Valley polarized magnetic state in hole-doped mono layers of transition metal dichalcogenides

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We compute the valley/magnetic phase diagram of mono layers of transition metal dichalcogenides in the hole doped region where spin-orbit effects are particularly relevant. Taking into account the moderate to high local electron-electron interactions due to the presence of transition metal atoms, we show that the system is unstable to an itinerant ferromagnetic phase where all charge carriers are spin and valley polarized. This phase shows an anomalous charge Hall and anomalous spin-Hall response, and may thus be detected experimentally.

Introduction.—The manipulation of quantum degrees of freedom such as the electron charge and spin is an essential ingredient in the development of better devices and novel quantum technologies. Yet charge and spin do not exhaust all quantum degrees of freedom associated with electrons in solids. In certain semiconductors, multiple degenerate valence band maxima or conduction band minima – the so called valleys – occur. Carriers are then characterized not only by charge and spin, but also by the valley degree of freedom indicating the region in momentum space where they are confined. Valleytronics aims to use this quantum degree of freedom in novel technological devices in much the same way the electron spin is used in spintronics. Individual valley manipulation is, however, a necessary requirement. Well known semiconductors such as Si and Ge display valleys [1], but it is difficult to have an external coupling to a single valley in these cases, which severely limits their manipulation.

The isolation of real 2D materials with hexagonal lattice like graphene have put valley physics on the spotlight again. The manipulation of the two valleys of graphene is, however, not easy to achieve [2]. Such manipulation has finally been clearly demonstrated for the new class of 2D materials known as semiconducting transition metal dichalcogenides (TMDs) [3], formula MX2, where M is a transition metal (ex. Mo, W) and X is a chalcogen (ex. S, Se) [4, 5]. The demonstration that electrons of either valley can be excited across the gap by conveniently choosing either left or right circularly polarized light paves the way to valleytronic devices [6–8]. The situation is even more interesting because of the non-negligible spin-orbit coupling in TMDs, which induces a sizable valence band spin-splitting [9]. Valley polarization may then be achieved by applying a perpendicular magnetic field [10–14], which combined with optical absorption makes coherent valley manipulation possible [15–18].

![Figure 1](https://example.com/figure1.png)

Figure 1: (a) Mean field phase diagram in the $n_{\text{hole}}$–$U$ plane, indicating the normal and the valley polarized ferromagnetic (VPF) phases, at a temperature of $T = 1$ K and $U' = 0$ for the TMD WS2. The dashed red line indicates the transition at $T = 100$ K. The vertical dashed line represents the estimated critical $U$ of 2.38 eV in the limit of low $T$ and $n_{\text{hole}}$ obtained using a low energy model. (b) Phase diagram in the $U$–$U'$ plane at a hole density of $n_{\text{hole}} = 0.2 \times 10^{13}$ cm$^{-2}$ and $T = 1$ K. The dashed red line, shows the transition line at the temperature of $T = 100$ K. The dashed black line indicates the critical line $U = U_c + 4U'$, estimated using the low energy model. Panels (c) and (e) show the band structure for the spin up (in red) and spin down (in blue) valence bands in the normal and VPF phases, respectively. The horizontal dashed line indicates the Fermi level for a constant particle number of $n_{\text{hole}} = 10^{13}$ cm$^{-2}$. The Fermi surfaces for the normal and VPF phases are represented in panels (d) and (f), respectively.
For systems with degenerate valleys like TMDs, an obvious question is whether a spontaneously valley polarized phase can emerge. The question is not only of fundamental interest, since possible device applications in valleytronics will require valley polarized materials in as much the same way spintronic devices require materials with long range magnetic order. Spontaneous valley polarization was predicted more than thirty years ago for Si inversion layers [19], and experimentally confirmed soon after [20]. This phase has nevertheless been elusive within the much recent field of novel 2D materials, and only in the Landau level regime it has some relevance [21–25]. Only recently have spontaneous valley polarization been used to explain magnetoluminescence results in electron doped WS$_2$ [26].

