Comparison of Coulomb Impurity, Longitudinal Acoustic Phonons, and Surface Optical Phonons Affecting the $n = 0$ Landau Level in Monolayer Graphene

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1. Introduction

In recent years, layered systems such as graphene with a substrate have been attracting a strong interest in applied physics since they have many unique physical properties. However, the gapless nature of graphene limits its application in electronic devices. Up to now, the most direct way to open the energy gap (EG) is to apply a magnetic field perpendicular to the graphene [1], in which the energy of an electron near the K-point is quantized into nonequidistant Landau levels, leading to the $n = 0$ Landau level (LL) splitting and the abnormal quantum Hall effect [2]. Besides, there are many methods to enhance the EG opening, such as electron-phonon interactions [3, 4], and doped impurity effects [5, 6].

In the presence of an external magnetic field, the effects of the electron-phonon longitudinal acoustic (LA) phonons in the graphene plane and the surface optical (SO) phonons on the substrate have been discussed for the assistant mechanism of EG opening. Li et al. [7] investigated the EG opened by the coupling between the electron and LA phonons and found both linear and square root relations between the EG and the magnetic field. Recently, Sun and Xiao [8] studied the effects of LA phonons in a monolayer graphene plane on the ground state energy of a magnetopolaron under different temperatures to indicate the energy splitting. But the energy gap opened by LA phonons in Refs. [7, 8] is only several meV. Wang et al. [9] investigated the effect of SO phonons from a polar substrate on the EG of $n = 0$ LL, and it was found to have a 40 meV constant of EG while increasing the external magnetic field. But it was confirmed that the EG can be enlarged with the increase of the magnetic field while an impurity appears in experiments [10, 11].

Xiao et al. [12] discussed both the effects of Coulomb impurities and SO phonons from the substrate on the $n = 0$ LL splitting. It was found the splitting energy could vary on a large scale due to a Coulomb impurity. Unfortunately, a constant relative dielectric function related to the screening effect was adopted in their calculation. Recently, we discussed the influences of a screened charge impurity with an inconstant dielectric function and carrier-SO phonons on the $n = 0$ LL in monolayer graphene [13]. A weak carrier-phonon coupling was adopted in our computation. However, it is more practical to discuss the arbitrary carrier-phonon coupling for monolayer graphene with a substrate since there are different kinds of phonons.

The influences of a charged Coulombic impurity with screened effect and carrier-phonon interaction on the $n = 0$ Landau level in monolayer graphene with a polar substrate under a high static magnetic field are discussed to compare the competition among the impurities, the longitudinal acoustic phonons in the graphene plane and the surface optical phonons on the substrate. A method of linear combination operators is used to deal with the position and momentum of a carrier in a magnetic field. The method of Lee-Low-Pines variation with an arbitrary carrier-phonon coupling is adopted to derive the effects of phonons. It is found that the energy gap of $n = 0$ Landau level opened by carrier-longitudinal acoustic phonons cannot be the main mechanism, whereas both the carrier-surface optical phonon interaction and the carrier-impurity interaction play the main roles in determining the energy splitting.

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In this work, the coupling between a carrier both with LA deformation phonons in the graphene plane and SO phonons on the substrate, and the influence of a screened Coulomb impurity from the substrate are considered to affect the splitting of $n = 0$ LL under a static magnetic field. An arbitrary carrier-phonon coupling is adopted to derive the effect of phonons by using the Lee-Low-Pines variation method [14]. The effect of the screened Coulomb potential induced by the charged impurity is examined by using the dielectric function under the random-phase approximation (RPA). A linear combination operator method [15] is adopted to derive the effect of the magnetic field. Our results show the competition of the above three effects on the EG of $n = 0$ LL splitting. Our model can provide a theoretical explanation for the experimental measurements [16, 17] of opening the EG in the monolayer graphene with a substrate.

