Berry curvature in monolayer MoS$_2$ with broken mirror symmetry

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(Dated: November 13, 2018)

An ideal 1H phase monolayer MoS$_2$ has the mirror reflection symmetry but this symmetry is broken in common experimental situations, where the monolayer is placed on a substrate. By using the k-p perturbation theory, we investigate the effect of the mirror symmetry breaking on the Berry curvature of the material. We find that the symmetry breaking may modify the Berry curvature considerably and the spin/valley Hall effect due to the modified Berry curvature is in qualitative agreement with a recent experimental result [Science 344, 1489 (2014)], which cannot be explained by previous theories that ignore the mirror symmetry breaking.

I. INTRODUCTION

In solids of two-dimensional (2D) hexagonal structure, an electron has not only spin but also valley degree of freedom, which acts as a pseudospin. The spin can be used for information storage, transport, and manipulation, and is the central degree of freedom for spintronics [1, 2]. It was recently realized [3–6] that the valley can play similar roles as the spin, opening the field of valleytronics. How to control the spin/valley degree of freedom is one of fundamental questions in spin/valleytronics, and the spin/valley Hall effect (SHE/VHE) is one possible way to achieve such control.

A prototypical material of 2D hexagonal structure is graphene, which has been studied extensively. Recently monolayer transition metal dichalcogenides (TMD) also have attracted huge attention as a 2D hexagonal material. Unlike the graphene, a monolayer TMD may have direct bandgap with suitable gap size and large spin-orbit coupling (SOC). It is thus a good candidate material for optoelectronic and spin/valleytronic devices [4].

A 1H phase monolayer MoS$_2$ [Figs. 1(a),1(b)] is probably most popular among the monolayer TMD materials. In this material, the mirror reflection symmetry is respected but the inversion symmetry is broken intrinsically. Energy bands are split by the SOC with electron spins quantized along the out-of-plane direction. Recent experiments on the monolayer MoS$_2$ investigated SHE/VHE [7, 8], spin-orbit torque [9, 10], valley magnetoelectric effect [11], valley relaxation [12–15], and spin relaxation [16–18]. Unfortunately many experimental results remain unexplained, which motivates further theoretical studies on this material.

In this paper, we investigate the SHE and VHE in a monolayer MoS$_2$ with the broken mirror symmetry. While the mirror reflection with respect to the mirror plane [Fig. 1(b)] within the monolayer MoS$_2$ may be a good symmetry for an ideal MoS$_2$ monolayer suspended in air, this symmetry is broken in common experimental situations where a MoS$_2$ monolayer is placed on a substrate and subject to a gate voltage. We demonstrate that the mirror symmetry breaking may significantly modify the monolayers Berry curvature, which is an important source of the SHE/VHE [19]. This provides an explanation as to why the experimental results [7, 11] on the SHE/VHE deviate from predictions of the previous theoretical studies [20] that assume the mirror symmetry. We calculate the spin and valley Hall conductivities as a function of the mirror symmetry breaking strength, which may be continuously modulated in experiments by applying a gate voltage. Qualitative agreement with recent experiments [7, 11] is found.

The paper is organized as follows. In Sec. II A, we introduce the k-p perturbed Hamiltonian near the K point of the monolayer MoS$_2$ with the mirror symmetry. In Sec. II B, we consider the mirror symmetry breaking effect in terms of the effective Hamiltonian. In Sec. III, we calculate the Berry curvature and orbital magnetic moment using the effective Hamiltonian and compare our result to recent experimental results. In Sec. IV, we discuss various technical issues related with this paper. Finally, our main results are summarized in Sec. V.
II. THEOREY