In this work we predict that hole doped TMDs, in particular those with large spin-splitting of the valence band like WS$_2$, display a valley polarized ferromagnetic (VPF) phase which should be robust in a wider range of parameters than its electron doped counterpart [26]. A typical phase diagram is shown in Figs. 1(a) and (b) in the plane of intra-orbital $U$ Coulomb interaction and hole density and, $U$ and inter-orbital $U'$ interaction, respectively. Even though the Coulomb repulsion parameters are largely unknown for TMDs, both the $T = 1$ K (full line) and the $T = 100$ K (dashed line) transition lines put the valley polarized phase within reach according to current parameter estimates [27]. As shown Figs. 1(c) and (d) in the normal phase there are degenerate hole pockets at both inequivalent valleys $K$ and $K'$. Even though in each valley the carriers are spin polarized due to spin-orbit interaction, since the two valleys are degenerate there is no net spin polarization. On the contrary, in the valley polarized phase only a single valley is occupied, as shown in Figs. 1(e) and (f). The system then realizes a valley polarized ferromagnet with a single Fermi pocket occupied. A key ingredient for this complete valley and spin polarization is the large spin-splitting of the valence band due to strong spin-orbit coupling. For the conduction band, the spin-splitting is smaller by one order of magnitude at least [28], given rise to a partially valley polarized [26], and thus less stable phase.

Model and variational mean field treatment.—We model electrons in TMDs using a M atom 3-orbital nearest neighbor tight-binding Hamiltonian. The free part of the Hamiltonian is given by

$$H_0 = \sum_{i,j} \sum_{\gamma,\gamma',\sigma} c_{i,\gamma,\sigma}^\dagger E_{\gamma\gamma'}^{ij}(r_{ij})c_{j,\gamma',\sigma} + H_{SO},$$

where $c_{i,\gamma,\sigma}^\dagger$ is a electron creation operator on lattice site $i$, M atom orbital $\gamma = d_{x^2−y^2}, d_{xy}, d_{x^2−y^2}$ and spin $\sigma = \uparrow, \downarrow$. $E_{\gamma\gamma'}^{ij}(r_{ij})$ are hopping integrals as given in Ref. [29] for the nearest neighbor model [37], and $H_{SO}$ is the spin-orbit coupling term. For the interacting part of the Hamiltonian, we consider on-site interactions, including the intra- ($U$) and inter-orbital ($U'$) Coulomb interactions, as well as Hund ($J$) and pair-hopping ($J'$) terms:

$$H_{\text{int}} = \frac{U}{2} \sum_{i,\gamma,\sigma} n_{i,\gamma,\sigma} n_{i,\gamma',\sigma'} + \frac{U'}{2} \sum_{i,\gamma,\sigma} n_{i,\gamma,\sigma} n_{i,\gamma',\sigma'}$$

$$+ \frac{J}{2} \sum_{i,\gamma \neq \gamma'} \sum_{\sigma,\sigma'} c_{i,\gamma,\sigma}^\dagger c_{i,\gamma',\sigma'} c_{i,\gamma',\sigma'} c_{i,\gamma,\sigma}$$

$$+ \frac{J'}{2} \sum_{i,\gamma \neq \gamma'} \sum_{\sigma,\sigma'} c_{i,\gamma,\sigma}^\dagger c_{i,\gamma',\sigma'} c_{i,\gamma',\sigma'} c_{i,\gamma,\sigma},$$

where we have written $n_{i,\gamma,\sigma} = c_{i,\gamma,\sigma}^\dagger c_{i,\gamma,\sigma}$. From the four parameters characterizing the on-site interaction only two are independent as by symmetry arguments one has for $d$ orbitals $J' = J = (U − U')/2$ [30].

