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Effect of off-center positively charged Coulomb impurity on Dirac states in graphene magnetic dot

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ABSTRACT

Using numerical diagonalization, we study the effect of the position of an off-center positively charged Coulomb impurity in a graphene magnetic dot, whose magnetic field profile is chosen as a Gaussian type. Numerical results show that the electron–hole symmetry is broken by the Coulomb potential and the originally zero energy states become nondegenerate and split into hole-like states. For the higher Landau levels shown, owing to the competition between the repulsive Coulomb potential and the magnetic confinement, the level orderings are reversed in the hole states at critical magnetic fields. Similar results are also obtained in the dot-size dependence of the low-lying spectra.

1. Introduction

Since the isolation of monolayer and few-layer graphene sheets by Novoselov et al. [1,2], extraordinary quantum properties [3], including room-temperature ballistic transports [4], unusual minimum conductivities [2] and anomalous quantum Hall effect [2,5,6], were subsequently reported. Of all these properties, quantum Hall effect is a useful tool for exploring the electronic structures. For graphene, the unusual sequence of the quantum Hall plateaus was observed and can be explained in terms of the Dirac-like chiral quasiparticles with a Berry phase π for the monolayer [7,8], and 2π for the bilayer [9]. This material is now emerging as a promising candidate for high density memory devices or spintronic devices, owing to its exceptionally high carrier mobility and long spin relaxation time.

Magnetic confinement of electron, or magnetic dots, in graphene is an interesting problem, since the electrons in the material, owing to the Klein effect [10], cannot be confined by pure electric field. Some possible schemes have been proposed to confine electrons by magnetic barriers. In experiments, an effective way to fabricate magnetic dots in graphene is by creating an inhomogenous magnetic field [11] using the existing technology. Deposition of appropriate ferromagnetic layers beneath the graphene layer substrate, placing thin superconducting materials on top of the samples and strain induced pseudo-magnetic fields are some of the examples. In theoretical studies, for monolayer graphene, Martino et al. have given earlier an interesting proposal to confine electrons by inhomogeneous magnetic fields [12–14]. Later on various inhomogeneous magnetic field configurations have been attempted to confine electrons or create electron bound states, including Gaussian fields [15], exponentially decaying fields [16], non-zero fields in a circular dot [17], fields corresponding to various potentials [18], and circular step fields [19]. In all these studies, discontinuous and/or inhomogeneous magnetic fields were considered to find out the field dependence of the low-lying spectra and the energy dependence of the transmission probability through the magnetic barriers, and the electron states, including bound, quasi-bound and scattering states. They all conclude that electrons can be confined by the magnetic barriers in monolayer graphene.

Doping of extrinsic impurities into these systems plays a key role in the study of this new material since it can modify the energy levels, and thus largely affects its electronic structure and optical properties. The Landau level (LL) laser is one of the potential applications in impurity-doped graphene-based quantum devices [20]. However, studies of those above-mentioned magnetic field configurations with impurities involved [21–23] in more realistic experimental situations are rare. In the present study, we are interested in the Dirac–Weyl (DW) model in the presence of an off-center positively charged Coulomb impurity and our focus is on the effect of its position on the low-lying spectra including both electron and hole states in a magnetic dot. The field profile is chosen as a Gaussian type. By employing numerical diagonalization, the low-lying spectra including positive energy,

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negative energy, and zero-energy states, and also the binding energies are calculated. Finally, we compare and analyze the qualitative difference of our numerical results between the electron and the hole states.

2. Theory

The massless DW Hamiltonian in graphene in the K and K' valley in the presence of a magnetic field describing a single electron bound to an off-center positively charged Coulomb impurity reads [21,22]

$$\hat{H} = v_F \boldsymbol{\sigma} \cdot (\mathbf{P} + e\mathbf{A}) - V_{\text{coul}}(d)\mathbf{I}, \tag{1}$$

where v_F is the electron's Fermi velocity, with the value of about 10^6 m s^{-1}. $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ and $\mathbf{I}$ are the 2×2 Pauli matrices in isospin space, and the identity matrix, respectively. $\mathbf{P}$ and $\mathbf{A}$ are the momentum operator and the vector potential in 2D space, respectively. The last term, for both diagonal matrix elements of the DW Hamiltonian, denotes the Coulomb potential between the electron and the off-center impurity:

$$V_{\text{coul}}(d) = \frac{e^2}{4\pi\varepsilon\sqrt{r^2 + d^2}}, \tag{2}$$

which depends on the separation d between the impurity and the plane of the magnetic dot. When $d=0$, the impurity is located at the center of the dot lying on the xy-plane. The minus sign in Eq. (1) indicates the Coulomb interaction between the electron and the impurity is attractive, and we suppose that this potential for the diagonalized term does not mix K and K'. Note that, in the presence of the Zeeman interaction that couples the single electron spin and the magnetic field, the whole low-lying spectra will be split and shifted by finite amounts without loss of main qualitative physical features and the Zeeman term can therefore be neglected in the present calculation. In the present case, we choose the Gaussian function as the profile of the magnetic field, which is perpendicular to the dot lying in the xy-plane, as

$$\mathbf{B} = \begin{cases} 0 & \text{for } 0 \le r < r_c, \\ B_0[1 - \exp(-(r - r_c)^2/r_0^2)]\hat{\mathbf{e}}_z & \text{for } r \ge r_c, \end{cases} \tag{3}$$

where $\hat{\mathbf{e}}_z$ is the unit vector in the z-direction. In such a profile, the field value is zero over the dot with a radius r_c and increases exponentially from zero at $r = r_c$ up to the maximum B_0 at sufficiently large r, with the overall dot size described by the effective dot radius $r_c + r_0$. The field value will be changed abruptly from zero to the maximum B_0 if r_0 approaches zero. Using the relationship between the closed line integral (the path is denoted by $\mathbf{l}$) of the vector potential $\mathbf{A}$ and the area (denoted by $\mathbf{S}$) integral of the magnetic field $\mathbf{B}$, i.e., the magnetic flux

$$\Phi(r) = \oint \mathbf{A} \cdot d\mathbf{l} = \int \mathbf{B} \cdot d\mathbf{S}. \tag{4}$$

