Optical signature of bipolaron in monolayer transition metal dichalcogenides: all coupling approach

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Abstract
We studied the optical signature of bipolaron and its effects on the bandgap modulation in the single-layer Transition Metal Dichalcogenides (TMDs) under magnetic field. Using the Huybrecht method, we derived the ground state energies in the modified zero Landau levels for all Fröhlich coupling constants. We take into account both intrinsic longitudinal optical phonon modes and surface optical phonon modes induced by the polar substrate. We observed that the higher the coupling strength, the stronger is the magnetic field effect. The highest amplitude of the bandgap modulation is obtained for the MoS2 monolayer and the lowest with the WSe2 monolayer. We also found that the bipolaron is stable in TMDs. It is seen that the optical absorption presents the threshold values and respectively increases for WSe2, MoSe2, WS2 and MoS2.

Keywords Bipolaron · Bandgap · Magnetic field, TMDs · Electron-phonon interaction

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1 Introduction

Transition metal dichalcogenides belong to the family of lamellar materials of formula MX$_2$. M is a transition metal of group IV, V or VI of the periodic classification table and X is a chalcogen. Electronically, it covers a wide range of properties from insulator to semiconductor and to the metal (Gordon et al. 2002). Two-dimensional (2D) TMDs is a new generation of thin atomic material with special physical properties. Today, these materials are the focus of much scientific research (Choi et al. 2017; Kenfack-Sadem et al. 2020). Compared to graphene, the direct bandgap of TMDs has been reduced, with potential applications for high electron mobility transistors and light-emitting diodes (Mak et al. 2010). Due to the ability to control the size of the 2D TMDs bandgap, the TMDs bandgap has become one of the most important studies in semiconductor physics (Kang et al. 2017; Lee et al. 2020).

Polaron is an entity discovered in 1933 by Landau (1993), it is used to describe interaction between free charge carriers and induced polarization coming from electron (hole)-atom coupling in solid material. This quasiparticle is characterized by some properties as effective mass, energy mobility and absorption coefficient, etc. These properties strongly depend on the interaction between charge carriers, crystal lattice and the frequency of charge carriers (Kandemir and Akay 2017; Fobasso et al. 2020). Depending on the way the size of lattice distortion is, comparing to lattice constant, there are two types of polarons: large polarons and small polarons (Emin 2018; Xin-Ran et al. 2013; Liu et al. 2019). The bipolaron is created when two identical polaron interact in the crystal lattice. Bipolaron formation is influenced by the difference between the coulombic repulsion of charge carriers and theirs attraction with lattice.

Many theoretical works investigated the polaron in 2D structure through the chemical composition (Yin et al. 2012), the geometrical shapes of the material (Lee et al. 2012), the lattice constant (Ni et al. 2012; Lee et al. 2017) and by applying an external electric field (Nguepnang et al. 2021). Other theoretical works exhibit high bandgap renormalization (Thygesen 2017; Ugeda et al. 2014). Experimental work shows that polar substrates are important in the study of the physical properties of TMDs (Liu et al. 2016; Raja et al. 2017) and also highlights the importance of the Van der Waals interaction (Ugeda et al. 2014; Withers et al. 2015; Trolle et al. 2017) in TMDs. Based on these results, it appears that the environment may affect the TMDs bandgap. In a recent paper (Xiao et al. 2017), the study of the modulated bandgap in 2D single-layer TMDs derived from carrier-optic phonon coupling in the Fröhlich model showed that the bandgap magnitude can be modulated in the range of 100-500meV by changing different polar substrates and by varying the internal distance between the TMDs and the polar substrates. This study only considered the weak coupling regime. Nevertheless, it is necessary to explore all coupling regimes while studying bipolarons in order to better understand the modulation bandwidth and the stability in TMDs. Optical conductivity and infrared absorption characterized by the optical absorption coefficient of the Fröhlich polaron have been studied in polar semiconductors and ion crystals (Devreese 2007; Devreese and Alexandre 2009; Devreese and Polaron 1611). Experimental and theoretical works have been used to derive the optical absorption (Koschorreck et al. 2012; Klimin and Devreese 2014; Sezen et al. 2015). Recently, Li and Wang studied the optical absorption coefficient of the Fröhlich polaron in single-layer TMDs taking into account both LO and SO phonons (Li and Wang 2018). They derived the optical absorption using the Devreese-Huybrechts-Lemmens model in the low temperature...
limit for the weak coupling between the electron and the phonon. However, the optical absorption of bipolaron in TMD, to our awareness, has not been sufficiently studied.

