Strain dependence of photoluminescence and circular dichroism in transition metal dichalcogenides: a $k \cdot p$ analysis

Shahnaz Aas and Ceyhun Bulutay

Department of Physics, Bilkent University, 06800, Bilkent, Ankara, Turkey
bulutay@fen.bilkent.edu.tr

Abstract: Within a two-band $k \cdot p$ method we analyze different types of strain for the $K$ valley optical characteristics of a freestanding monolayer MoS$_2$, MoSe$_2$, WS$_2$ and WSe$_2$. We predict that circular polarization selectivity for energies above the direct transition onset deteriorates/improves by tensile/compressive strain. Wide range of available strained-sample photoluminescence data can be reasonably reproduced by this simple bandstructure combined with accounting for excitons at a variational level. According to this model strain impacts optoelectronic properties through its hydrostatic component, whereas the shear strain only causes a rigid wavevector shift of the valley. Furthermore, under the stress loading of flexible substrates the presence of Poisson’s effect or the lack of it are examined individually for the reported measurements.

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1. Introduction

Transition metal dichalcogenides (TMDs) possess direct optical gap together with mechanical flexibility up to 10% range [1] which enables wide strain tunability of their optoelectronic properties [2, 3]. As a consequence, the associated body of literature is rapidly growing, while a number of milestones have been reached. The tuning of the electronic structure by applying a uniaxial tensile bending to monolayer MoS$_2$ on flexible substrates has been demonstrated by several groups within a short time span [4–10]. For a suspended monolayer MoS$_2$ membrane, Lloyd et al. showed the continuous and reversible tuning of the optical bandgap over an ultralarge range of applied biaxial strain [11]. More recently, deterministic two-dimensional array of quantum emitters from thin TMDs due to a localized strain pattern is achieved that becomes instrumental to construct scalable quantum architectures [12, 13]. Additional experimental [14–21] as well as theoretical [22–25] studies substantiated strain as a viable control mechanism for these two-dimensional materials.

Our aim in this work is to consolidate accumulating experimental photoluminescence (PL) data on strained TMD samples with the aid of a simple $K$-valley-specific two-band $k \cdot p$ theory. Particularly, for the measurements performed by uniaxial bending of flexible substrates, this analysis can reveal the extent of Poisson’s contraction over the TMD layer for each individual case. It also governs the circular dichroism which refers to the helicity-selective optical absorption [26], and in which way it can be altered by strain.

2. Theory

2.1. Two-band strained $k \cdot p$ approach for TMDs

The conduction and valence bands of TMDs around the direct bandgap at the $K$ valleys can be represented by a two-band basis $\{|\phi_c\}, |\phi_v\rangle$ which primarily accounts for the $d$-orbitals $|d_{x^2-y^2}\rangle$ and $|d_{xy}\rangle \pm i|d_{xy}\rangle$ [27]. The corresponding strained $k \cdot p$ Hamiltonian has been very
recently suggested by Fang et al., which in this basis attains the matrix form
\[
H = \begin{bmatrix}
\left(f_0 + \frac{4}{3}\right) + (f_3 + f_4)(\varepsilon_{xx} + \varepsilon_{yy}) & f_2a(k_x - ik_y) + f_3(\varepsilon_{xx} - \varepsilon_{yy} + 2i\varepsilon_{xy}) \\
- f_2a(k_x + ik_y) + f_3(\varepsilon_{xx} - \varepsilon_{yy} - 2i\varepsilon_{xy}) & \left(f_0 - \frac{4}{3}\right) + (f_3 - f_4)(\varepsilon_{xx} + \varepsilon_{yy})
\end{bmatrix},
\]

where \(a\) is the lattice constant, \(f_i\)’s are the strained \(k \cdot p\) parameters fitted to first-principles electronic bandstructure, also listed in Table 1 for convenience [28]. Among these six \(k \cdot p\) parameters, \(f_0\) and \(f_3\) do not play a role in homogeneous systems (as in this work). Their significance emerges in vertical heterostructures [29] for \(f_0\). In Eq. (1) as well as in the remainder of this work, without loss of generality we refer to \(K_+\) valley, which is assumed to be the origin for the wavevector \(k = \hat{x}k_x + \hat{y}k_y\), where \(\hat{x}\) points from \(\Gamma\) to \(K_+\) in reciprocal space, that matches with the “zigzag” direction in direct space. Expressions for the \(K_-\) valley, if required, can be obtained by complex conjugation, as the \(K_\pm\) points are connected through time-reversal symmetry [30]. The spin and the spin-orbit coupling are discarded in Eq. (1), although the spin-splitting can be easily incorporated to this framework [28]. For our purposes this is not necessary as we are interested in the so-called \(A\)-excitons only [5].