We performed a mean field analysis of the interacting Hamiltonian $H = H_0 + H_{\text{int}}$. We focused on homogeneous phases that are diagonal in the spin and orbital degrees of freedom. The mean field Hamiltonian thus reads

$$H_{MF} = H_0 + \sum_{\gamma,\sigma} \phi_{\gamma,\sigma} \sum_{i} n_{i,\gamma,\sigma}$$

where $\phi_{\gamma,\sigma}$, the molecular fields for atomic orbital $\gamma$ and spin $\sigma$, constitute variational parameters. Due to the spin-valley coupling in TMDs, we have that magnetic instabilities, which break time reversal symmetry, also lift valley degeneracy. We therefore focus on magnetic phases and assume a minimum set of variational parameters, with

$$\phi \equiv \phi_\uparrow \equiv \phi_{d_{x^2−y^2},\uparrow} = \phi_{d_{xy},\uparrow} = \phi_{d_{x^2−y^2},\downarrow} = -\phi_\downarrow.$$

This ansatz corresponds to a relative shift in energy of the spin up and down states keeping the same electronic dispersion relation for each spin component. We analyze the possible phases at fixed hole concentration, $n_{\text{hole}}$, by minimizing the mean field functional

$$\mathcal{F}[\phi] = \Omega_{MF} + \mu \langle N_e \rangle_{MF} + \langle H - H_{MF} \rangle_{MF},$$

where $\Omega_{MF} = -k_B T \log \text{Tr} \left\{ e^{-\beta (H_{MF} - \mu N_e)} \right\}$ is the grand potential for the mean field Hamiltonian, with $N_e$ the total electron number operator, and $\langle ... \rangle_{MF}$ is the thermodynamical average with respect to $H_{MF}$. In the previous equation, the chemical potential is determined by the condition

$$2 - n_{\text{hole}} = \frac{1}{N} \sum_{k,n,\sigma} f \left( \epsilon_{k,n,\sigma}^{MF} - \mu \right),$$

where $N$ is the number of lattice sites, $n_{\text{hole}}$ is the density of holes per unit cell, $f(\epsilon) = (e^{\beta \epsilon} + 1)^{-1}$ is the Fermi-Dirac function and $\epsilon_{k,n,\sigma}^{MF}$ are the bands of $H_{MF}$ [38].

In the following, we focus on the large valence band spin-splitting TMD, WS$_2$, for hole dopings where the
chemical potential lies within the spin-splitting of the valence bands. In Figs. 1(a-b), we show the phase diagram of WS$_2$. As can be seen in In Fig. 1(a), for a given hole density $n_{\text{hole}}$ and $U'$ value, there is a critical value of $U$ above which the system goes into a valley polarized ferromagnetic phase. Using a low energy model, which correctly captures interactions between holes and the full band as well as the multi-orbital character of the system, we estimate $U_c \approx 2.38$ eV in the limit of low temperature and hole density with $U' = 0$. For finite $U'$, the low energy model predicts that the system will be ferromagnetic provided $U > U_c + 1.4U'$, which is in good agreement with the tight-binding results shown in Fig. 1(b). As represented in Fig. 1(c-f), in the VPF phase the system becomes fully valley and spin polarized, with one of the spin polarized bands becoming fully occupied, while the opposite polarized band remaining partially occupied. This is further shown in Fig. 2, where we plot the behavior of the mean field functional $\mathcal{F}[\phi]$ as a function of $\phi$ for a hole density of $n_{\text{hole}} = 10^{13}$ cm$^{-2}$. The plateau region seen in $\mathcal{F}[\phi]$ signals the case where the system becomes fully valley and spin polarized, with one of spin polarized bands becoming fully occupied, while the opposite polarized band remains partially occupied. In the zero temperature limit, once one of the spin bands becomes fully occupied $\mathcal{F}[\phi]$ no longer depends on $\phi$. At finite temperature, there will always be some hole density in the minority band and therefore $\mathcal{F}[\phi]$ will have a weak dependence on $\phi$ as shown in the inset of Fig. 2(b), where, within numerical precision, the minimum of $\mathcal{F}[\phi]$ indicating the stability of the VPF phase can be seen. The spin and orbit resolved densities are plotted in Fig. 3(a-b) for the case of $U = 6$ eV and $U' = 0$ eV, at $n_{\text{hole}} = 10^{13}$ cm$^{-2}$ and $T = 1$ K. As can be seen in Fig. 3(a) for the $d_{z^2}$ orbital, and in Fig. 3(b) for the degenerate orbitals $d_{xy}$ and $d_{x^2-y^2}$, the system becomes a spin polarized metal. The evolution of the chemical potential is shown in panel (c). Similar results are obtained for other TMDs of the semiconducting family.