In this work, we first present the effect of the bipolaron for all coupling regime on the modulated bandgap in a two-dimensional TMDs quantum dot supported by a polar substrate in the presence of an external magnetic field in the third direction. We study the optical absorption of bipolaron in TMDs for all coupling regime. The optical phononic modes are strongly coupled with the carriers in 2D TMDs (Chow et al. 2017), which leads to the formation of the polar state (Chen et al. 2017). We have taken into account the intrinsic longitudinal optical phononic modes (LO) and the surface optical phononic modes (SO) induced by the polar substrate.

We organized the article as follows: in Sect. 2, we present the conceptual model and the calculations. The results are given and discussed in Sect. 3, and in Sect. 4, we conclude.

2 Model and calculations

2.1 Ground state energies

Let us consider a monolayer of TMDs situated on a polar substrate in presence of uniform magnetic field applied on the third dimensions in a quantum dot (Fig. 1). The total Hamiltonian of the bipolaron can be written in this form

$$ H_{bp} = H_e + H_{ph} + H_{e-ph} + u(r) + U(|r_1 - r_2|) $$

where $H_e$ describes the energy of the electron defined as:
\[ H_e = \gamma V_F \sum_{i=1,2} \left( \sigma_1 (p_{ix} - 2eA_x) + \sigma_2 (p_{iy} - 2eA_y) + \sigma_3 (p_{iz} - 2eA_z) + \sigma_3 G \right) \]  

(2)

with \( \sigma_1, \sigma_2, \sigma_3 \) the Pauli matrices, \( V_F \) the Fermi velocity, \( 2G \) the bandgap, \( (\gamma = \pm 1) \) for electrons and holes respectively and \( A \) is the vector potential.

The second term \( H_{ph} \) stands for the phonon energies including SO and LO modes defined as:

\[ H_{ph} = \sum_{k,\nu} \hbar \omega_\nu a_k^+ a_k \]

(3)

where \( a_k^+, a_k \) are respectively creation and annihilation operators for the phonon with \( k \) being wave vector where \( \omega_\nu \) is the frequency of the phonon.

The third term \( H_{e-ph} \) is the Hamiltonian of interaction between electron and phonon

\[ H_{e-ph} = \sum_{k,\nu} M_{k,\nu} (a_k^+ + a_k) \exp(i k r) \]

(4)

where \( M_{k,\nu} \) is the coupling element of Fröhlich (Xiao et al. 2017).

The term \( u(r) \) is the confinement potential (Liu et al. 2014) in the quantum dot

\[ u(r) = \begin{cases} 
0 & r < R - \frac{L}{2} \\
\frac{V}{2} \left( \frac{\tanh \left( \frac{r - R}{c} \right) R}{\tanh \left( \frac{R}{c} \right)} + 1 \right) & R - \frac{L}{2} \leq r \leq R + \frac{L}{2} \\
V & r > R + \frac{L}{2}
\end{cases} \]

(5)

whereas \( R \) and \( V \) are respectively the length and the depth of the quantum dot and \( L \) is the smoothness of quantum dot. \( C \) is a constant. The last term of Eq. (1). is the coulomb interaction potential between the two electrons. Since the bipolaron is a composite particle, it is convenient to introduce the center of mass and relative coordinate and momenta,

\[ P_x = p_{1x} + p_{2x}, P_y = p_{1y} + p_{2y}, P_z = p_{1z} + p_{2z}, \quad r = r_1 - r_2, \quad R_1 = \frac{r_1 + r_2}{2}. \]