Table 1. \(k \cdot p\) parameters \(f_i\) (eV), lattice constant \(a\) (Å) [28], 2D polarizability \(\chi_{2D}\) (Å) [31] for different TMDs.

| Materials | \(f_0\) | \(f_1\) | \(f_2\) | \(f_3\) | \(f_4\) | \(f_5\) | \(a\) | \(\chi_{2D}\) |
|-----------|--------|--------|--------|--------|--------|--------|-----|--------|
| MoS\(_2\) | -5.07  | 1.79   | 1.06   | -5.47  | -2.59  | 2.2    | 3.182| 6.60   |
| MoSe\(_2\) | -4.59  | 1.55   | 0.88   | -5.01  | -2.28  | 1.84   | 3.317| 8.23   |
| WS\(_2\)  | -4.66  | 1.95   | 1.22   | -5.82  | -3.59  | 2.27   | 3.182| 6.03   |
| WSe\(_2\) | -4.23  | 1.65   | 1.02   | -5.26  | -3.02  | 2.03   | 3.316| 7.18   |

Neglecting any displacement perpendicular to TMD that lies on the two-dimensional (2D) \(xy\)-plane, the tensor strain components for most common types are:

- **Biaxial strain**: \(\varepsilon_{yy} = \varepsilon_{xx}, \quad \varepsilon_{xy} = \varepsilon_{yx} = 0\),
- **Uniaxial strain**: \(\varepsilon_{xx} \neq 0, \quad \varepsilon_{yy} = \varepsilon_{xy} = \varepsilon_{yx} = 0\),
- **Shear strain**: \(\varepsilon_{yy} = -\varepsilon_{xx}, \quad \varepsilon_{xy} = \varepsilon_{yx} \neq 0\),
- **Uniaxial stress**: \(\varepsilon_{yy} = -\nu \varepsilon_{xx}, \quad \varepsilon_{xy} = \varepsilon_{yx} = 0\),

where \(\nu\) is the Poisson’s ratio. To simplify our expressions, also we make use of the (areal) hydrostatic component of strain, \(\varepsilon_H = \varepsilon_{xx} + \varepsilon_{yy}\). Regarding the terminology, we should caution that the term uniaxial strain is in widespread use in TMD literature [3,5,20,21], although with the assumed Poisson’s effect, as explicitly mentioned in these works, it needs to be referred to as uniaxial stress; also note that we use tensor and not the engineering strain [32].

The strained eigenstates of Eq. (1) can be readily solved analytically. The direct bandgap becomes \(E_K = f_1 + 2f_4\varepsilon_H\). If we introduce \(k_{x0} \equiv (\varepsilon_{xx} - \varepsilon_{xy})f_2/(f_2a), k_{y0} \equiv 2\varepsilon_{xy}f_2/(f_2a), q_x \equiv k_x - k_{x0}, q_y \equiv k_y - k_{y0}\), with their magnitude \(q = \sqrt{q_x^2 + q_y^2}\), the energy dispersion for the conduction and valence bands can be expressed as

\[
E_{c/v}(q) = f_0 + f_3\varepsilon_H \pm \frac{E_K}{2} \sqrt{1 + 4[r(q, \varepsilon_H)]^2},
\]
in terms of an auxiliary function that depends on the (valley edge-centered) wavenumber and the hydrostatic strain as
\[ r(q, \varepsilon_H) = \frac{f_2 a q}{f_1 + 2 f_3 \varepsilon_H}, \tag{3} \]
which quantifies the degree of mixing between basis states \(|\phi_c\rangle, |\phi_v\rangle\) as to be justified below.

Hence, the valley edge shifts from \((k_x = 0, k_y = 0)\) to \((k_x 0, k_y 0)\) because of strain. So that for \(\varepsilon_{xx} > \varepsilon_{yy}\), \(k_x 0 > 0\), and band extremum at \(K\) shifts away from \(\Gamma\) (toward neighboring zone \(M'\)) point, while for \(\varepsilon_{xx} > \varepsilon_{yy}\), \(k_x 0 < 0\) it shifts toward \(\Gamma\) point. Thus, according to this simple model the shear strain rigidly displaces it along \(k_y\) direction without affecting the bandgap. As a matter of fact the terms proportional to \(f_5\) in Eq. (1) were referred to as the pseudogauge field in the graphene literature, responsible for shifting the Dirac cone from the \(K\) point [28].