We can then get the following expression for the corresponding vector potential A, with circular symmetry, and in polar coordinate as

$$\mathbf{A} = \begin{cases} 0 & \text{for } 0 \le r < r_c, \\ \left\{ \dfrac{B_0}{2}\dfrac{(r^2 - r_c^2)}{r} \right. & \\ \left. - \dfrac{B_0 r_0^2}{2r}\left[1 - \exp\left(-\dfrac{(r - r_c)^2}{r_0^2}\right)\right] \right. & \\ \left. - \dfrac{B_0 r_c r_0 \sqrt{\pi}}{2r}\,\text{erf}\left(\dfrac{r - r_c}{r_0}\right) \right\}\hat{\mathbf{e}}_\theta & \text{for } r \ge r_c, \end{cases} \tag{5}$$

where $\hat{\mathbf{e}}_\theta$ is the unit vector in the azimuthal direction and erf(x) is an error function. In experiments, the inhomogeneous magnetic fields in such a system can be created by placing a superconducting material of circular shape on top of the graphene to repel an external magnetic field, and the field at the boundary may be smoothed as a Gaussian profile due to the edge effect.

Before numerical diagonalization, the DW Hamiltonian is first simplified and separated into two parts:

$$\hat{H} = \hat{H}_0 + \hat{V}, \tag{6}$$

where the unperturbed term $\hat{H}_0$ and the residual potential term are given by

$$\hat{H}_0 = v_F \begin{pmatrix} 0 & \hat{\pi}_0^- \\ \hat{\pi}_0^+ & 0 \end{pmatrix} \tag{7}$$

with

$$\hat{\pi}_0^{\pm} = \pm j \exp(\pm j\theta)\left[\mp\hbar\frac{\partial}{\partial r} + \frac{l\hbar}{r} + \frac{erB_0}{2}\right], \tag{8}$$

and

$$\hat{V} = \begin{pmatrix} \hat{V}_{\text{coul}} & \hat{V}_+ \\ \hat{V}_- & \hat{V}_{\text{coul}} \end{pmatrix}, \tag{9}$$

respectively. The two-component spinor, as bases for numerical diagonalization, with each component corresponding to the sublattice of graphene, is written as

$$\Psi_{nl}^T = (\phi_{N-1,l-1} \;\; j\phi_{N,l}), \tag{10}$$

where the symbol j in Eqs. (8) and (10) is the imaginary unit. $\phi_{N,l}$ can be chosen as the well-known 2D harmonic product basis states [15], with nonnegative integer LL index $N[\equiv n + (l + |l|)/2]$. n and $l\hbar$ are the radial quantum number and the orbital angular momentum, respectively. The phase factor $\exp(\pm j\theta)$ for both off-diagonal matrix elements in $\hat{H}_0$ and also in $\hat{V}$, as given later, can be canceled out after integration, since the angular momenta of the two spinor components are differed by one unit. The two operators in $\hat{H}_0$ are regarded as raising and lowering operators. Therefore, the corresponding eigenvalue for the $\hat{H}_0$ is obtained by $E_{N,l} = \pm N^{1/2}$ in the energy unit of $\hbar\omega(\equiv \sqrt{2}v_F\hbar/a)$ with the magnetic length $a(\equiv \sqrt{\hbar/eB_0})$. The $\pm$ sign represents the electron–hole symmetry. Although the quantum states of the two spinor components are different, see Eq. (10), for easy comparison, we use the same notations for the quantum states of those electron–hole pairs in the present article without affecting our analysis, according to their LL indices, N. Here we use the following typical parameters for realistic experiment to illustrate one point for the Hamiltonian (Eq. (1)). B_0 is set to be 1.00 mT, and a will be 800 nm which is greater than the lattice spacing. The transformation $\mathbf{P} \to \mathbf{P} + e\mathbf{A}$ is therefore valid in this continuum model.

In Eq. (9), the matrix elements of the residual potential are rewritten in dimensionless unit, after simplification, as

$$\hat{V}_{\text{coul}} = \frac{C}{\sqrt{r^2 + d^2}}, \tag{11}$$

$$\hat{V}_{\pm} = \mp j \exp(\mp j\theta) \times \frac{-F(r)}{2\sqrt{2}r}, \tag{12}$$

where

$$F(r) = \begin{cases} r^2 & \text{for } 0 \le r < r_c, \\ r_c^2 + r_0^2\left[1 - \exp\left(-\dfrac{(r - r_c)^2}{r_0^2}\right)\right] & \\ \quad + r_c r_0 \sqrt{\pi}\,\text{erf}\left(\frac{r - r_c}{r_0}\right) & \text{for } r \ge r_c, \end{cases} \tag{13}$$