2. Model and Theory

As shown by Figure 1(a), the monolayer graphene is taken along the $x$-$y$ plane under a uniform static magnetic field $B$ along the $z$ direction and the carrier (electron and hole) is located at $\mathbf{R} = (r, 0)$, where $r = (x, y)$ is the position vector in the graphene plane. A single charged impurity with charge number $Z$ is located at $\mathbf{R}_0 = (0, -z_0)$ and provides a Coulomb potential in the graphene plane as plotted in Figure 1(b). The Hamiltonian of the carrier, LA phonons, SO phonons, and the impurity [5, 7, 12] can be expressed as

$$H = H_c + H_{LA} + H_{c-LA} + H_{SO} + H_{c-SO} + H_{c-i},$$

where

$$H_c = V_F \begin{pmatrix} 0 & \pi_x - i\pi_y \\ \pi_x + i\pi_y & 0 \end{pmatrix},$$

$$H_{LA} = \sum_k \hbar \omega_{LA} a_k^\dagger a_k,$$

$$H_{c-LA} = \sum_{k,\nu} M_{LA,\nu} \begin{pmatrix} i 0 \\ 0 i \end{pmatrix} (a_k^\dagger + a_k) e^{ikr},$$

$$H_{SO} = \sum_{k,\nu} \hbar \omega_{SO,\nu} b_{k,\nu}^\dagger b_{k,\nu},$$

$$H_{c-SO} = \sum_{k,\nu} M_{SO,\nu} \begin{pmatrix} b_k^\dagger + b_k \end{pmatrix} e^{ikr},$$

$$H_{c-i} = \frac{\beta Z e^2}{4\pi\varepsilon_0 |\mathbf{R} - \mathbf{R}_0|}.$$  

Equation (2a) is denoted by $H_c$, stands for the carrier (electron and hole) kinetic energies and $V_F$ is the Fermi velocity of carriers. The magnetic field $\mathbf{B}$ is in a symmetric gauge and satisfies $\pi_x = (p_x + \beta eB y/2)$ and $\pi_y = (p_y - \beta eB x/2)$ with $p_x$ and $p_y$ as the electron (hole) momentum operators. In the Hamiltonian $\beta = +$ and $\beta = -$ denote hole and electron, respectively. Equations (2b)–(2e) represented by $H_{LA}, H_{c-LA}, H_{SO},$ and $H_{c-SO}$ describe the LA phonon energy, electron (hole)–LA phonon coupling energy, the SO phonon energy, and electron (hole)–SO phonon coupling energy, respectively. In equations (2b) and (2d), $a_k^\dagger$ and $b_k^\dagger$ are the creation (annihilation) operators of LA and SO phonons with wave vector $k$, respectively. Subscript $v$ ($v = 1, 2$) is the branch of SO phonons with frequency $\omega_{SO,v}$. In equation (2f), $M_{SO,\nu} = D k \sqrt{\omega_{SO,\nu}}/\hbar$ is the electron (hole)–LA phonon interaction with the phonon dispersion relation $\omega_{LA} = \nu LA k$ in the graphene plane, and $\nu_{LA}$ is the velocity of the LA wave. Here, $A$ represents the area of the monolayer graphene, $D$ is the deformation potential constant, and $\rho$ is the mass density. In equation (2e), $M_{SO,k,\nu} = \sqrt{(\varepsilon_0^2 \eta \omega_{SO,v})/ (2\varepsilon_0^2 \kappa_0)} \exp(-kz')$ is the electron (hole)–SO phonon interaction with the parameter of polarization strength $\eta = (\kappa_0 - \kappa_\infty)/[(\kappa_0 + 1)(\kappa_\infty + 1)]$ for the substrate, with $\kappa_0$ as the static dielectric constant and $\kappa_\infty$ as the electric dielectric constant, $z'$ represents the distance from the graphene to the substrate. Equation (2f) denoted by $H_{c-i}$ is the carrier-impurity Coulomb energy describes the interaction between the electron (hole) and impurity, $\varepsilon_0$ as the permittivity of vacuum, and $\varepsilon$ as the relative static dielectric constant for impurity in the substrate, respectively.