The Hamiltonian in Eq. (1). can be rewritten after averaging over a relative wavefunction \( \psi(r) \) as:

\[ H_{bp} = \gamma V_F \sum_{i=1,2} \left( \sigma_1 \pi_{ix} + \sigma_2 \pi_{iy} + \sigma_3 \pi_{iz} + \sigma_3 G \right) + \sum_{k,\nu} B_{k,\nu} (a_k^+ + a_k) \exp(i k R_1) + \sum_{k,\nu} \hbar \omega_\nu a_k^+ a_k + E_r + u(r) \]

(6)

With \( B_{k,\nu} = 2M_{k,\nu} \left( \cos \left( \frac{k r}{2} \right) \right) \) and \( E_r = \left\langle \frac{U}{2} \right\rangle \).

\( \langle . \rangle \) denoting an averaging over the oscillator wavefunction \( \psi_0^\nu(r) = c \exp \left( -\frac{br^2}{4} \right) \) as used in reference (Ruan and Chen 2007).

The Huybrechts method is applied by using the two following unitary transformations: 
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where $E_{byp0+}$ is the modified zero Landau level due to the bipolaron effect for the electron. Following the same rules, $E_{byp0-}$ is for the case of the hole and also can be obtained in the top of the valence band. Finally, the eigenvalues of the energies in the zero Landau Levels can be written as:

$$E_{byp0±} = \pm \sqrt{(V_F G)^2 + \left( 4hV_F a \sum_{k,\nu} M_{k,\nu}^* \exp \left[ -(1 - \alpha)^2 \frac{h}{m_0 k^2} \exp \left( -\frac{k^2}{b} \right) \right] \right)^2} \pm U \mp 4\pi^2 \left( \frac{b}{2\pi} \right)^{1/2} \frac{e^2}{\varepsilon_\infty b} + \sum_{k,\nu} \frac{M_{k,\nu}^* \exp \left[ -(1 - \alpha)^2 \frac{h}{m_0 k^2} \exp \left( -\frac{k^2}{b} \right) \right]}{(V_F a h + \hbar \omega_o)^2} \frac{2}{V_F a h + \hbar \omega_o}$$

(13)

Surface optical phonons strongly coupling with carriers in monolayer TMDs are described by the third term in Eq. (1). with the coupling element (Devreese et al. 1971; Berman and Roman 2017; Kormányos et al. 2015):

$$M_{k,0} = \sqrt{\frac{\varepsilon^2 \eta \omega_{SO0} \hbar}{2\varepsilon_0 k}} \exp \left( -k_{z0} \right)$$

(14a)

$\eta$ is the polarizability of the substrate, $\varepsilon_0$ is low frequency dielectric constant, $z_0$ is the internal distance between the TMDs and substrate, $\hbar \omega_{SO0}$ is the energy of SO phonon with two branches $\nu = 1, 2$. Carriers coupled with intrinsic longitudinal optical phonon coupling in monolayer TMDs have been studied extensively (Kaasbjerg et al. 2012; Kuc et al. 2011; Sohier et al. 2016). The coupling element in Fröhlich model is given by
\[ M_{k,LO} = \sqrt{\frac{e^2 \eta_0 L_m \hbar \omega_{LO}}{2A\epsilon_0}} \operatorname{erfc}\left(\frac{k\sigma}{2}\right) \] (14b)

where \( L_m \) is the atomic thickness of the monolayer, \( \eta_0 \) is the intrinsic polarizability of material, \( \hbar \omega_{LO} \) represents the energy of LO phonon and \( \operatorname{erfc} \) is the complementary error function. \( \sigma \) denotes the effective width of the electronic Bloch states reflecting the confinement effect between LO phonons and carriers in 2D materials (Kaasbjerg et al. 2012; Sohier et al. 2016). Replacing Eqs. (14a), or (14b), we obtain the following results for different coupling regime and for SO and LO phonons:

The energies of SO and LO in the weak coupling (\( \alpha = 1 \)) are respectively:

\[
\begin{align*}
(E_{\text{bipolaron}})_{SO} &= \pm \sqrt{(V_F G)^2 + \frac{h V_F e^2 \eta}{\pi \epsilon_0} \sum_{\omega_{SO}} \frac{k_{\omega}}{0} \int \frac{dk}{k} \left( \operatorname{erfc} \left( \frac{k a}{2} \right) \right)^2 \frac{\exp \left( -2k c_0 \right) \exp \left( -\frac{\epsilon^2}{b} \right)}{(V_F \hbar k + \hbar \omega_{SO})^2}} \\
&\pm 2 \frac{e^2 \eta}{\pi \epsilon_0} \sum_{\omega_{SO}} \frac{k_{\omega}}{0} \int \frac{dk}{k} \left( \operatorname{erfc} \left( \frac{k a}{2} \right) \right)^2 \frac{\exp \left( -2k c_0 \right) \exp \left( -\frac{\epsilon^2}{b} \right)}{(V_F \hbar k + \hbar \omega_{SO})^2} \\
\end{align*}
\] (15a)

and

\[
\begin{align*}
(E_{\text{bipolaron}})_{LO} &= \pm \sqrt{(V_F G)^2 + \frac{h V_F e^2 \eta_0 L_m \hbar \omega_{LO}}{\pi \epsilon_0} \frac{k_{\omega}}{0} \int \frac{dk}{k} \left( \operatorname{erfc} \left( \frac{k a}{2} \right) \right)^2 \frac{\exp \left( -2k c_0 \right) \exp \left( -\frac{\epsilon^2}{b} \right)}{(V_F \hbar k + \hbar \omega_{LO})^2}} \\
&\pm 2 \frac{e^2 \eta_0 L_m \hbar \omega_{LO}}{\pi \epsilon_0} \frac{k_{\omega}}{0} \int \frac{dk}{k} \left( \operatorname{erfc} \left( \frac{k a}{2} \right) \right)^2 \frac{\exp \left( -2k c_0 \right) \exp \left( -\frac{\epsilon^2}{b} \right)}{(V_F \hbar k + \hbar \omega_{LO})^2} \\
\end{align*}
\] (15b)

The energies of SO and LO bipolaron in the intermediate coupling (\( 0 < \alpha < 1 \)) are respectively:

\[
\begin{align*}
(E_{\text{bipolaron}})_{SO} &= \pm \sqrt{(V_F G)^2 + \frac{h V_F e^2 \eta}{\pi \epsilon_0} \sum_{\omega_{SO}} \frac{k_{\omega}}{0} \int \frac{dk}{k} \left( \operatorname{erfc} \left( \frac{k a}{2} \right) \right)^2 \frac{\exp \left( -2k c_0 \right) \exp \left[ -(1 - \alpha)^2 \frac{\hbar^2}{m_k} k^2 \right] \exp \left( -\frac{\epsilon^2}{b} \right)}{(V_F \hbar k + \hbar \omega_{SO})^2}} \\
&\pm U \pm 4 \pi^2 \left( \frac{b}{2\pi} \right)^{1/2} \frac{e^2 \eta}{\pi \epsilon_0} \sum_{\omega_{SO}} \frac{k_{\omega}}{0} \int \frac{dk}{k} \left( \operatorname{erfc} \left( \frac{k a}{2} \right) \right)^2 \frac{\exp \left( -2k c_0 \right) \exp \left[ -(1 - \alpha)^2 \frac{\hbar^2}{m_k} k^2 \right] \exp \left( -\frac{\epsilon^2}{b} \right)}{(V_F \hbar k + \hbar \omega_{SO})^2} \\
&\pm 2 \frac{e^2 \eta}{\pi \epsilon_0} \sum_{\omega_{SO}} \frac{k_{\omega}}{0} \int \frac{dk}{k} \left( \operatorname{erfc} \left( \frac{k a}{2} \right) \right)^2 \frac{\exp \left( -2k c_0 \right) \exp \left[ -(1 - \alpha)^2 \frac{\hbar^2}{m_k} k^2 \right] \exp \left( -\frac{\epsilon^2}{b} \right)}{(V_F \hbar k + \hbar \omega_{SO})^2} \\
\end{align*}
\] (16a)

