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The properties of strong couple bound polaron in monolayer graphene

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Based on the Hamiltonian of the interaction energy between electron on the surface of the graphene and longitudinal acoustic phonon on the surface of the substrate, the paper studies the properties of strong couple polaron in monolayer graphene considering the coulomb doping problem. The conventional Lee-Low-Pine unitary transformation method and linear combination operator method are used to calculate the ground state energy of the polaron. The results show that the ground state energy of the system has a linear relationship with the magnetic field strength, the cut-off wave number, the coulomb bound parameter, the distance between the graphene and the substrates, meanwhile, the ground state energy will split into two branches near the Dirac point.

1. Introduction

Graphene is a kind of only one atom thick material, not only it is the thinnest material that people get, but also it is the most solid material. Because of its unique structure, inspire people's enthusiasm for its research. In recently years, many researchers domestic and overseas have researched properties of graphene from the aspects of theory and experiment. So far the influence of the magnetic field effect and the Rashba effect on properties of the graphene has been discussed, the results show that solutions to the impurity problem which are qualitatively different from those of zero magnetic field has been found by numerical diagonalization of the large Hamiltonian matrices; the properties of the polaron on the electronic structure of zigzag graphene nanoribbon with different width have been researched by a unitary transformation to get an effective Hamiltonian for nanoribbon in the case of considering electron-phonon interaction [1,2]. Apart from these impurity factors, the Coulomb impurity problem in graphene has also been addressed. The result that below the supercritical impurity magnitude within the Wentzel-Kramers-Brillouin (WKB) approximation can solve the problem has been shown. Without impurity the semiclassical energies correctly reproduce the Landau level spectrum. When a given Landau level is given, the relation of the WKB energy and the absolute value of angular momentum in a way which is consistent with the exact diagonalization result [3]. The problem of screening of an electrically charged impurity and the rate of valley relaxation induced by charged impurities in graphene have been also considered and calculated. When Coulomb interaction is neglected, a special model of graphene is applied, the screening charge has a sign opposite to that of the impurity; the valley relaxation rate by solving the Boltzmann equation can be obtained [4,5]. The effects of spin-orbit couplings on the electron (hole) − E_{2g} phonon (The degeneration mode of iTO and LO phonon is called E_{2g} near G peak in the graphene Raman

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spectroscopy) interaction in graphene has been investigated. The effects of spin-orbit couplings on electron and hole polaron formation as well as direct-current conductivity, and spin polarizations of charge carriers have been examined. The Frohlich type Hamiltonian has be used to describe the electron-phonon system within the continuum limit [6]. All the possible stable macromolecules that unit charges can form on graphene in magnetic field have been classified. The result that the binding survives the high temperatures has been argued. Which opens the perspective to nanoscopic manipulation of ions on graphene by using macroscopic tools [7]. The key properties of cloaked states in circularly symmetric potentials have been discussed, and cloaking should be observable in quantum corral geometries via scanning tunneling probe measurements [8]. The results of full numerical Hartree-Fock study of coherent and crystalline ground states of the interacting balanced electron-hole graphene systems in small and intermediate separations with each layer occupying up to four lowest lying Landau levels have been reported. It is shown that the capacitance of some crystallized states as well as uniform coherent states are significantly enhanced compared to geometrical values solely due to Coulomb interactions and quantum corrections [9]. The problem of an unscreened Coulomb charge in graphene has been addressed and the local density of states and displaced charge as a function of energy and distance from the impurity has been calculated [10].

While most of the results of the study have concerned on electron transport properties on graphene, in fact the other properties of graphene still need to be researched. The magnetopolaron is studied in the presence of a magnetic field in monolayer graphene. The phenomenon the energy gap will be opened in the zero-energy Landau level due to the effect of polaron has been found. And the result the EG depends on square-root forms of the magnetic field strength is consistent with recent experimental measurements [11]. But the study on the phonon effect of polaron properties in monolayer graphene is rare. Because of this reason when different substrates are considered, the study on the phonon effect of polaron properties in monolayer graphene is less. Recently the polaron effects are investigated in the presence of a magnetic field based on the carrier-surface optical phonon coupling induced by the polar substrates under the graphene [12]. Meanwhile the research also become a hot research topic. But so far the research of the phonon effect on the coulomb impurity problem has almost no in monolayer graphene with different substrate. In this paper, in the case of considering the coulomb impurity problem we study the phonon effect of polaron in monolayer graphene with different substrate by using the linear combination operator and the Lee-Low-Pine variational methods. The results that we obtained are in agreement with the cyclotron resonance experiment results.

2. Theoretical model and calculations

This model assume single layer graphene is sandwiched between the substrate and the air, the strong interaction between longitudinal acoustic phonon on the surface of the substrate and the electronic (hole) in the graphene happens, and this system is supplied a perpendicular and uniform magnetic field. Its Hamiltonian is as follows:

$$H = H_e + H_{ph} + H_{e-ph} - \frac{e^2}{\mathbf{4}\pi\varepsilon\mathbf{r}} \tag{1}$$

$$H_e = V_F\begin{pmatrix} 0 & \pi_x - i\pi_y \\ \pi_x + i\pi_y & 0 \end{pmatrix} \tag{2}$$

$$\pi_x = (p_x - eBy/2) \tag{3}$$

$$\pi_y = \left(p_y + eBx/2\right) \tag{4}$$

$$H_{ph} = \sum_{k,v} \hbar\omega_{so,v} a_k^+ a_k \tag{5}$$

$$H_{e-ph} = \sum_{k,v} M_{k,v}\left(a_{-k}^+ + a_k\right) e_k^{ik\cdot r} \tag{6}$$

$$M_{k,v} = \sqrt{(Q^2 - \eta\hbar\omega_{so,v})/(2\varepsilon_0 k)}e^{-kz} \tag{7}$$

Here $\eta = (k_0 - k_{-\infty})/[(k_\infty + 1)(k_0 + 1)]$, k_∞ represents the high frequency dielectric constant, k_0 represents the low frequency dielectric constant, ε_0 represents the vacuum dielectric constant, η represents the dielectric constant of the substrate, $\omega_{sa,v}$ represents the surface acoustic phonon frequencies, the of the creation and annihilation linear combination operators b_j^+ and b_j [13] are represented as:

$$p_j = \left(\hbar\lambda\big/\sqrt{2}\right)\left(b_j^+ + b_j\right) \tag{8}$$