A two-dimensional transform of the Fourier series for equation (2f) can be performed as [12, 18, 19]

$$H_{c-i} = \frac{\beta Z e^2}{2\varepsilon_0 \varepsilon k} \sum_k \frac{1}{|k|} \exp(i\mathbf{k} \cdot \mathbf{r}) \exp(-kz_0).$$

Applying the well-known Lee-Low-Pines (LLP) theory [14] which was extensively used to deal with the problem of polaron, a unitary transformation can be performed by [15]

$$U_1 = \exp \left(-i\alpha_1 \sum_k \mathbf{k} \cdot \mathbf{r} a_k^\dagger a_k - i\alpha_1 \sum_{k,\nu} \mathbf{k} \cdot \mathbf{r} b_k^\dagger b_k \right),$$

$$U_2 = \exp \left(\sum_k (g_k f_k^\dagger a_k + g_k^* f_k b_k^\dagger b_k) + \sum_{k,\nu} (g_{k,\nu} f_k^\dagger b_{k,\nu} + g_{k,\nu}^* f_k b_{k,\nu}) \right),$$

where $f_k, f_k^*$, $g_{k,\nu},$ and $g_{k,\nu}^*$ are the variational parameters, $\alpha_1$ and $\alpha_2$ are variational parameters related to the carrier-phonon coupling. The linear combination of creation and annihilation operators $B_j^\dagger$ and $B_j$ for the position and momentum of an electron (hole) is adopted by

$$j = \left(\frac{i}{\sqrt{2\lambda}} \right) (B_j - B_j^\dagger),$$

$$p_j = \left(\frac{\hbar k}{\sqrt{2}} \right) (B_j^\dagger + B_j),$$

where index $j$ refers to the coordinates $x, y$ and $\lambda = \sqrt{\varepsilon B/2\hbar}.$

Substituting equations (4)–(7) into equation (1), and performing the LLP transformation, one can get

$$H' = U_{c-i}^\dagger U_{c-i} H U_{c-i} U_{c-i}^\dagger.$$
where
\[ H'_c = U^{-1}_c U^{-1}_c H_c U_c U_2 = V_F \left\{ \begin{array}{cc} 0 & H'_{c,12} \\ H'_{c,21} & 0 \end{array} \right\}, \]
with
\[ H'_{c,12} = \left( \frac{\hbar a}{\sqrt{2}} (B'_x + B'_z) - \left( \frac{\beta e B}{2\hbar} \right) (B_x - B'_z) \right) \]
\[ - \left( \frac{i eB}{\sqrt{2}} \right) (B'_x + B'_y) + \left( \frac{i eB}{2\hbar} \right) (B_y - B'_y) \]
\[ - \alpha_1 h \sum_k k_x (a'_k + f'_k) (a_k + f_k) \]
\[ + \alpha_2 h \sum_k k_x (b'_k + g'_k) (b_k + g_k) \]
\[ H'_{c,21} = \left( \frac{\hbar a}{\sqrt{2}} (B'_x + B'_z) - \left( \frac{\beta e B}{2\hbar} \right) (B_x - B'_z) \right) \]
\[ + \left( \frac{i eB}{\sqrt{2}} \right) (B'_x + B'_y) + \left( \frac{i eB}{2\hbar} \right) (B_y - B'_y) \]
\[ - \alpha_1 h \sum_k k_x (a'_k + f'_k) (a_k + f_k) \]
\[ - \alpha_1 h \sum_k k_x (a'_k + f'_k) (a_k + f_k) \]
\[ - \alpha_2 h \sum_k k_x (b'_k + g'_k) (b_k + g_k) \]
\[ - \alpha_2 h \sum_k k_x (b'_k + g'_k) (b_k + g_k) \]
\[ H_{L,k} = U^{-1}_c U^{-1}_c H_{L,k} U_c U_2 \]
\[ = \sum_k \hbar \omega_{L,k} (a'_k a_k + a_k f_k' + f_k' a_k + f_k f_k'), \]
\[ H_{c-L,k} = U^{-1}_c U^{-1}_c H_{c-L,k} U_c U_2 \]
\[ = \left\{ \begin{array}{ccc} i & 0 & \left\{ \sum_k M_{L,k} (a'_k + f'_k) \exp[-(1 - \alpha_1)^2 k^2/4\lambda^2] \right\} \\ 0 & i & \exp\left( \frac{1}{\sqrt{2} \lambda} \sum_j k_j B'_j \right) \exp\left( \frac{1}{\sqrt{2} \lambda} \sum_j k_j B_j \right) \right. \]
\[ + \sum_k M_{L,k} (a_k + f_k) \exp[-(1 - \alpha_1)^2 k^2/4\lambda^2] \]
\[ \times \exp\left( \frac{1}{\sqrt{2} \lambda} \sum_j k_j B'_j \right) \exp\left( \frac{1}{\sqrt{2} \lambda} \sum_j k_j B_j \right) \right\}. \]
\[ H_{SO} = U^{-1}_c U^{-1}_c H_{SO} U_c U_2 \]
\[ = \sum_{k,v} \hbar \omega_{SO,v} (b^+_k g_k + g^+_k b_k) \exp\left[ -\left(1 - \alpha_1\right)^2 k^2/4\lambda^2 \right] \]
\[ \times \exp\left( \frac{1}{\sqrt{2} \lambda} \sum_j k_j B'_j \right) \exp\left( \frac{1}{\sqrt{2} \lambda} \sum_j k_j B_j \right) \]
\[ + \sum_{k,v} M_{SO,k,v} (b^+_k g_k + g^+_k b_k) \exp\left[ -\left(1 - \alpha_1\right)^2 k^2/4\lambda^2 \right] \]
\[ \times \exp\left( \frac{1}{\sqrt{2} \lambda} \sum_j k_j B'_j \right) \exp\left( \frac{1}{\sqrt{2} \lambda} \sum_j k_j B_j \right). \]
\[ H_{c-SO} = U^{-1}_c U^{-1}_c H_{c-SO} U_c U_2 \]
\[ = \sum_{k,v} M_{c-SO,k,v} (b^+_k g_k + g^+_k b_k) \exp\left[ -\left(1 - \alpha_1\right)^2 k^2/4\lambda^2 \right] \]
\[ \times \exp\left( \frac{1}{\sqrt{2} \lambda} \sum_j k_j B'_j \right) \exp\left( \frac{1}{\sqrt{2} \lambda} \sum_j k_j B_j \right). \]
\[ H_{c-i} = U^{-1}_c U^{-1}_c H_{c-i} U_c U_2 \]
\[ = \sum_{k} \left[ \beta Z e^2 \left\{ \begin{array}{c} \frac{1}{2 A \epsilon e k} \exp\left( \frac{1}{\sqrt{2} \lambda} \sum_j k_j B'_j \right) \\ \exp\left( \frac{1}{\sqrt{2} \lambda} \sum_j k_j B_j \right) \right. \right\} \right]. \]

