Generalized many-body exciton g-factors: magnetic hybridization and non-monotonic Rydberg series in monolayer WSe_2

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Magneto-optics of low dimensional semiconductors, such as monolayer transition metal dichalcogenides, offers a vast playground for exploring complex quantum phenomena. However, current *ab initio* approaches fail to capture important experimental observations related to brightening of excitonic levels and their g-factor dependence. Here, we develop a robust and general first principles framework for many-body exciton g-factors by incorporating off-diagonal terms for the spin and orbital angular momenta of single-particle bands and many-body states for magnetic fields pointing in arbitrary spatial directions. We implement our framework using many-body perturbation theory via the GW-Bethe-Salpeter equation (BSE) and supplement our analysis with robust symmetry-based models, establishing a fruitful synergy between many-body GW-BSE and group theory. Focusing on the archetypal monolayer WSe_2, we accurately reproduce the known results of the low-energy excitons including the Zeeman splitting and the dark/grey exciton brightening. Furthermore, our theory naturally reveals fundamental physical mechanisms of magnetic-field hybridization of higher-energy excitons (s- and p-like) and resolves the long-standing puzzle of the experimentally measured non-monotonic Rydberg series (1s–4s) of exciton g-factors. Our framework offers a comprehensive approach to investigate, rationalize, and predict the non-trivial interplay between magnetic fields, angular momenta, and many-body exciton physics in van der Waals systems.

Introduction. Semiconducting transition metal dichalcogenides (TMDCs) are a family of two-dimensional, atomically thin layered van der Waals materials [1–5] that display unique electronic and optical properties, making them promising candidates for ultrathin optoelectronic, photovoltaic, and valleytronic applications [6–14]. Particularly, optical properties in TMDC systems are dominated by strongly bound excitons – quasiparticles resulting from the electron-hole Coulomb interaction [15–19]. For monolayers, the combination of broken inversion symmetry and strong spin-orbit interaction imprints selective coupling to circularly polarized light at the inequivalent K and −K points in the Brillouin zone[20, 21]. As a consequence, direct excitons display valley-dependent optical properties [22, 23]. Moreover, excitons carry intrinsic magnetic moments and effectively couple to external magnetic fields, revealing important effects such as many-body Zeeman shifts and magneto-optical selection rule modifications [24–47].

A fundamental framework for understanding magneto-exciton phenomena is provided by symmetry-based low-energy Hamiltonians [48, 49]. Such models explain why optically inactive (dark) excitons brighten under in-plane fields in TMDC monolayers due to spin-flip and valley-mixing terms [33, 50, 51]. However, a drawback of such approach is that these models do not offer quantitative insights into the coupling terms. Conversely, *ab initio* methods based on the many-body GW-Bethe-Salpeter equation (BSE) [52–55] explicitly evaluate the underlying Coulomb interactions between the involved quantum states (conduction and valence bands), providing parameter-free information absent in purely symmetry-based models. In particular, the GW-BSE approach captures not only the spatial structure of the single-particle (Bloch) states but also of the excitonic states, achieved by explicitly considering the electron-hole basis and evaluating their many-body interactions. Within this formalism, the microscopic information about the crystal geometry, atomic nature, and orbital details of the wavefunctions can be incorporated perturbativelly to calculate electronic and excitonic magnetic moments (g-factors) in TMDCs [38, 46, 56–58]. However, existing numerical evaluations of exciton g-factors remain incomplete by neglecting two critical aspects: (1) insights from group-theory analysis and (2) off-diagonal matrix elements (valley, orbital, and spin mixing) in the electronic and excitonic basis. These limitations severely hinder our ability to understand the fundamental aspects, such as spin-valley mixing, decoherence, and relaxation in realistic systems using reliable first principles techniques.