A monolayer MoS$_2$ has a direct band gap at the K and K’ points [21]. Since these two points are the time reversed images of each other, study on one point, say the K point, is sufficient to understand properties of the both points. We thus study only the K point which is highly symmetric and has the property of $C_{3h}$ point group. From the irreducible representations of $C_{3h}$ point group [22], K point basis functions of the two lowest conduction and the two highest valence bands may be written as

$$ |\phi_c\rangle = |d_{z^2}\rangle, \quad |\phi_v\rangle = \frac{1}{\sqrt{2}}(|d_{x^2-y^2}\rangle - i|d_{xy}\rangle), \quad (1) $$

where the subscript $c/v$ indicates conduction/valence bands. It is useful to introduce the Pauli matrix $\hat{\sigma}$ to distinguish conduction and valence bands with $\hat{\sigma}$ defined by $\hat{\sigma}_z |\phi_{c/v}\rangle = \pm |\phi_{c/v}\rangle$.

A. WITH MIRROR SYMMETRY

In the presence of the mirror symmetry, the k-p perturbation near the K point results in the effective Hamiltonian $H_0$ [20],

$$ H_0 = \frac{\hat{I} + \hat{\sigma}_z}{2} (\varepsilon_{c/\uparrow}(q) \frac{\hat{I} + \hat{\sigma}_z}{2} + \varepsilon_{c/\downarrow}(q) \frac{\hat{I} + \hat{\sigma}_z}{2}) + \frac{\hat{I} - \hat{\sigma}_z}{2} (\varepsilon_{v/\uparrow}(q) \frac{\hat{I} + \hat{\sigma}_z}{2} + \varepsilon_{v/\downarrow}(q) \frac{\hat{I} - \hat{\sigma}_z}{2}) + \alpha (-q_x \hat{\sigma}_x + q_y \hat{\sigma}_y), \quad (2) $$

where $\hat{\sigma}$ is the Pauli matrix for spin, $q$ is the Bloch momentum measured with respect to the K point, and $\varepsilon_{c/v/\uparrow/\downarrow}(q)$ is quadratic energy-momentum dispersion near the K point for the conduction/valence band with spin $\hat{\sigma}_z = +1/-1$. Thus $H_0$ describes the two lowest conduction bands and the two highest valence bands near the K point [Fig. 1(c)]. The last term in Eq. (2) describes the wavefunction hybridization between $|\phi_c\rangle$ and $|\phi_v\rangle$ as $q$ moves away from the K point [20]. Recalling that the Berry curvature arises from the $q$-dependent change of the wavefunction, the hybridization is crucial for the Berry curvature. In principle, the Berry curvature arises not only by the hybridization within the conduction and valence bands depicted in Fig. 1(c) but also by the hybridization between $|\phi_{c/v}\rangle$ and higher conduction and lower valence bands not shown in Fig. 1(c). However the DFT calculation [23] indicates that when the mirror symmetry is present, such hybridization with outer bands has negligible effect on the Berry curvatures of the two lowest conduction bands and the two highest valence bands, although it affects $\varepsilon_{c/v/\uparrow/\downarrow}(q)$. Thus for the coefficient $\alpha$ in the last term of $H_0$, we take its value $\alpha = 3.512$ eV·Å from the previous work [20] that captures the hybridization between $|\phi_c\rangle$ and $|\phi_v\rangle$ only. On the other hand, the quadratic dispersion $\varepsilon_{c/v/\uparrow/\downarrow}(q)$ is chosen in such a way that the energy eigenvalues $E_{c/v/\uparrow/\downarrow}(q)$ of $H_0$ agrees with the band structure from the DFT calculation [24].