The wavefunctions of the n = 0 LL system in a magnetic field can be written as [1]
\[ |\psi_{0,e}\rangle|0 >_{LA}|0 >_{SO} = \left( \begin{array}{c} 0 \\ |0 >_{LA} \end{array} \right) |0 >_{LA}|0 >_{SO}, \]
\[ |\psi_{0,h}\rangle|0 >_{LA}|0 >_{SO} = \left( \begin{array}{c} |0 >_{LA} \\ 0 \end{array} \right) |0 >_{LA}|0 >_{SO}, \]
for the electron in the K' valley and
\[ |\psi_{0,e}\rangle|0 >_{LA}|0 >_{SO} = \left( \begin{array}{c} 0 \\ |0 >_{LA} \end{array} \right) |0 >_{LA}|0 >_{SO}, \]
for the hole in the K valley, where |y > 0 e (|y > 0 h) denotes the eigenfunction of the electron (hole). In equations (11a) and (11b), |0 >_{LA} and |0 >_{SO} represent the zero LA and SO phonon states, respectively, which satisfies \[ a'_k |0 >_{LA} = |1 >_{LA}, \]
\[ b'_k |0 >_{SO} = |1 >_{SO}, \]
and \[ a_k |0 >_{LA} = b_k |0 >_{SO}. \] The eigenenergy of the system \[ H_c \] can be obtained via [12, 16]
\[ E_{c,0}^2 = SO < |0 >_{LA}|\psi_0|H_{c}^2|\psi_0|0 >_{LA}|0 >_{SO}. \]

Furthermore, one can get
\[ E_{c,0} = \pm \sqrt{E_{c,0}^2} = \beta \left( \sum_k \alpha_k V F h k f'_k f_k + \sum_{k,v} \alpha_k V F h g_k g'_k f_k f_k' \right). \]

The eigenenergy of the total system corresponding to the n = 0 LL can be expressed as
E_0 = \beta \left( \sum_k \alpha_1 V_p \hbar k f_k^* f_k + \sum_k \alpha_2 V_p \hbar k g_k^* g_k \right) + \sum_{n=0} \left| \psi_0 \right| H_{n,LA} |\psi_0 \rangle + H_{c-LA} + H_{c-SO} + H_{c-\epsilon_0} \left| \psi_0 \right| \langle 0_{n} | 0_{SO} \rangle