The eigenvectors of the two-band Hamiltonian in Eq. (1) corresponding to the conduction and valence states are given by
\[ |U_c\rangle = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad |U_v\rangle = \begin{pmatrix} x_2 \\ -x_1^* \end{pmatrix}, \tag{4} \]
where in terms of \(\phi = \tan^{-1}(q_y / q_x)\), an \(r\) defined in Eq. (3) the entries are given by
\[ x_1 = \frac{e^{-i\phi}}{\sqrt{1 + r^2}}, \tag{5} \]
\[ x_2 = \frac{r}{\sqrt{1 + r^2}}. \tag{6} \]

### 2.2. Degree of circular polarization

For a light polarized along a unit vector \(\mathbf{u}\), the dipole matrix element connecting valence \(|U_v\rangle\) and conduction \(|U_c\rangle\) states is given by [27]
\[ \mathcal{P}_u(\mathbf{k}) \equiv \frac{m_0}{\hbar} \langle U_c | \frac{\partial \hat{H}}{\partial k_u} | U_v \rangle, \tag{7} \]
where \(m_0\) is the free electron mass. For the \(\pm\) circularly polarized light defined by the unit vectors \(\mathbf{u}_\pm = (\mathbf{\hat{x}} \pm i\mathbf{\hat{y}})/\sqrt{2}\). Eq. (7) can be expressed in terms of Pauli spin raising/lowering operators \(\hat{\sigma}_\pm\) as
\[ \mathcal{P}_\pm(\mathbf{k}) = \frac{m_0 f_2 a}{\sqrt{2} \hbar} \langle U_c | \hat{\sigma}_\pm | U_v \rangle. \tag{8} \]

Though it is not directly apparent from this expression, these momentum matrix elements are actually strain dependent through the eigenkets in Eq. (4) and the mixing function \(r(q, \varepsilon_H)\) from Eq. (3).

The so-called circular dichroism (CD) corresponds to a difference in the absorption of the right- and left-hand circularly polarized radiation, where the \(k\)−resolved degree of helicity selectivity is quantified as [26],
\[ \eta(\mathbf{k}) \equiv \frac{[\mathcal{P}_+(\mathbf{k})]^2 - [\mathcal{P}_-(\mathbf{k})]^2}{[\mathcal{P}_+(\mathbf{k})]^2 + [\mathcal{P}_-(\mathbf{k})]^2}. \tag{9} \]

We should note that inclusion of spin and the spin-orbit coupling does not affect the above helicity selection rules [33]. For isotropic and electron-hole symmetric bands as in our case, its wavevector dependence simplifies as \(\eta(\mathbf{k}) \rightarrow \eta(q) = \eta(E)\). By inserting the associated states from Eq. (4) it acquires a simple analytical form
\[ \eta(q, \varepsilon_H) = \frac{1 - [r(q, \varepsilon_H)]^4}{1 + [r(q, \varepsilon_H)]^4}. \tag{10} \]
2.3. Exciton binding and PL energies

To compare with the experimental PL data under a given strain, we need to include excitonic effects as the associated binding energies significantly exceed the thermal energy at room temperature [5]. For that, we first extract the valley edge effective masses $m^*_c/v$ from the energy dispersion relation (Eq. (2)) via,

$$m^*_c/v = \frac{\hbar^2}{\left( \frac{D}{\partial k_x} \right)_0} = \pm \frac{\hbar^2 (f_1 + 2f_4 \varepsilon_H)}{2(f_2 a)^2},$$

(11)

where the curvatures are evaluated at the strained band extremum, $(k_x, k_y)$. Within our two-band $k \cdot p$ model electron and hole effective masses are equal, i.e., $m^*_e = m^*_h = m^*_0 = -m^*_0$, and furthermore they are spatially isotropic, but note that here these effective masses are strain-dependent. Thus, the corresponding exciton effective mass for its relative degrees of freedom follows from $\mu = m^*_e m^*_h / \left( m^*_e + m^*_h \right)$.