B. WITHOUT MIRROR SYMMETRY

Until now, we have considered the ideal monolayer MoS$_2$ which has the mirror symmetry with respect to its 2D plane. However, the mirror symmetry is broken when the monolayer MoS$_2$ is placed on a substrate, which may generate an atomic scale potential gradient (or electric field) and modify the effective onsite and hopping energies of the S atoms in the bottom sublayer of MoS$_2$. These effects can lead to the coupling between the spin $\hat{\sigma}$ and the Bloch momentum $q$ (spin-momentum coupling) [25–31]. Figure 2(a) illustrates the microscopic process by which the spin-momentum coupling may emerge. $n_{\uparrow/\downarrow}$ denotes one of the four conduction or valence bands shown in Fig. 1(c) whereas $n_{\uparrow/\downarrow}'$ denotes outer bands not shown in Fig. 1(c), both with the given spin. The left panel in Fig. 2(a) illustrates the effect of atomic SOC, which induces the spin-orbit interaction between $n_{\uparrow}$ and $n_{\downarrow}$ and between $n_{\downarrow}$ and $n_{\uparrow}'$. The middle panel illustrates the effect of the mirror-symmetry-breaking, which induces the hybridization between $n_{\uparrow}$ and $n_{\uparrow}'$, and between $n_{\downarrow}$ and $n_{\downarrow}'$. The right panel summarizes the combined effect of the atomic SOC and the mirror symmetry breaking; $n_{\uparrow}$ and $n_{\downarrow}$ now couple to each other through the virtual transitions to $n_{\uparrow}'$ and $n_{\downarrow}'$.

As a result, the effective Hamiltonian of the monolayer
MoS$_2$ with the broken mirror symmetry becomes $H = H_0 + H_1$ [27], where

$$H_1 = \frac{i + \sigma_z}{2} [\beta_i (q \times \hat{s}) \cdot \hat{z} + \beta_r q \cdot \hat{s}]. \quad (3)$$

Here $\beta_i$ and $\beta_r$ are the spin-momentum coupling constants which depend on the degree of mirror symmetry breaking. Note that in addition to the conventional Rashba spin-momentum coupling $q \times \hat{s} \cdot \hat{z}$, the Weyl spin-momentum coupling $q \cdot \hat{s}$ coexists. The corresponding couplings for the valence bands are ignored for the reason specified below.

Both the Rashba and Weyl couplings induce $q$-dependent spin character change of the wavefunction. Thus the couplings can affect the Berry curvature. For the valence bands, however, this effect is strongly suppressed (and thus ignored) since the intrinsic spin-dependent splitting of the valence bands, $\Delta_v \approx 148\text{ meV}$ [Fig. 1(c)], which exists even without the mirror symmetry breaking, is much stronger than the Rashba and Weyl couplings. For the conduction bands, on the other hand, this effect can be significant since the intrinsic spin-dependent splitting of the conduction bands, $\Delta_c \approx 3\text{ meV}$, is much weaker.

The next section shows that the Berry curvature depends on $\beta_i$ and $\beta_r$ only through the combination $\beta = \sqrt{\beta_i^2 + \beta_r^2}$. Here we thus estimate $\beta$. A recent experiment on electron-doped MoS$_2$ placed on a SiO$_2$ substrate [32] reports that the product $\beta k_F$ ranges 1 $\sim$ 3 meV (see Fig. 3 in Ref. [32]), where $k_F$ is the Fermi wavelength. Considering that the electron density $n_{2D} = k_F^2/2\pi$ in the experiment is of the order of $10^{14}$ cm$^{-2}$, we conclude that $\beta_i$ is of the order of 10 meV $\cdot$ Å. For $\beta_i$, we do not have any direct estimation but we expect $\beta_i$ to be comparable to or smaller than $\beta_i$. This leads to the estimation of $\beta \sim 10\text{ meV} \cdot \text{Å}$. Here we remark that this estimation is at odds with the freestanding monolayer model. A recent DFT calculation [27] examines the effect of a perpendicular electric field $E_z$ on a suspended ideal monolayer MoS$_2$ and finds $\beta = 0.033E_z \text{ eV} \cdot \text{Å}$, where $E_z$ is in units of V/Å. Combined with $E_z \sim 0.03\text{ V/Å}$ [33] estimated from gate voltages in experiments [7, 11], this calculation leads to $\beta \sim 1\text{ meV} \cdot \text{Å}$, which is one order of magnitude smaller than the above estimation obtained from the experiment [32]. We attribute this difference to the neglect of interatomic hopping between MoS$_2$ and substrates (SiO$_2$) in the freestanding monolayer model [27]. Recent studies [28, 29, 31] report that interatomic hopping with environment atoms can enhance the spin-momentum coupling strength more than one order of magnitude than estimated from the electric field strength. As a reference for estimation of this hopping effect, we use results on a monolayer MoS$_2$–monolayer graphene heterostructure [34–37], for which it is reported that the graphene acquires the spin-momentum coupling strength of $\sim 160\text{ meV} \cdot \text{Å}$ [34]. Efficient electrical gate control of spin current is also demonstrated [35, 36]. To obtain the estimation of $\beta$ for our problem, one should take into account the fact that the hopping effect is inverse quadratically proportional to the energy spacing (Fig. 2) between bands connected by the hopping, and the energy spacing $(1.8 - 8.9)/2 = 3.6\text{ eV}$ between MoS$_2$ (energy gap 1.8 eV) and SiO$_2$ (8.9 eV) bands is about factor 4 larger than that $(1.8 - 0)/2 = 0.9\text{ eV}$ between MoS$_2$ and graphene (0 eV) bands. This consideration implies that $\beta$ for the MoS$_2$–SiO$_2$ system is about factor 16 smaller than the corresponding value $\sim 160\text{ meV} \cdot \text{Å}$ for the MoS$_2$-graphene structure. One thus obtains $\beta \sim 10\text{ meV} \cdot \text{Å}$ for the MoS$_2$–SiO$_2$ system, which agrees with the above estimation obtained from the experiment [32].