and
\[
(E_{bp0\pm})_{LO} = \pm \left( V_F G \right)^2 + \frac{\hbar V_F e^2 n_0 L_m h_{0LO}}{\pi \epsilon_0} \int k^2 dk \left( \frac{1}{2} \right) \exp \left[ \frac{\epsilon k^2}{2} \right] \exp \left\{ \frac{1}{2} \left[ \epsilon k^2 - \frac{1}{\pi} \right] \right\} \exp \left[ \frac{-\left( 1 - \alpha \right)^2}{\alpha \epsilon k^2} \exp \left( -\frac{k^2}{\alpha} \right) \right] \left( V_F h + h_{0LO} \right)^2
\]

\[
\pm U \pm 4\pi^2 \left( \frac{b}{2\pi} \right) e^2 \epsilon_{\omega b} \exp \left( -2kz_0 \right) \exp \left[ -\frac{\hbar}{m\alpha} k^2 \right] \exp \left( -\frac{k^2}{b} \right) \left( V_F h + h_{0LO} \right)^2
\]

\[
\pm 2 e^2 n_0 L_m h_{0LO} \frac{K_c}{\pi \epsilon_0} \int k^2 dk \left( \frac{1}{2} \right) \exp \left[ \frac{\epsilon k^2}{2} \right] \exp \left[ -\frac{\hbar}{2m\alpha} k^2 \right] \exp \left( -\frac{k^2}{b} \right) \left( V_F h + h_{0LO} \right)^2
\]

(16b)

The energies of SO and LO bipolaron in the strong coupling (\(\alpha = 0\)) are respectively:

\[
(E_{bp0\pm})_{SO} = \pm V_F G \pm e^2 n_0 L_m \frac{K_c}{\pi \epsilon_0} \int k^2 dk \left[ \frac{1}{2} \right] \exp \left[ -\frac{\hbar}{m\alpha} k^2 \right] \exp \left( -\frac{k^2}{b} \right) \left( V_F h + h_{0LO} \right)^2
\]

(17a)

and

\[
(E_{bp0\pm})_{LO} = \pm V_F G \pm e^2 n_0 L_m \frac{K_c}{\pi \epsilon_0} \int k^2 dk \left[ \frac{1}{2} \right] \exp \left[ -\frac{\hbar}{m\alpha} k^2 \right] \exp \left( -\frac{k^2}{b} \right) \left( V_F h + h_{0LO} \right)^2
\]

(17b)

The binding energy (BE) given as in (Ruan and Chen 2007)

\[
BE = 2E_p - E_{bp}
\]

characterises the stability criteria. Here, \(E_p\) is the single polaron ground state energy in the same approximation. In this case the BE is given by:

\[
BE = 2E_{p0} - E_{bp0}
\]

(18)

2.2 Magnitude of the banggap modulation

As the energy difference \(E_{bp0+} - E_{bp0-}\) denotes the modulated bandgap, it is important to derive it in order to analyse qualitatively the bipolaron effects on the bandgap. The magnitude of the bandgap modulation is defined as (Xiao et al. 2017):

\[
2\Delta G = 2G - \left[ (E_{bp0+})_{SO,LO} - (E_{bp0-})_{SO,LO} \right]
\]

(19)

Using Eq. (19) we obtained the magnitude of the bandgap modulation for all coupling regimes and both for LO and SO phonons. From Eq. (15a, b), we observe that \(E_{bp0+}\) and \(E_{bp0-}\) are independant of the magnetic field which is different from other Landau level energies and...
other couplings (Eqs. (16a, b) and (17a, b)). So the magnitude of bandgap modulation in weak coupling regime can not be altered by an external magnetic field. This result is similar to the case of polaron (Xiao et al. 2017; Wang et al. 2015). In other coupling regimes (intermediate and strong), the magnitude of the bandgap is a function of the magnetic field.

