Erratum: Robust optical emission polarization in MoS_2 monolayers through selective valley excitation [Phys. Rev. B 86, 081301(R) (2012)]

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Following publication, it was noticed that some labels for the conduction- and valence-band states in Fig. 2(a) were erroneous. We present the corrected figure below in Fig. 1. This has no consequence on the interpretation of the experimental data, and the final conclusions of the article are still valid.

Here, we proceed to the detailed symmetry analysis to clarify the labeling of the states. Hereafter, we will use the notations of Koster *et al*. [1]. The K_+ and K_- valleys correspond to the C_{3h} point group. The conduction band is formed from orbital states [2–4],

$$|\phi^c\rangle = d_{z^2}, \tag{1}$$

which transforms according to the scalar Γ_1 representation [1]. Valence bands are formed from intermixed d- and p-shell orbitals [4–6] and can be written

$$|\phi^v_\tau\rangle = \frac{\alpha_\pm}{\sqrt{2}}(d_{x^2-y^2} + i\tau d_{2xy}) + \frac{\beta_\pm \tau}{\sqrt{2}}(p_x - i\tau p_y). \tag{2}$$

Here, $\tau = \pm 1$ represents the valley index. State $|\phi^v_+\rangle$ transforms according to the Γ_3 representation, whereas, $|\phi^v_-\rangle$ transforms according to the Γ_2 representation of C_{3h}. Note that

$$|\phi^v_-\rangle = \hat{K}|\phi^v_+\rangle, \tag{3}$$

where $\hat{K}$ is the Kramers' time-reversal operator so that $\alpha_- = \alpha_+^*$ and $\beta_- = \beta_+^*$ (in Fig. 1, $\alpha \equiv \alpha_+$, $\beta \equiv \beta_+$).

Now, taking the spin into account, the conduction-band states $|\phi^c\rangle \uparrow$ and $|\phi^c\rangle \downarrow$ transform according to the Γ_7 and Γ_8 representations, respectively (in Fig. 1, we note $K^c_{\pm,7}$ and $K^c_{\pm,8}$, respectively, for $K_\pm$ valleys). For the valence band, one has

$$\begin{aligned} (K_+)&: \quad \Gamma_3 \times \Gamma_7 = \Gamma_{10}, \quad \Gamma_3 \times \Gamma_8 = \Gamma_{12}, \\ (K_-)&: \quad \Gamma_2 \times \Gamma_7 = \Gamma_{11}, \quad \Gamma_2 \times \Gamma_8 = \Gamma_9 \end{aligned} \tag{4}$$

(in Fig. 1, we have labeled these states $K^v_{10(12)}$ for the K_+ valley and $K^v_{9(11)}$ for the K_- valley, respectively). Hence, the eigenfunctions in the K_+ valley belonging to the Γ_{10} (Γ_{12}) representation transform like the $\phi(5/2,+5/2)$ [$\phi(3/2,+3/2)$] angular momentum, whereas, the eigenfunctions in the K_- valley belonging to the Γ_9 (Γ_{11}) representation transform like the $\phi(5/2,-5/2)$ [$\phi(3/2,-3/2)$] angular momentum [1]. All these states are eigenstates of the spin-orbit Hamiltonian at the $K_\pm$ points of the Brillouin zone.

The optical selection rules are then deduced straightforwardly. The complex electric-field component [7] $e_+ \equiv -(e_x - ie_y)/\sqrt{2}$ [$e_- \equiv (e_x + ie_y)/\sqrt{2}$] transforms according to the Γ_3 (Γ_2) representations, respectively. The same is true for the electron linear

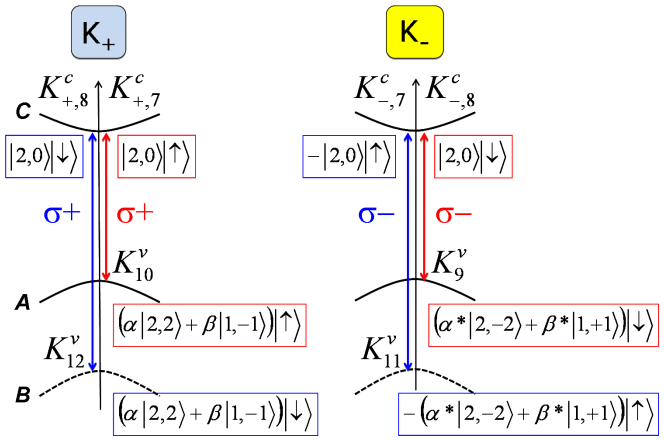

FIG. 1. (Color online) Selection rules for optical dipole transitions in a simple single-particle picture in K_+ and K_- valleys at zero magnetic field. The small spin-orbit splitting of the conduction bands does not appear at this scale [4].

momentum operator components $\hat{p}_+$ ($\hat{p}_-$) with similar definitions. Recalling the optical Hamiltonian $\hat{H}_{\rm opt}$ for light propagating along the **z** axis is proportional to $e_+^*\hat{p}_+ + e_-^*\hat{p}_- \equiv -(e_-\hat{p}_+ + e_+\hat{p}_-)$ and since [1]

$$\begin{aligned}(K_+):&\quad \Gamma_2\times\Gamma_{10}=\Gamma_7,\quad \Gamma_2\times\Gamma_{12}=\Gamma_8,\\ (K_-):&\quad \Gamma_3\times\Gamma_9=\Gamma_8,\quad \Gamma_3\times\Gamma_{11}=\Gamma_7,\end{aligned}\tag{5}$$

under σ^+-polarized light ($e_+=-1$, $e_-=0$; $\hat{H}_{\rm opt}\sim\hat{p}_-$), the interband matrix element $\langle\psi_+^c\uparrow|\hat{p}_-|\psi_+^v\uparrow\rangle$ transforms along $\Gamma_7^*\times\Gamma_2\times\Gamma_{10}=\Gamma_8\times\Gamma_7=\Gamma_1$, whereas, the matrix element $\langle\psi_+^c\downarrow|\hat{p}_-|\psi_+^v\downarrow\rangle$ transforms along $\Gamma_8^*\times\Gamma_2\times\Gamma_{12}=\Gamma_7\times\Gamma_8=\Gamma_1$. Conversely, under σ^--polarized light ($e_+=0, e_-=1$; $\hat{H}_{\rm opt}\sim-\hat{p}_+$), the matrix element $\langle\psi_+^c\uparrow|\hat{p}_+|\psi_+^v\uparrow\rangle$ transforms along $\Gamma_7^*\times\Gamma_3\times\Gamma_{10}=\Gamma_8\times\Gamma_{11}=\Gamma_2$, whereas, $\langle\psi_+^c\downarrow|\hat{p}_+|\psi_+^v\downarrow\rangle$ transforms along with $\Gamma_8^*\times\Gamma_3\times\Gamma_{10}=\Gamma_7\times\Gamma_{11}=\Gamma_6$. As neither of these irreducible representations coincides with the scalar representation, these transitions are forbidden. The other matrix elements are spin forbidden. Similar operations can be performed for transitions in the K_- valley. Finally, the only possible optical transition scheme is the one represented in Fig. 1.

Note the above description for state symmetries and optical selection rules is generally valid for any group-VIB transition-metal dichalcogenide compound MX_2 (M = Mo, W; X = S, Se, Te) of C_{3h} symmetry.

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