**Anomalous Hall and other responses.**— Although TMDs possess a bands with a locally non-vanishing Berry curvature, intrinsic time-reversal symmetry (TRS) voids them of an anomalous Hall (AH) response other than the valley Hall effect [9]. The spontaneous breaking of TRS
in an itinerant magnetic phase provides a richer response, in
virtue of the simultaneous polarization in the spin and
valley degrees of freedom.

The AH conductivity can be expressed in terms of the
Berry connection as [31]

\[ \sigma^{AH} = -\frac{e^2}{h} \frac{1}{A_c N} \sum_{\mathbf{k},n,\sigma} \left( \epsilon_{\mathbf{k},n,\sigma}^{MF} - \mu \right) \Omega_{\mathbf{k},n,\sigma}, \]

where \( \Omega_{\mathbf{k},n,\sigma} \) is the Berry curvature and \( \epsilon_{\mathbf{k},n,\sigma}^{MF} = \epsilon_{\mathbf{k},n,\sigma}^0 + \sigma \phi \) is the mean-field dispersion relation, with \( \epsilon_{\mathbf{k},n,\sigma}^0 \) the
eigenenergies of Eq. (1), and we use \( A_c \) the unit cell area.

For hole doping, we can write the AH conductivity as a
contribution from the full bands \( \sigma^{AH} \) and a contribution
from the holes \( \sigma_h^{AH} \), i.e. \( \sigma^{AH} = \sigma_h^{AH} + \sigma_{\mathbf{k}}^{AH} \),
where the full band contribution is null. For weak doping, the
main contribution to \( \sigma_{\mathbf{k}}^{AH} \) comes from the valence band
pockets at the \( K \) and \( K' \) points, which have, respectively,
spin up and spin down polarizations. Therefore we can
write \( \sigma_{\mathbf{k}}^{AH} \simeq \sigma_{h,\tau,\sigma}^{AH} + \sigma_{h,\sigma}^{AH} \), where

\[ \sigma_{h,\tau,\sigma}^{AH} = \frac{e^2}{h} \frac{1}{A_c N} \sum_{\mathbf{k}} [1 - f(\epsilon_{\mathbf{k},\tau,\sigma} - \mu)] \Omega_{\mathbf{k},\tau,\sigma}, \]

with \( \tau \) indicating valence band. Neglecting the momentum
dependence of the Berry curvature, which is valid in the
limit of small doping, we approximate

\[ \sigma_{h,\tau,\sigma}^{AH} \simeq \frac{e^2}{h} \Omega_{\mathbf{k},\tau,\sigma} n_{\text{hole},\uparrow/\downarrow}, \]

where \( n_{\text{hole},\uparrow/\downarrow} \) is the spin up/down hole density per area
and \( \Omega_{\mathbf{k},\tau,\sigma} = \Omega_{\mathbf{k},\tau,\sigma}^0 = -\Omega_{\mathbf{k},\tau,\sigma}^0 \) is the Berry curvature at the
\( K/K' \) point. The Berry curvature at the \( K \) and \( K' \)
points can be computed within a low energy, continuum
model. Using \( k \cdot p \) theory, we can write an effective two-
band model valid close to the \( \tau K \) point

\[ H_{\mathbf{k},\tau,\sigma} = \left( \mathcal{E}_0 + \sigma \tau \frac{\lambda}{2} + a^2 k^2 \right) \mathbf{I} + \left( \Delta - \sigma \tau \frac{\lambda}{2} + \beta a^2 k^2 \right) \mathbf{\sigma} + u a \mathbf{\sigma} \cdot \mathbf{k}, \]