### 2.3 Absorption coefficient

The absorption coefficient $\Gamma(h\Omega)$ of the incident light with the energy $h\Omega$ of a free polaron, according to Fermi’s golden rule, is (Devreese and Alexandre 2009; Devreese and Polaron 2011; Devreese et al. 1971):

$$
\Gamma(h\Omega) = \frac{\pi}{\hbar c n \epsilon^2} \sum_f \left| \langle \psi_0 | V | \psi_f \rangle \right|^2 \delta(E_0 + h\Omega - E_f)
$$

(20)

where $n$ is the refractive index of the medium, $c$ equals the speed of light, $\epsilon$ stands for the permittivity of free space, and $F$ represents the intensity of the electric field vector of the incident photon. $V = eFr$ indicates the time-dependent perturbation, $\psi_0$ denotes the ground state of a free polaron and $E_0$ represents the energy of the ground state. $\psi_f$ represents the wave functions of all possible end states with the corresponding energies $E_f$. To prevent complicated summation on the final states, a simple model in which the wave functions of the excited states have been suppressed by the Lee Löw Pines unit transformations have been developed (Devreese et al. 1971). It was noted that Eq. (20) concerns the weak and intermediate coupling regimes. Thus, in the weak coupling regime using the same formula we obtain, the absorption coefficient for SO and LO bipolarons as

$$\Gamma_{\text{W-bp}}(h\Omega) = \left\{ \begin{array}{ll}
\frac{e^4 \eta}{h^2 V_f c n \epsilon^3 m^2 (h\Omega)^3} \sum_{i=1,2} \hbar \omega_{SO,i} (h\Omega - \hbar \omega_{SO,i})^2 \exp \left[ \frac{2\zeta_0 (h\Omega - \hbar \omega_{SO,i})}{h V_f} \right] \exp \left[ -\frac{(h\Omega - \hbar \omega_{SO,i})}{b V_f h} \right]
\\
\frac{e^4 \eta}{h^2 V_f c n \epsilon^3 m^2 (h\Omega)^3} \sum_{i=1,2} \hbar \omega_{LO,i} (h\Omega - \hbar \omega_{LO,i})^2 \exp \left[ -\frac{(h\Omega - \hbar \omega_{SO,i})}{b V_f h} \right]
\\
\frac{e^4 \eta}{h^2 V_f c n \epsilon^3 m^2 (h\Omega)^3} \sum_{i=1,2} \hbar \omega_{LO,i} (h\Omega - \hbar \omega_{LO,i})^2 \exp \left[ -\frac{(h\Omega - \hbar \omega_{SO,i})}{b V_f h} \right]
\\
\end{array} \right.
$$

(21)

In the intermediate coupling, the absorption coefficient of SO and LO bipolarons is given by:

$$\Gamma_{\text{int-bp}}(h\Omega) = \left\{ \begin{array}{ll}
\frac{e^4 \eta}{h^2 V_f c n \epsilon^3 m^2 (h\Omega)^3} \sum_{i=1,2} \hbar \omega_{SO,i} (h\Omega - \hbar \omega_{SO,i})^2 \exp \left[ \frac{2\zeta_0 (h\Omega - \hbar \omega_{SO,i})}{h V_f} \right] \exp \left[ -\frac{(h\Omega - \hbar \omega_{SO,i})}{b V_f h} \right]
\\
\frac{e^4 \eta}{h^2 V_f c n \epsilon^3 m^2 (h\Omega)^3} \sum_{i=1,2} \hbar \omega_{LO,i} (h\Omega - \hbar \omega_{LO,i})^2 \exp \left[ -\frac{(h\Omega - \hbar \omega_{SO,i})}{b V_f h} \right]
\\
\frac{e^4 \eta}{h^2 V_f c n \epsilon^3 m^2 (h\Omega)^3} \sum_{i=1,2} \hbar \omega_{LO,i} (h\Omega - \hbar \omega_{LO,i})^2 \exp \left[ -\frac{(h\Omega - \hbar \omega_{SO,i})}{b V_f h} \right]
\\
\end{array} \right.
$$