We remark that the estimated value of $\beta \sim 10\text{ meV} \cdot \text{Å}$ is about two orders of magnitude smaller than the corresponding value of $\sim 1\text{ eV} \cdot \text{Å}$ in strong spin-momentum coupling systems such as Bi/Ag(111) [38]. Thus it is reasonable to expect that $H_1$ in Eq. (3) would generate only weak effects. One example is the spin-conservation violation. Whereas $H_0$ in Eq. (2) conserves $\hat{z}$, $H_1$ does not. But since $\beta$ is very small, the spin conservation is violated only weakly. Figure 2(b) shows that for most values of $q$, the expectation value $\langle \hat{z} \rangle$ of the lowest conduction bands stay close to +1 or −1, confirming the weakness of the spin-conservation violation. The spin-conservation induces sizable deviation of $\langle \hat{z} \rangle$ from ±1 only for narrow range of $q$ in which the lowest and the second lowest conduction bands become degenerate. However our study in the next section is focused on electronic states very close to the K point ($|q| \ll 0.1\text{ Å}^{-1}$), so the spin-conservation violation is a weak effect and we use a spin index $s$ to denote eigenstates.

### III. RESULT

In this section, we demonstrate that $H_1$ can induce sizable correction to the Berry curvature even though $\beta$ is small. This becomes possible since the two spin branches of the lowest conduction bands are separated by a small energy spacing of 3 meV. Its demonstration goes as follows.

The Berry curvature $\Omega_{n,s}(q) = \nabla_q \times \langle \psi_{n,s} | \nabla_q | \psi_{n,s} \rangle : \hat{z}$ at each band [39, 40] is given by

$$\Omega_{n,s}(q) = i \sum_{n',s'} \left[ \langle \psi_{n,s} | \frac{\partial}{\partial q_x} | \psi_{n',s'} \rangle \langle \psi_{n',s'} | \frac{\partial}{\partial q_y} | \psi_{n,s} \rangle \right]$$

$$- \left( \frac{\partial}{\partial q_x} \leftrightarrow \frac{\partial}{\partial q_y} \right), \quad (4)$$