= \beta \sum_k \left[ \alpha_1 V_p \hbar k f_k^* f_k + \alpha_2 V_p \hbar k g_k^* g_k \right] + \sum_k \left[ M_{LA,k} f_k^* f_k + h\omega_{LA} f_k^* f_k \right] + \sum_{k,\nu} \left[ \alpha_1 V_p \hbar k g_k^* g_k + h\omega_{SO,k} g_k^* g_k \right] + M_{SO,k,v} g_k^* g_k + \frac{Ze^2}{2\lambda\eta\varepsilon_k} \left( \frac{k^2}{4\lambda^2} - k z_0 \right) .

(14)

Minimizing equation (14) with respect to \( f_k, f_k^*, g_k, g_k^* \), and \( g_{k,v}^* \), one has

\[ f_k = \left( \frac{-iM_{LA,k}}{\alpha_1 V_p \hbar k + h\omega_{LA}} \right) \exp \left[ -(1 - \alpha_1)^2 \frac{k^2}{4\lambda^2} \right] , \quad (15) \]

\[ f_k^* = \left( \frac{-iM_{LA,k}^*}{\alpha_1 V_p \hbar k + h\omega_{LA}} \right) \exp \left[ -(1 - \alpha_1)^2 \frac{k^2}{4\lambda^2} \right] , \quad (16) \]

\[ g_k = \left( \frac{-M_{SO,k,v}}{\alpha_2 V_p \hbar k + h\omega_{SO,v}} \right) \exp \left[ -(1 - \alpha_2)^2 \frac{k^2}{4\lambda^2} \right] , \quad (17) \]

\[ g_k^* = \left( \frac{-M_{SO,k,v}^*}{\alpha_2 V_p \hbar k + h\omega_{SO,v}} \right) \exp \left[ -(1 - \alpha_2)^2 \frac{k^2}{4\lambda^2} \right] . \quad (18) \]

Substituting equations (15)–(18) into equation (14), one can obtain

\[ E_{0,k} = E_{c-LA,k} + E_{c-SO,k} + E_{c-\epsilon_0,k} \]

\[ = \sum_k \left[ \left| M_{LA,k} \right|^2 \exp \left[ -(1 - \alpha_1)^2 \left( \frac{k^2}{2\lambda^2} \right) \right] \right] \frac{\alpha_1 V_p \hbar k + h\omega_{LA}}{\alpha_1 V_p \hbar k + h\omega_{LA}}

\[ + \sum_{k,\nu} \left[ \left| M_{SO,k,v} \right|^2 \exp \left[ -(1 - \alpha_2)^2 \left( \frac{k^2}{2\lambda^2} \right) \right] \right] \frac{\alpha_2 V_p \hbar k + h\omega_{SO,v}}{\alpha_2 V_p \hbar k + h\omega_{SO,v}}

\[ + \sum_k \left[ \frac{Ze^2}{2\lambda\eta\varepsilon_k} \exp \left( \frac{k^2}{4\lambda^2} - k z_0 \right) \right] \frac{k}{2\pi\nu_{LA}} \exp \left[ -(1 - \alpha_2)^2 \left( \frac{k^2}{2\lambda^2} \right) \right] - 2k z_0 \right] \frac{dk}{4\pi\varepsilon_0 (\alpha_2 V_p \hbar k + h\omega_{SO,v})}

\[ + \int_0^\infty \sum_{k,\nu} \frac{Ze^2}{4\pi\varepsilon_0 k} \exp \left( \frac{k^2}{4\lambda^2} - k z_0 \right) \frac{dk}{4\pi\varepsilon_0 (\alpha_2 V_p \hbar k + h\omega_{SO,v})} . \quad (19) \]