(22)
3 Results and Discussion

This section presents the numerical results, we used some constants outlined in Table 1 in our calculations. We assume the Fermi velocity to be equal for all TMDs selected.
in this paper since it varies slightly for different TMDs (Kormányos et al. 2015). The values of the bandgap are adopted in Table 2. For LO phonons, the evaluation of the amounts of bandgap modulation and the relative ratio for the different TMDs are shown in Table 3 and fixed values of $L m = 0.5\,\text{nm}$, $\sigma = 0.6\,\text{nm}$ are taken in all TMDs monolayer (Thilagam 2016).

In Fig. 2(a), we present the dependences of MBM on the magnetic field for bipolaron in different monolayer TMDs at intermediate coupling regime. It can be seen that the MBM increases with magnetic field. For various TMDs, the MBM are also shown, one can observe that it varies with TMDs monolayer. The most important MBM is obtained with WS$_2$ and the least with MoSe$_2$. Thus among the selected TMDs the latter strongly enhances the conductivity. A significant change of MBM relates to each TMDs highlights the impact of the magnetic field on the bandgap modulation in TMDs monolayer.

Figure 2(b), presents the dependence of MBM on the magnetic field in different monolayer at strong coupling regime. As in the intermediate regime we can see that MBM increases with magnetic field. We also observe that the MBM varies with TMDs monolayer, then the most important is obtained with MoS$_2$ and the less with WSe$_2$ which is not the case in intermediate coupling regime. Thus the electron phonon coupling affects the MBM for different TMDs monolayer in the presence of bipolaron. Fig. 2(c), presents the MBM versus $\eta_0$ for different monolayers in weak coupling regime. One can observed that MBM increases with increasing the coupling parameter $\eta_0$. Same result was obtained by (Xiao et al. 2017). These results show that the bipolaron strongly affects the bandgap of TMDs. Since the coupling parameter characterizes the material, strong coupling favor the modulation of the bandgap. The WSe$_2$ presents the highest MBM. In the investigation of carriers LO phonon coupling in monolayer TMDs, we defined a new parameter $g_f$ defined by sohier (Sohier et al. 2016) as the coupling strength, which is analogous to the parameter

![Fig. 3 Binding energy of the bipolaron versus magnetic field $B$ in MoS$_2$ for different polar substrate (intermediate coupling regime)](image-url)
and pointed out that the 2D Fröhlich coupling is much stronger in TMDs. Moreover, we noticed that the values obtained for the bandgap modulation due to carrier-LO phonon coupling are very close to experimental results (Tongay et al. 2012; Arora et al. 2015). Then, the LO phonons increase the modulated bandgap then consequently decrease conductivity in TMDs. Among the selected TMDs, the one with highest performance in conductivity is the MoS$_2$.

**Fig. 4** Binding energy of the bipolaron with parameter $\eta_0$ in weak coupling regime for different TMDs monolayer

**Fig. 5** Optical absorption coefficient versus photon energy in LO phonon in different monolayer TMDS materials for bipolaron in weak coupling regime

$\eta_0$ and pointed out that the 2D Fröhlich coupling is much stronger in TMDs. Moreover, we noticed that the values obtained for the bandgap modulation due to carrier-LO phonon coupling are very close to experimental results (Tongay et al. 2012; Arora et al. 2015). Then, the LO phonons increase the modulated bandgap then consequently decrease conductivity in TMDs. Among the selected TMDs, the one with highest performance in conductivity is the MoS$_2$. 
In Fig. 3, the binding energy with magnetic field is presented for intermediate coupling regime. One can observe that the binding energy decrease with increasing magnetic field. The increase of magnetic field enhances the average of coulomb repulsion between the electrons, this result is in accordance with the work of Brosens and Devreese (Brosens and Devreese 1996). Thus, despite the enhancement of coulomb repulsion, the phonon mediated attractive electron-electron attraction still dominates. That is the reason why the binding energy remains positive and this is an indication that in all selected TMDs monolayer, the bipolaron is stable. From Fig. 4, the binding energy decreases as $\eta_0$ increases, then the bipolaron is stable in the different monolayer TMDs as the binding energy remains positif.