In this paper, we present a robust and general first-principles formalism to describe many-body exciton g-factors by incorporating off-diagonal elements of spin and orbital angular momenta, both in the single-particle and the exciton basis. These off-diagonal matrix elements are essential for capturing the correct spectral struc-

ture in degenerate many-body subspaces and therefore, exciton hybridization under arbitrarily oriented external magnetic fields. Our approach synergistically combines many-body perturbation theory within the GW-BSE framework with systematic symmetry-based analysis. We validate it by studying the exciton fine structure of monolayer WSe_2, a prototypical TMDC, reproducing the known results for the exciton Zeeman splitting, as well as the brightening dark/grey excitons in several magnetic field orientations [33, 50, 51]. Importantly, we demonstrate that off-diagonal angular momentum terms drive the brightening and hybridization of higher-energy excitons, including s–p mixing, and provide a natural resolution to the long-standing puzzle of the non-monotonic behavior in the excitonic Rydberg series g-factors (1s–4s) [36–39]. Our formalism opens new opportunities to investigate and predict the role of many-body effects on the non-trivial spin-valley physics of excitons in complex van der Waals systems.

General theory of exciton g-factors. The Hamiltonian describing two-particle excitations in the presence of an external magnetic field reads $\hat{H} = \hat{H}^{\mathrm{BSE}} + \hat{\mathbf{g}} \cdot \boldsymbol{\mathcal{B}}$ (further details in Sec. II of the Supplemental Material (SM) [59]). The term $\hat{H}^{\mathrm{BSE}}$ represents the BSE Hamiltonian, $\hat{\mathbf{g}} = (\hat{g}^x, \hat{g}^y, \hat{g}^z)$ corresponds to the g-factor, $\mathcal{B}_\epsilon := \mu_B B_\epsilon$, $B_{\epsilon=x,y,z}$ is the external magnetic field, and μ_B the Bohr magneton. In the exciton basis, the BSE Hamiltonian is diagonal, $\langle S|\hat{H}^{\mathrm{BSE}}|S'\rangle = \Omega_S \delta_{S,S'}$ with Ω_S being the exciton energies. The magnetic coupling within degenerate and between different exciton subspaces is driven by the external magnetic field and characterized by the Hamiltonian matrix elements $\langle S|\hat{H}|S'\rangle = \sum_\epsilon g^\epsilon_{SS'} \mathcal{B}_\epsilon$, which are excitonic-dressed "generalized" g-factor matrix elements

$$g^\epsilon_{SS'} = \sum_{vc\mathbf{k}} (\mathcal{A}^S_{vc\mathbf{k}})^* \left[\sum_{c'} \mathcal{A}^{S'}_{vc'\mathbf{k}} g^\epsilon_{cc'\mathbf{k}} - \sum_{v'} \mathcal{A}^{S'}_{v'c\mathbf{k}} g^\epsilon_{vv'\mathbf{k}} \right]. \tag{1}$$

Here, $g^\epsilon_{\alpha\alpha'\mathbf{k}} = \langle \alpha\mathbf{k}|\hat{L}^\epsilon + \hat{\Sigma}^\epsilon|\alpha'\mathbf{k}\rangle$ are the electronic g-factor matrix elements [60] accounting for the direct magnetic coupling, $\hat{L}^\epsilon$ ($\hat{\Sigma}^\epsilon$) the components of the orbital (spin) angular momentum operator in the Bloch basis, $|\alpha\mathbf{k}\rangle$, and $\mathcal{A}^S_{vc\mathbf{k}}$ the exciton amplitude obtained from the solution of the BSE. Eq. (1) extends on previous derivations [56, 57] by considering off-diagonal terms in the exciton g-factor, not only in the excitonic but also in the single-particle electron/hole manifold (band g-factors). For the latter, we need to consider off-diagonal matrix elements of single-particle operators in the Bloch basis. For instance, the orbital angular momentum in $\hat{\mathbf{z}}$ reads

$$L^z_{\alpha\alpha'\mathbf{k}} = \frac{1}{\mathrm{i} m_0} \left[\sum_{\beta\neq\alpha}{}' \frac{p^x_{\alpha\beta\mathbf{k}} p^y_{\beta\alpha'\mathbf{k}} - p^y_{\alpha\beta\mathbf{k}} p^x_{\beta\alpha'\mathbf{k}}}{\epsilon_{\alpha\mathbf{k}} - \epsilon_{\beta\mathbf{k}}} - \sum_{\beta\neq\alpha'}{}' \frac{p^y_{\alpha\beta\mathbf{k}} p^x_{\beta\alpha'\mathbf{k}} - p^x_{\alpha\beta\mathbf{k}} p^y_{\beta\alpha'\mathbf{k}}}{\epsilon_{\alpha'\mathbf{k}} - \epsilon_{\beta\mathbf{k}}} \right] \tag{2}$$

with $p^\epsilon_{\alpha\beta\mathbf{k}} = \langle \alpha\mathbf{k}|\hat{p}^\epsilon|\beta\mathbf{k}\rangle$ [61], i being the imaginary unit, and m_0 the bare electron mass. The $'$ in the first (second) summation indicates that the α' (α) state must be excluded if α and α' are in the same degenerate subset.

