquad (14)$$

with the *DA* interaction vertex defined as

$$\left|V_q\right|^2 = \hbar^2 q v_{DA} / \left(p_0^2 \bar{\tau}\right)$$

by introducing the nominal scattering time

$$1/\bar{\tau} = D^2 p_0^2 / \left(2\hbar\rho v_{DA}\right) \qquad (15)$$

the new Hamiltonian can be written as

$$H = \frac{P^2}{2m} + \sum_q \hbar\omega_q a_q^\dagger a_q + \sum_q V_q^* a_q^\dagger e^{-i\vec{q}\cdot\vec{r}} + h.c. \qquad (16)$$

Introducing the dimensionless bulk e-LA-p coupling constant

$$\alpha = \frac{D^2 m^2}{8\pi\rho\hbar^3 c} \qquad (17)$$

Using the Huybrechts variational approach and adopting Hou's treatment [17], we can obtain the ground state energy

$$E_0 = \frac{1}{2}\lambda(1-a)^2 - 2\alpha \int_0^{q_0} \frac{q^2}{1+a^2 q/2} \exp\left(-\frac{(1-a)^2 q^2}{2\lambda}\right) dq \qquad (18)$$

this formula is coincide with the expression of ground state energy of polaron in pure two dimensional system of Ref. [17].

4. Numerical results and discussions

The ground state energy of polaron in graphene system is calculated. The criterion of self-trapping transition of acoustic polaron in graphene is also established by using the product of cut-off wave vector and coupling constant. The correctness of the criterrion is confirmed by the result of electron-acoustic phonon interaction at the location that deviation from Dirac point.

The formula (13) and (18) are the expressions of ground state energies near the Dirac point and far from the point, respectively. Expressing the energies in units of mc^2, the lengths in units of $\hbar/mc$, and the phonon wave vector in units of $mc/\hbar$. Thus all variables will be dimensionless. Equation (13) shows that the ground state energy has only integral term about wave vector, and (18) shows that the energy consists of two parts, integral term about wave vector and the constant term of variational parameters. Based on previous studies on polaron energy [18], we can see that the constant term containing variational parameters originates from the linear combination operators that introduced into the momentum in the electronic kinetic energy term. That is to say, it represents the characteristics of the electron itself. The integral term of wave vector is the result of the interaction between electron and phonons. Self-trapping is the binding state of electron in phonon cloud, which is the result of the coexistence of electron and phonons. The calculation shows that when the electron is near the Dirac point, there is only interaction term but no electron kinetic energy term in the ground state energy formula. Therefore, in this state, the electron can not form a normal polaron, and thus self-trapping transition can not occur.

For the non-relativistic effect, the relationship between the ground state energy of the acoustic polaron and the coupling constant is numerically calculated as shown in Fig. 1.

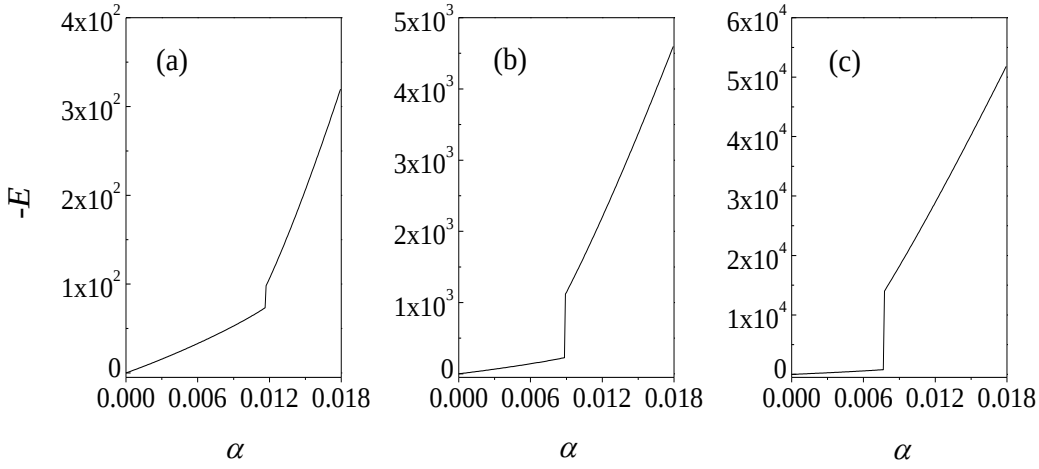

Fig. 1. Ground-state energies of the acoustic polaron in 2D graphene as a function of the e-p coupling constant α for (a) q_0 = 50, (b) q_0 = 100 and (c) q_0 = 200 respectively

From Fig. 1 we can see that the electronic behavior is the normal electron in the crystal when it is far from the Dirac point, and the ground state energy decreases with the increases of the coupling constant. When the coupling constant α increases to a certain value, the energy curve turns to an inflection point, and the polaron energy suddenly decreases, which is the transition from near-free state to self-trapping state. Defining the coupling constant as a critical coupling constant α_c, we can get the condition of the self-trapping transition is $\alpha_c q_0 \geq 0.6$, which is consistent with Hou's work [17] that obtained in the ideal model of general two-dimensional system.

The explanation for the case of abnormal polaron and non-self-trapping near the Dirac point is as follows: Due to the special band structure of graphene, electrons exist in the form of massless near the zero band gap junction, which means that electrons have relativistic effects. But polaron is a quasi-particle of the interaction system between slow electron and lattice vibrating phonons, which is the characteristic of slow moving electrons in crystals. When the electrons have relativistic effect in a particular structure, the vibration frequency of phonons unable to respond to the nearest electrons due to the very fast migration rate of electrons. So that it is impossible to form the normal polaron, let alone form the self-trapping state.

5. Conclusion

The ground state energies of acoustic polarons near the Dirac point and non-Dirac point of graphene are calculated by Huybrechts variational method, respectively. The results show that the normal polarons can not be formed due to the relativistic effect for the electrons near the Dirac point. The relationship between the ground state energy of acoustic polaron and the electron-phonon coupling constant is consistent with the conclusions obtained in the ideal two dimensional theory when the electrons deviated from the Dirac point. Furthermore, the self-trapping criterion of the acoustic polaron in two dimensional material is verified by graphene material.

Acknowledgment

This work is supported by the Applied and Basic Research Program of Shanxi Province (No. 201901D111290) and the Science and Technology Innovation Project of Shanxi Province (No. 20191017) in China.

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