Figure 5 illustrates the optical absorption of the bipolaron versus the incident photon energy for LO phonons in different layers of TMDs with a weak coupling regime. It can be noted that there is no absorption for $h\Omega < h\omega_{LO}$. The threshold value of absorption is at $h\Omega = h\omega_{LO}$. At this value the optical absorption increases and arrives at a maximum and decreases slowly with an increase of photon energy. In fact, these optical absorption behaviours are consistent with previous works on monolayer TMDs and others (Devreese and Polarons 1611; Li and Wang 2018; Sohier et al. 2017). Optical absorption is similar for different TMDs but the strength are not the same for each TMD. This behaviour may be attributed to the fact that the optical absorption is proportional to the phononic energy of the bipolaron in the different TMDs. This suggests that the lower the phononic energy of the bipolaron in the TMDs, the lower the optical absorption of a bipolaron. A number of past works have been carried out to study the coupling force in such monolayers (Sohier et al. 2016; Thilagam 2016; Kaasbjerg et al. 2014) Then in MoS$_2$, bipolaron has enough energy to absorb photon than WSe$_2$, this can be due to the dominance of electron-phonon and photon-phonon interations. Comparing the optical absorption in intermediate coupling regimes (not shown) with the one in weak coupling regime we observe a similar behavior. This can explain why both couplings can be considered identically in some cases.

Figure 6 displays the dependences of optical absorption with magnetic field for the monolayer MoS$_2$ on SiO$_2$ substrate at various values of internal distance between TMDs monolayer and polar substrate. One can observe that the optical absorption is the same.
for different internal distance. When $B = 0$, it increases slowly and become constant with magnetic field. We also observe that optical absorption increases with internal distance separating the monolayer from polar substrates, proving that the strength of the electron-SO coupling directly depends on the internal distance between the TMDs and the polar substrates. This result is in agreement with that of Li and Wang (Li and Wang 2018). In fact, in some studies (Ryou et al. 2016; Chen et al. 2018), carrier phonon coupling between 2D materials and the polar substrate has also been recognized, where the trends are comparable for the coupling strength with the internal distance. The optical absorption of SO bipolaron at intermediate coupling regime in monolayer MoS$_2$ for different polar substrates is shown in Fig. 7. One can observe the variation of optical absorption with the polar substrates. For $B < 0.6$, no absorption is observed in MoS$_2$ then for $B = 0.6$ a significant change of absorption relates to each substrates highlights the impact of the magnetic field on the optical absorption in MoS$_2$ monolayer. The greatest optical absorption is observed in SiO$_2$ polar substrate this result is in agreement with those of Hein et al. (Hien et al. 2020) and lowest for h-BN.

4 Conclusion

We theoretically studied optical absorption of bipolaron and its effects on the bandgap modulation in quantum dot of single layer transition metal dichalcogenides under magnetic field for all coupling regime, where both LO and SO phonon are taken into account. Huybrechts method and simple unitary transformation are used. We show that the MBM of TMDs are flexible. We also found that magnetic field strongly affects the MBM in intermediate and strong coupling regime, thus enhances the conductivity of TMDs monolayer and that in weak coupling regime, the magnetic field cannot be used to tune the MBM. Investigating the optical absorption we found that both the magnetic field and the internal distance separating the monolayer and polar substrates affects the optical absorption in the TMDs. We showed that in MoS$_2$, the bipolaron has enough energy to absorb than in WSe$_2$. This study is necessary for high performance in optoelectronic and nanoelectronic device.
applications. Due to the flexibility of the MBM and the stability of bipolaron in TMD, it is important to investigate the decoherence of bipolaron in future works.

Declarations

Conflict of interest  The authors declare that they have no conflict of interest.

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