In the previous works, \( \alpha_1 = \alpha_2 = 0 \) as a strong coupling [7] and \( \alpha_1 = \alpha_2 = 1 \) as a weak coupling [13] for carrier-phonon interaction were discussed, respectively. However, we take the variational minimum of equation (19) with respect to \( \alpha_1 \) and \( \alpha_2 \) as arbitrary coupling in our calculation. In equation (19), the ground state \( E_0 \) splits into two branches \( E_{0,+} \) and \( E_{0,-} \) for the hole and electron in the \( n = 0 \) LL under a high magnetic field, respectively. Therefore, the EG of \( n = 0 \) LL splitting can be determined by 2\( A = E_{0,+} - E_{0,-} \). Here, \( E_{c-LA,k} \), \( E_{c-SO,k} \), and \( E_{c-\epsilon_0,k} \) are the carrier-LA phonon, carrier-SO phonon, and carrier-impurity interaction splitting energy, respectively. The upper limit of the integral for the first term on the right side of equation (19) was adopted as a larger cut-off wave number \( k_c \) [7, 9].

In the present work, the \( c-i \) interaction potential can be represented by the Coulomb potential intensity \( V_k = 2n\beta Z e^2 / 4\pi\varepsilon_0 k \) in the third term on the right side of equation (19). Taking into account the usual RPA, the screened \( c-i \) Coulomb interaction potential is obtained as
In our computation, the parameters used in Sec. 2 are adopted as $V_F \approx 10^8 m/s$ [9], $D = 50 eV/LA = 2.0 \times 10^4 m/s$, $\rho = 7.5 \times 10^{-7} kg/m^3$ [7, 23], $Z = 1$ and $zt = 0$. For $z_0 = 0$ since the impurity is in the graphene plane, static dielectric constants $\varepsilon = 2.50$ and $2.30$ [1] are the average of the dielectric constant of the vacuum and that of the substrate for SiO$_2$ and h-BN, respectively. For $z_0 > 0$, since the impurity is in the substrate, $\varepsilon = 3.90$ and 3.57 are adopted as shown in Table 1. The other parameters used in our computation are given in Table 1.

The comparisons of the splitting of $n = 0$ LL for SiO$_2$ (a) and h-BN (b) substrate with $z_0 = 2.0 nm$ and $k_c = 5.0 \times 10^8 m^{-1}$ are depicted in Figure 2. It can be seen that the EG of $n = 0$ LL split by LA phonons varies only 1–2 meV with the magnetic field both on SiO$_2$ and on h-BN substrate, and the splitting increases gradually with the increase of the magnetic field. The dependence of $n = 0$ LL splitting on magnetic field changes into the form of square root from linear form as considering the effect of SO phonons and $c-i$ interaction. Such a relationship is in agreement with experiments [10, 17].

Figure 3 gives each component of splitting energy $\Delta \varepsilon$ as a function of the magnetic field for SiO$_2$ (a) and h-BN (b) substrate with $z_0 = 2.0 nm$ and $k_c = 5.0 \times 10^8 m^{-1}$. The EG of the $n = 0$ LL opened by LA phonons has a gentle linear relationship with the magnetic field both for SiO$_2$ and h-BN as substrates. It can be clearly seen that the splitting energy can be expanded significantly by the screened Coulombic potential of the charged impurity and increases with the increase of the magnetic field. It can be found that the contribution from the carrier-SO phonons on a substrate and the carrier-impurity interaction play the main roles.

Figure 4 shows the splitting energy $\Delta \varepsilon$ as a function of the magnetic field for SiO$_2$ and h-BN as substrates with $k_c = 5.0 \times 10^8 m^{-1}$ and different $z_0$. It can be seen that $\Delta \varepsilon$ increases with increasing the magnetic field due to the Lorenz

### Table 1: Physical parameters for graphene with SiO$_2$ and h-BN substrates used in the computation.

| Quantity (units) | $\hbar \omega_{SO,1}$ (meV) | $\hbar \omega_{SO,2}$ (meV) | $\kappa_0 (\varepsilon_0)$ | $\kappa_{\infty} (\varepsilon_0)$ |
|------------------|----------------------------|----------------------------|---------------------------|-----------------------------|
| SiO$_2$          | 146.5$^a$                  | 60.0$^a$                   | 3.90$^a$                  | 2.50$^a$                    |
| h-BN             | 195.7$^b$                  | 101.7$^b$                  | 3.57$^c$                  | 2.95$^c$                    |

$^a$ Reference [24]. $^b$ Reference [25]. $^c$ Reference [26].