Low-energy excitons. We demonstrate our theoretical approach for the archetypal monolayer WSe_2, extensively studied via magneto-optics [28, 33, 36–40, 50, 51, 62, 63]. The top view of the TMDC crystals (D_{3h} symmetry group) and the first Brillouin zone are depicted in Figs. 1(a,b), respectively. We focus on the subspace of low-energy excitons visible in typical magneto-photoluminescence experiments. These excitons arise from the top valence band, VB_+, and the lowest conduction bands, $CB_\pm$, in the vicinity of the K-valleys. In Fig. 1(c) we show VB_+ and $CB_\pm$, highlighting their irreducible representations (*irreps*) and the direction of

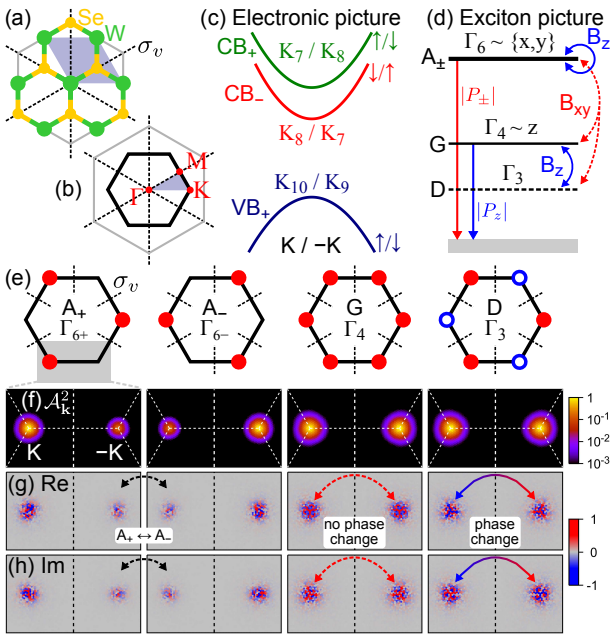

Figure 1. (a) Top view of the monolayer WSe_2. The colored parallelogram indicates the primitive unit cell. (b) First Brillouin zone. The colored triangle indicates the irreducible wedge. The dashed lines in panels (a,b) indicate the mirror planes σ_v. (c) Low-energy bands at K/−K valleys, including the irreps and spin orientation. (d) Low-energy exciton states at the Γ-point, identified by their labeling and irreps (see main text). Vertical arrows indicate the allowed optical transitions. Curved arrows indicate couplings via the magnetic field (solid for $\mathbf{B} \parallel z$ and dashed for $\mathbf{B} \parallel x, y$). (e) Schematic representation of the exciton wavefunctions. Closed (open) circles indicate positive (negative) amplitudes. For irrep Γ_6, the subindex $+(-)$ refers to the exciton wavefunction mainly localized in the $+(-)K$-valley. (f) Absolute, (g) real, and (h) imaginary values of the calculated GW-BSE exciton wavefunctions. The arrows in panels (g,h) emphasize the effect of σ_v, i. e., $\Gamma_{6+}(A_+) \leftrightarrow \Gamma_{6-}(A_-)$, no phase change for Γ_4 (G), and phase change for Γ_3 (D).

the spin expectation value in the out-of-plane direction (Σ^z) at ±K valleys (C_{3h} point group with complex double group irreps). The interband optical selection rules at ±K can be readily evaluated within group theory (see Sec. III of the SM [59]), revealing that the transitions $\mathrm{CB}_- \to \mathrm{VB}_+ \sim K_4$ are optically active with z polarization at ±K points, while $\mathrm{CB}_+ \to \mathrm{VB}_+ \sim K_3(K_2)$ are optically active with s_+ (s_-) polarization at K (−K) point, in agreement with previous results [21, 64, 65]. Here, we adopt the group theory nomenclature of Ref. 66.