where $|\psi_{n,s}\rangle$ and $E_{n,s}(q)$ are respectively the energy eigenstate and the corresponding energy eigenvalue of $H$, and the summation over $(n',s')$ runs over the four bands of $H$ excluding the case $(n',s') = (n,s)$. The prime symbol $(\prime)$ above $\Sigma$ is introduced to denote this exclusion. The second line of Eq. (4) contains $\partial H/\partial q_{x,y} = \partial H_0/\partial q_{x,y} + \partial H_1/\partial q_{x,y}$ and allows one to
separate $\Omega_{n,s}(q)$ into three contributions. When $\partial H/\partial q_x$ and $\partial H/\partial q_y$ are replaced by $\partial H_0/\partial q_x$ and $\partial H_0/\partial q_y$, one obtains the first contribution, which depends on $\beta_{ji}$ only implicitly through $|n s q\rangle$, $|n's' q\rangle$, $E_{n,s}(q)$, $E_{n',s'}(q)$, and captures the hybridization effect between $(c, \uparrow / \downarrow)$ and $(v, \uparrow / \downarrow)$ bands (orbital hybridization) due to the last term of $H_0$ [Eq. (2)]. When $\partial H/\partial q_x$ and $\partial H/\partial q_y$ are replaced by $\partial H_1/\partial q_x$ and $\partial H_1/\partial q_y$, one obtains the second contribution, which depends explicitly on $\beta_{ji}$ and captures the hybridization between $(c, \uparrow / \downarrow)$ and $(c, \downarrow / \downarrow)$ bands (spin hybridization) [see Eq. (3)]. “Mixed” contributions coming from $\partial H_0/\partial q_x$ and $\partial H_1/\partial q_y$, for instance, vanish since $\partial H_0/\partial q_x$ and $\partial H_1/\partial q_y$ induce completely different types of hybridization. Thus only two contributions survive. When $(n, s)$ denotes $(c, \downarrow)$, for instance, straightforward calculation produces

$$
\Omega_{c,\downarrow}(q) = \Omega_{c,\downarrow}^e(q) + \Omega_{c,\downarrow}^s(q),
$$

$$
\Omega_{c,\downarrow}^e(q) = \frac{2\alpha^2 \Delta}{[E_{c,\downarrow}^e(q) - E_{v,\downarrow}^e(q)]^3},
$$

$$
\Omega_{c,\downarrow}^s(q) = \frac{2\beta^2 \Delta_c}{[E_{c,\downarrow}^s(q) - E_{c,\uparrow}^s(q)]^3},
$$

where $\Omega_{n,s}^e(q)$ and $\Omega_{c,s}^e(q)$ are the Berry curvatures from the orbital and the spin hybridizations, respectively. $\Omega_{c,\downarrow}(q)$, $\Omega_{v,\downarrow}(q)$, and $\Omega_{v,\uparrow}(q)$ can also be evaluated in a similar way.

The Berry curvatures $\Omega_{c/v,\uparrow/\downarrow}(q)$ are evaluated for $\beta = 0$ meV $\cdot$ Å [Fig. 3(a)] and 20 meV $\cdot$ Å [Fig. 3(b)] as a function of $q_x$ with $q_y = 0$. Note that $\Omega_{c,\uparrow/\downarrow}(q)$ is more than one order of magnitude enlarged due to the mirror-symmetry breaking whereas $\Omega_{c,\downarrow}(q)$ is only very weakly affected. This difference between $\Omega_{c,\uparrow/\downarrow}(q)$ and $\Omega_{c,\uparrow}(q)$ stems from $H_1$, which affects the wavefunction character only for the conduction bands. In case of $\Omega_{c,\uparrow}(q)$, $\Omega_{c,\downarrow}^e(q)$ is responsible for the enlargement of $\Omega_{c,\downarrow}(q)$. We emphasize that $\Omega_{c,\downarrow}^e(q)$ is much larger than $\Omega_{c,\downarrow}^s(q)$ not because of its numerator but because of its denominator [Eq. (6)]. At the K point, for $\beta = 20$ meV $\cdot$ Å, its numerator $2\beta^2$ is about $(175)^2$ times smaller than the numerator $2\alpha^2$ of $\Omega_{c,\downarrow}^s(q)$, but its denominator $\Delta_c^2 \sim (3$ meV$)^2$ is about $(600)^2$ times smaller than the corresponding denominator $\Delta_c^2 \sim (1.82$ eV$)^2$. Their combined effect is more than one order of magnitude enlargement. Figure 3(c) shows the $\beta$ dependence of the Berry curvature at the K point. While $\Omega_{v,\uparrow/\downarrow}(q)$ remains almost independent of $\beta$, $\Omega_{v,\uparrow/\downarrow}(q)$ grows quadratically as $\beta$ grows. We also calculate the orbital magnetic moment [41]