To retain the simplicity of our approach, the binding energies for neutral excitons in TMDs can be calculated following [31] by a variational method based on the exciton Hamiltonian (switching to Hartree atomic units in the remainder of this subsection),

$$H_X = -\frac{\nabla^2}{2\mu} + V_{2D}(\rho).$$

(12)

Here, the in-plane interaction between an electron and a hole separated by $\rho = \sqrt{x^2 + y^2}$ is,

$$V_{2D}(\rho) = \frac{-\pi}{(\kappa_a + \kappa_b)\rho_0} \left[ H_0(\rho/\rho_0) - Y_0(\rho/\rho_0) \right],$$

(13)

where, $\kappa_a$ and $\kappa_b$ are dielectric constants for the media above and below the TMD (for a freestanding case, $\kappa_a = \kappa_b = 1$), $H_0$ and $Y_0$ are the Struve and the Bessel function of the second kind; the screening length is given by $\rho_0 = 2\pi \chi_{2D}$, and $\chi_{2D}$ is the 2D polarizability of the TMD, which is listed in Table 1 [31].

The wave function for the neutral exciton with a single variational parameter $\lambda$ is chosen as,

$$\Psi_X(\rho, \lambda) = \sqrt{\frac{2}{\pi \lambda^2}} \exp\left(-\rho/\lambda\right).$$

(14)

In such a case the kinetic energy has the analytical form, $T(\lambda) = 1/(2\mu \lambda^2)$, while potential energy requires the following integration to be evaluated numerically,

$$V(\lambda) = -\frac{2\pi}{\rho_0 \lambda^2} \int_0^\infty \left[ H_0(\rho/\rho_0) - Y_0(\rho/\rho_0) \right] \exp\left(-2\rho/\lambda\right) \rho \, d\rho.$$  

(15)

The total exciton energy is found by minimizing $E_X(\lambda) = T(\lambda) + V(\lambda)$, where the optimum value of $\lambda$ corresponds to the mean the exciton radius. For a bound exciton $E_X < 0$, and the PL energy is obtained from $E_{PL} = E_X + E_X$.

2.4. A critique of the two-band Hamiltonian

The Hamiltonian of Eq. (1) was originally derived from a simplified tight binding model for TMDs [34]. Alternatively, starting from the well-known unstrained $k \cdot p$ model [27], it can be arrived through the substitutions

$$k_x \to k_x + \alpha (\varepsilon_{yy} - \varepsilon_{xx}), \quad k_y \to k_y + \alpha 2 \varepsilon_{xy},$$

(16)
that resembles a minimal coupling to a strain-related gauge field with a coupling constant $\alpha$ (which is $f_3$ in our case) [35]. A group-theoretic basis of this substitution is that for the $C_{3v}$ point symmetry of the $K$ point in TMDs, both $k_x - ik_y$ and $(e_{xx} - e_{yy}) + i2e_{xy}$ transform according to $K_2$ ($\Gamma_3$ in the notation of [36]), while $k_x + ik_y$ and $(e_{xx} - e_{yy}) - i2e_{xy}$ transform according to $K_3$ ($\Gamma_2$) irreducible representations [37]. Moreover, both $\Gamma_2$ and $\Gamma_3$ transform the same way under time-reversal symmetry [36].

Even though the substitution recipe in Eq. (16) when applied to the unstrained Hamiltonian of [27] generates strain terms respecting the symmetry of $K$ point, it fails to produce higher-order strain effects. The rigorous approach following the method of invariants [38] allows calculations with the data from numerous experimental references. For MoS$_2$

Figure 2 shows the PL peak shift for the four TMDs under uniaxial strain, comparing our 3.2. PL peak shift under strain

calculation with the data from numerous experimental references. For MoS$_2$ and WSe$_2$ we have a good agreement between our theory and the best fit to the experimental data, taking
Fig. 1. Effect of uniaxial/biaxial strain on the degree of optical polarization of TMDs for compressive/tensile strain at different excess energies $\Delta E$, as measured from the conduction band minimum.

into account the spread in the latter. At variance to this, for WS$_2$ our results do not agree with two reports [18, 19]. To resolve this case, we also plot the bandgap variation for WS$_2$ under uniaxial strain from a first-principles calculation [24] (yellow-dashed). If we add to this the strained excitonic correction we get a closer agreement with our calculations (purple-dotted vs. blue-solid). Therefore, we believe that some slipping may have occurred on the TMD layer while applying strain to the substrate in [18, 19], whereas other measurements in Fig. 2 such as [5, 20, 21] have taken measures to clamp the TMD to the substrate. For MoSe$_2$, we see that the uniaxial stress condition using the Poisson’s ratio of the substrate, $\nu = 0.37$ (blue-dashed) matches perfectly with the data, in agreement with their assertion in [21]. In other words, unlike the other measurements in Fig. 2, for this experiment the TMD layer fully complies with the Poisson’s contraction of the substrate.