$V_{sc}^R = V_k^R k^R \varepsilon_{PL}(k)$, where $\varepsilon^R(k) = \varepsilon^R \varepsilon(k, \omega = 0)$ is the static dielectric function in graphene on polar substrates. Therefore, the screened carrier-impurity Coulomb interaction potential in equation (19) can be replaced by $V_{sc}^R$ and $\varepsilon \rightarrow \varepsilon^R(k, \omega = 0)$ [19–21]. Here, $\varepsilon^R(k, \omega = 0)$ in graphene with air on one side and SiO$_2$ substrate on the other for $n = 0$ LL has been discussed in detail in Ref. [21, 22] and it can be expressed as

$$\varepsilon^R(k, \omega = 0) \approx 1 + \frac{k k^c_{vac}(k^2)}{\sqrt{2}},$$

where $l = 1/\sqrt{2} \lambda$ is the magnetic length and $\xi_{vac}(k^2)$ is the vacuum polarization function, whose specific form was given by equation (4.4) in Ref. [22]. The relation curves between $\varepsilon^R(k)$ of $n = 0$, LL and $k/\lambda$ for SiO$_2$ and h-BN substrate have plotted in our previous work [13]. Substituting equation (20) into equation (19), the numerical results can be obtained.

### 3. Results and Discussion

In our computation, the parameters used in Sec. 2 are adopted as $V_F \approx 10^8 m/s$ [9], $D = 50 eV/LA = 2.0 \times 10^4 m/s$, $\rho = 7.5 \times 10^{-7} kg/m^3$ [7, 23], $Z = 1$ and $zt = 0$. For $z_0 = 0$ since the impurity is in the graphene plane, static dielectric constants $\varepsilon = 2.50$ and 2.30 [1] are the average of the dielectric constant of the vacuum and that of the substrate for SiO$_2$ and h-BN, respectively. For $z_0 > 0$, since the impurity is

\[ V_{sc} = V_k^R k^R \varepsilon_{PL}(k), \] where $\varepsilon^R(k) = \varepsilon^R \varepsilon(k, \omega = 0)$ is the static dielectric function in graphene on polar substrates. Therefore, the screened carrier-impurity Coulomb interaction potential in equation (19) can be replaced by $V_{sc}^R$ and $\varepsilon \rightarrow \varepsilon^R(k, \omega = 0)$ [19–21]. Here, $\varepsilon^R(k, \omega = 0)$ in graphene with air on one side and SiO$_2$ substrate on the other for $n = 0$ LL has been discussed in detail in Ref. [21, 22] and it can be expressed as

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### 3. Results and Discussion

In our computation, the parameters used in Sec. 2 are adopted as $V_F \approx 10^8 m/s$ [9], $D = 50 eV/LA = 2.0 \times 10^4 m/s$, $\rho = 7.5 \times 10^{-7} kg/m^3$ [7, 23], $Z = 1$ and $zt = 0$. For $z_0 = 0$ since the impurity is in the graphene plane, static dielectric constants $\varepsilon = 2.50$ and 2.30 [1] are the average of the dielectric constant of the vacuum and that of the substrate for SiO$_2$ and h-BN, respectively. For $z_0 > 0$, since the impurity is
effect and decreases with increasing $z_0$ since the increase of $z_0$ can weaken the carrier-impurity interaction. Therefore, the energy of the $n = 0$ LL splitting can be modulated by the position of a charged impurity. Significantly, there is an obvious change in the splitting energy $2\Delta$ (from the black line to the red line) when the impurity moves from the graphene plane to the substrate due to the change in the dielectric environment around the impurity. In addition, there is only the impurity energy correction corresponding to angular momentum $j = \pm 1/2$ of $n = 0$ LL in Ref. [11], and the effects of different angular momentums on the modification of impurity energy will be the subject of further work.

4. Conclusion

In summary, the influence of carrier-LA phonons, carrier-SO phonons, and the carrier-impurity interaction on the EG of $n = 0$ LL splitting in monolayer graphene with a substrate under a static magnetic field is investigated theoretically. The dependence of splitting energy on the magnetic field strength and position of the charged Coulombic impurity are also discussed. Our results show that the EG split by LA phonons is smaller enough to be neglected, the main contributions to the splitting depend on SO phonons and the screened Coulombic impurity, and our model could provide a possible theoretical explanation for previous experiments.
Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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