$$
m_{n,s}(q) = \frac{e}{2k} \sum_{n',s'} \left[ \langle n s q | \frac{\partial H}{\partial q_x} | n' s' q \rangle \langle n' s' q | \frac{\partial H}{\partial q_y} | n s q \rangle - \left( \frac{\partial}{\partial q_x} \leftrightarrow \frac{\partial}{\partial q_y} \right) \right],
$$

The result is shown in Fig. 3(d). Note that the mirror symmetry breaking barely affects the orbital magnetic moment in contrast to its significant effects on the Berry curvature. This difference arises since $m_{n,s}(q)$ is inversely proportional to the energy difference in contrast to the difference square in case of $\Omega_{n,s}(q)$. This difference in the energy denominator makes the $\beta$ effect much weaker.

Next we compare our calculation results with experiments [7, 11]. In the recent experiment [7], right/left circularly polarized light is used to selectively excite electrons near the K/K’ point from $(v, \uparrow / \downarrow)$ to $(c, \downarrow / \downarrow)$ and the Hall conductivity is measured for the optically excited states as a function of the gate voltage and the light intensity, which controls the number of excited carriers. In the degenerate limit, the Hall conductivity from the intrinsic and side-jump contributions [7, 41] is

$$
\sigma_H \approx -\frac{e^2}{h} \Omega_{c,\downarrow}(0) \cdot n_{c,\downarrow}^K,
$$

where $n_{c,\downarrow}^K$ is the photocarrier density under the assumption that excitation occurs only to the $(c, \downarrow)$ band near the K point. The minus sign in Eq. (9) arises since the side-jump contribution is two times bigger and of opposite sign to the intrinsic contribution. The result is shown in Fig. 4(a). Note that (i) $\sigma_H$ is essentially linear in $n_{c,\downarrow}^K$ and (ii) the slope of the $\sigma_H$ vs $n_{c,\downarrow}^K$ curve grows roughly as $\beta^2$. In comparison, the experimental data (Fig. 3 in Ref [7]) indicates that (iii) $\sigma_H$ grows linearly with the density $\Delta_{nph}$ of the photoexcited carriers and (iv) the slope of the linear dependence varies with the gate voltage $V_g$. Here $\Delta_{nph}$ and $n_{c,\downarrow}^K$ are related by $n_{c,\downarrow}^K \equiv \Delta_{nph} P$, where the ratio $P$ is reported to be much smaller than 1 since it is suppressed by valley relaxation [12–15] and more significantly by the spin relaxation within the conduction bands [16, 17]. Such spin relaxation is crucial since.
The activity is given by symmetry breaking effect appears to be weak. In the from the chemical potential variation and the mirror-symmetry breaking effect which can be obtained from Eq. (10) by multiplying each term by the proper spin expectation value. Note that for large $\beta$, $\sigma_{H}^{\text{spin}}$ is significantly larger than $\sigma_{H}^{\text{valley}}$ [Fig. 4(b)] since the two spin-split conduction band contributions now add up.