where \( \mathbf{\sigma} = (\sigma_x, \sigma_y) \) and \( \mathcal{E}_0 \simeq 0.84 \text{ eV}, \Delta \simeq 0.9 \text{ eV}, \alpha \simeq 0.26 \text{ eV}, \beta \simeq 0.38 \text{ eV}, \) and \( u \simeq 1.69 \text{ eV}, \) with \( \alpha \simeq 3.191 \text{ Å} \)
the lattice parameter and \( \lambda \simeq 0.211 \text{ eV} \) the spin-orbit
coupling. From the eigenstates of this Hamiltonian we
can evaluate the Berry curvature as [9],

\[ \Omega_{\mathbf{k},\tau,\sigma} = a^2 \tau \frac{u a^2}{2} \frac{(\Delta - \sigma \tau \frac{\lambda}{2} - \beta a^2 k^2)}{[\Delta - \sigma \tau \frac{\lambda}{2} + \beta a^2 k^2]^{3/2}}, \]

from which we obtain \( \mathcal{E}_0 = \mathcal{E}_0_{\tau,\tau,\uparrow} = \mathcal{E}_0_{\tau,\tau,\downarrow} = a^2 (u a^2)^2 / 2 (\Delta - \frac{\lambda}{2}) \simeq 20 \text{ Å}^2. \)
Therefore the AH response is proportional to the magnetization of the
system \( \sigma^{AH} \simeq \frac{e^2}{h} \Omega_0 \left( n_{\text{hole},\uparrow} - n_{\text{hole},\downarrow} \right). \) Besides the
charge response, we can also consider spin and spin-valley
responses, which can be obtained as \( \sigma^{AH}_s = -\sum_{\tau,\sigma} \epsilon_{\tau,\sigma}^{\mathbf{k}} \sigma_{\mathbf{k},\tau,\sigma}^{AH} / \mathcal{E}_0, \) with \( \epsilon_{\tau,\sigma}^{\mathbf{k}} = \sigma \) for the spin Hall and \( \epsilon_{\tau,\sigma}^{\mathbf{k}} = \sigma \tau \) for the spin-valley Hall responses. In the VPF
phase, only one of the valleys is populated with holes
(for concreteness we assume that is the \( K \) point) implying
\( \sigma^{AH} \simeq \frac{e^2}{\hbar} \Omega_0 n_{\text{hole},\uparrow} \) and \( \sigma^{AH} = e \sigma^{AH} = -\sigma^{AH}. \)
We conclude that this phase has a transversal response
that is polarized in both the spin and valley degrees of
freedom.

Further responses can be qualitatively inferred from the
structure of the magnetic bands depicted in Fig. 1(e).
Besides the transversal component computed above, the
system will respond with a longitudinal component, in
virtue of its metallic state, that is just as well spin- and
valley-polarized. Moreover, optical transitions in this
phase will also be polarized, in virtue of the inequival-
ent valleys having differing optical gaps. Note that the
physics of the latter response differs from that of earlier
reports such as in Refs. [6–8], since the magnetic ground-
state spontaneously breaks TRS, whereas previously this
symmetry has been explicitly broken using circularly po-
larized photons.

Conclusions.—Based in the present mean field calcu-
lations, we have shown that TMDs are unstable to a spin-
valley polarized metal. For the phase to be observed it is
required that \( U > U_c \simeq 2.38 \text{ eV} \) and \( U' < 0.7 (U - U_c) \),
which are realistic conditions given the transition metal
atoms involved. Experimentally, this phase could be
detected by the measurements of the anomalous Hall
and/or longitudinal response, both of which are spin and
valley polarized. Interestingly, the spin and valley po-
larization is opposite for the two responses. Also, the
presence of a valley polarized, magnetic field tunable,
positively charged exciton (X trion) in the PL spec-
trum of hole doped TMDs would be a clear indication
by optical means of this phase [26]. Even though defects
make TMDs naturally electron doped [32], holes can be
induced by electric field effect and the observation of X+2
excitations is possible [33]. The present results show that
a valley polarized phase can be achieved in TMDs with-
out the need of an exchange coupling to a permanent
magnet [14, 34]. They also agree with a recent non self-
consistent approach [35] and with DFT calculations for
a monolayer of 2H-VSe2 [36].

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