In the case of biaxial strain displayed in Fig. 3, for MoS$_2$ we have an excellent agreement with the widest-range strain data by Lloyd et al. [11] which goes up to 6%. Once again we plot the variation in the bandgap (green-dashed in upper-left panel); the notable offset from PL line indicates the extent of excitonic contribution on the strain variation of the PL energy. Here, our results as well as [11] are for freestanding monolayer TMDs, on the other hand the remaining biaxial strain data from [45] was originally reported with respect to polypropylene substrate strain. Therefore, to convert substrate strain results in [45], we multiplied all strain data from this reference by the 0.573 scale factor. This brings their data in agreement with the freestanding case of [11]. However, for MoSe$_2$ we still have a disagreement with [45]; noting the leveling off in their data beyond about 0.15% strain, we again suspect that a slipping might be responsible.

In Table 2 we compare our PL peak strain shift results with the quantities from various experimental references. For our results, both uniaxial strain and uniaxial stress cases are presented, where in the former no transverse contraction takes place in the direction perpendicular to axial deformation (i.e., $\nu = 0$). For uniaxial stress we use $\nu = 0.37$ value which is typical for
Fig. 2. Uniaxial strain dependence of A-exciton PL peak energy shift for monolayer TMDs, comparing our calculations (in blue) with experimental data (symbols) along with their best fit line (red-dashed). References: Conley et al. [5], Island et al. [21], Wang et al. [18], Zhang et al. [19], Schmidt et al. [20], Maniadaki et al. [24].

the flexible substrates in use [20,21]. As mentioned above, the uniaxial stress condition applies only for the MoSe$_2$ experiment of [21]. We also quote in parentheses our results excluding the variation of exciton binding energy under strain. It can be observed that sulfur-TMDs are more responsive to strain for PL peak shift and the amount of change is larger for biaxial strain than uniaxial one for each material considered.

Table 2. PL peak redshift under uniaxial or biaxial strain in comparison with results from literature. Our results (this work) have both uniaxial strain/stress (i.e., $\nu$ : 0/0.37) cases with the values in parentheses corresponding those without the excitonic contribution.

|         | MoS$_2$       | MoSe$_2$      | WS$_2$       | WSe$_2$      |
|---------|---------------|---------------|--------------|--------------|
|         | Uniaxial (\%) | Biaxial (\%) | Uniaxial (\%) | Biaxial (\%) |
| This Work | 49.4/31.1 (51.8/32.6) | 98.8 (103.6) | 43.6/27.5 (45.6/28.7) | 87.2 (91.2) |
| Literature | ~45$^a$, ~70$^b$, ~48$^c$ | 99.9/6$^d$, (90.15), 90.1$^e$ | 27$^f$/2$^f$ | 53.74$^e$ |
| Literature | 68.5/43.2 (71.8/45.2) | 113.8$^g$, 10$^h$ | 157$^e$ | 54$^i$ |

References: $^a$ [5], $^b$ [4], $^c$ [6], $^d$ [11], $^e$ [45], $^f$ [21], $^g$ [18], $^h$ [19], $^i$ [20]
Fig. 3. Biaxial strain dependence of A-exciton PL peak energy shift for monolayer TMDs, comparing our calculations (blue-solid) with experimental data (symbols) along with their best fit line (red-dashed). References: Lloyd et al. [11], Frisenda et al. [45].

4. Conclusions
A simple two-band $k \cdot p$ approach within minimal coupling to strain as applied to TMDs shows that the bandgap and effective masses are affected by the hydrostatic component of the strain, whereas the shear strain does not alter the optoelectronic properties, but merely shifts the wavevector of the valley extrema. A mixing of the valley edge states occurs away from the extrema which is either amplified or diminished depending on the tensile or compressive nature of strain, respectively. This also manifests itself on the CD that can be tuned in either direction by applying tensile or compressive strain which is more pronounced for the biaxial case. Comparison of strain-dependent PL peak shifts with a wide range of experimental data for monolayer TMDs demonstrates a satisfactory agreement provided that excitonic effects are included, and it reveals whether Poisson’s effect takes place in a certain experiment. This analysis can easily be extended to other TMDs with the availability of their $k \cdot p$ parameters. It can also act as a benchmark for more refined theories.

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