Another interesting implication of our study is the Rashba-Edelstein effect [42]. When the mirror symmetry is broken, in-plane chiral spin component arises from the Rashba and Weyl spin-momentum coupling between the two lowest conduction bands in monolayer MoS$_2$ [Ref. $(7)$]. The in-plane spin component and the Berry curvature are maximized at the degenerate points [Fig. 1(c)] with completely hybridized eigenstates. In such a situation, an electric field can generate spin accumulation (Rashba-Edelstein effect). A similar enhancement of the Berry curvature has been theoretically proposed [43, 44] for graphene in the context of the quantum anomalous Hall effect. There is also an experimental paper which reported the change of the inverse Rashba-Edelstein effect depending on the Fermi energy in 2D Rashba system [45]. A recent experiment [8] on a heterostructure made of a n-doped monolayer MoS$_2$ and a ferromagnet Co reported large inverse Rashba-Edelstein effect, which may be related to the strong spin-momentum coupling effects near the degenerate points. This relation may be tested experimentally through the material variation since the monolayer MoX$_2$ (X=S, Se, Te) all exhibits the degenerate points whereas WX$_2$ does not [24].

### IV. DISCUSSION

Here we discuss a few related issues. The first issue is the substrate effect. In Sec. II B, the substrate effect was taken into account through $H_1$. But substrates may generate other types of perturbations as well, which are ignored in this paper. Here we argue that when the coupling with the substrate is weak, the neglect of other perturbations can be a good approximation and $H_1$ describes the most important perturbation in terms of the Berry curvature correction. This point can be seen from the general expression of the Berry curvature in Eq. (4). When a perturbation is weak, it usually induces only minor corrections to the Berry curvature. But an exceptional situation can occur when a perturbation induces a hybridization between energy bands with small energy.
spins. Thus they should contain a spin current in a conventional way (spin current edge spin accumulation. In Sec. III, we defined a spin current and argued that the modified definition can improve the connection between the bulk spin Hall conductivity and the edge spin accumulation. In Sec. III, we defined a spin current in a conventional way (spin current \( \propto \) spin times velocity) since this definition is more commonly used and also the modified definition becomes identical to the conventional definition at the K and K’ points \( (q = 0) \). 

Lastly we discuss possible effects of the skew scattering briefly. In case of the anomalous Hall effect, it is well known [48] that the skew scattering is the dominant mechanism in very clean systems whereas the intrinsic Berry curvature is dominant in relatively dirty systems. In case of the MoS\(_2\) experiment [7], the measured Hall conductivity \( \sigma_H \) is in rough agreement with the prediction of the Berry curvature theory [20] that neglects the mirror symmetry breaking effect. Thus we suspect that the intrinsic Berry curvature is more important in this experiment. This has also motivated us to investigate the deviation between the measured \( \sigma_H \) and the theory \([20]\) in terms of the Berry curvature modification by the mirror symmetry breaking. However there is a possibility that the skew scattering contributes to the deviation as inferred in Ref. [7], although the skew-scattering-based theory of the deviation has not developed yet. Refined experiments are needed to determine whether the mirror symmetry breaking or the skew scattering is the main reason of the deviation.

V. SUMMARY

In summary, we calculated the Berry curvature in a monolayer MoS\(_2\) in realistic situations where the mirror symmetry is broken. Our focus was not the well-known Rashba spin momentum coupling at the \( \Gamma \) point, but the spin momentum coupling at the K point which is a direct band gap point. We found that the symmetry-breaking contribution to the Berry curvature, which varies with the gate voltage, may be larger than the previously known Berry curvature in an ideal monolayer MoS\(_2\) with the symmetry. However we estimated that the symmetry breaking barely affects the orbital magnetic moment. This provides an explanation to the gate voltage dependence of VHE in the recent experiment on VHE [7]. It also provides an explanation as to why the two recent experiments [7, 11] show different results with regards to the gate voltage dependence of the VHE. Large inverse Rashba-Edelstein effect [8], which is reported recently in a monolayer MoS\(_2\) and a ferromagnet heterostructure, may be related to our result.

We acknowledge helpful discussion with Jieun Lee and Jonghwan Kim. Recently we were informed that Ref. [49] reports similar results as ours although it does not discuss its connection with the experiment [7]. Through Ref. [49], we became aware of a recent experiment [32], which provides valuable data for the estimation of \( \beta \). This work was supported by the National Research Foundation of Korea grant (No. 2011-0030046).

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