To evaluate the irreps of the direct (1s-like) excitons, we map the irreps from the K-valleys to the Γ-point. Using the compatibility relations ($C_{3h} \to D_{3h}$), we find $K_2 \oplus K_3 \to \Gamma_6$ and $K_4 \to \Gamma_3/\Gamma_4$, with $\Gamma_6 \sim x, y$ and $\Gamma_4 \sim z$. The two possibilities of mapping K_4 to Γ_3 or Γ_4 arise from their distinct behavior under the mirror plane σ_v operation, identified in Figs. 1(a,b), as a consequence of the intervalley exchange coupling [33, 64, 67]. We employ the typical nomenclature for these excitons [33, 50, 51]: bright (A $\sim \Gamma_6$), grey (G $\sim \Gamma_4$), and dark (D $\sim \Gamma_3$). From the symmetry perspective, A excitons are two-fold degenerate while the D exciton has zero oscillator strength. The resulting low-energy subspace, optical selection rules, and coupling to an external **B**-field are summarized in Fig. 1(d), with the schematic representation of the exciton wavefunctions given in Fig. 1(e).

Our GW-BSE calculations provide the exciton energies and oscillator strengths (Table II in the SM [59]), supplying a clear identification of these 4 exciton states. Notably, the symmetry analysis also allows us to identify the numerical precision of the GW-BSE calculations. The energy values (oscillator strengths) fully satisfy the symmetry constraints up to 0.1 meV ($10^{-3}\ e^2a_0^2$). The exciton energy splitting between G and A excitons is ∼52.4 meV while the D-G exciton splitting is ∼2.4 meV, in excellent agreement with experimental observations in hBN encapsulated samples [33, 50, 51, 65]. One relevant aspect of the numerical effects in the GW-BSE calculations is the mixing of the A exciton states, *i.e.*, the two states do not emit light with completely circular polarization. This is a common effect in first-principles calculations whenever the irreps are (nearly) numerically degenerate [68, 69]. To verify the features from Fig. 1(e) at the GW-BSE level, we display in Figs. 1(f-h) the density ($\rho^S_{\mathbf{k}} = \sum_{vc} |\mathcal{A}^S_{vc\mathbf{k}}|^2$), real ($\mathrm{Re}\{\mathcal{A}^S_{\mathbf{k}}\} = \sum_{vc} \mathrm{Re}\{\mathcal{A}^S_{vc\mathbf{k}}\}$), and imaginary ($\mathrm{Im}\{\mathcal{A}^S_{\mathbf{k}}\} = \sum_{vc} \mathrm{Im}\{\mathcal{A}^S_{vc\mathbf{k}}\}$) values of the computed *ab initio* exciton wavefunctions. Because of the numerical degeneracy in the A exciton subspace, the wavefunctions are not fully localized in ±K but are still connected by the mirror plane σ_v. For the G and D excitons, the sign change is visible in the real and imaginary parts, evidenced by the dashed (G) and solid (D) arrows.

Knowing the excitons' symmetry allows us to incorporate the effect of external magnetic fields, which transform as pseudovector objects ($B_{x,y} \sim \Gamma_5$ and $B_z \sim \Gamma_2$). The resulting symmetry-allowed couplings in the low-energy excitons are shown in Fig. 1(d), revealing that out-of-plane fields ($\mathbf{B} \parallel z$) yield Zeeman splitting physics for the A exciton subset and mixing of D and G excitons, while in-plane fields ($\mathbf{B} \parallel x, y$) introduce exciton mixing between A and D/G states. We emphasize here the relevance of our general formalism: mixing effects can only be captured by off-diagonal matrix elements, which are also relevant for degenerate subsets such as the A exciton. The details of the symmetry analysis and connection to the microscopic contributions of electron g-factors in the exciton basis are given in Sec. III of the SM [59]. We incorporate the magnetic field within GW-BSE by numerically evaluating Eq. (1), including the **k**-space extension of the exciton wavefunctions coupled via the full matrices Σ and L.

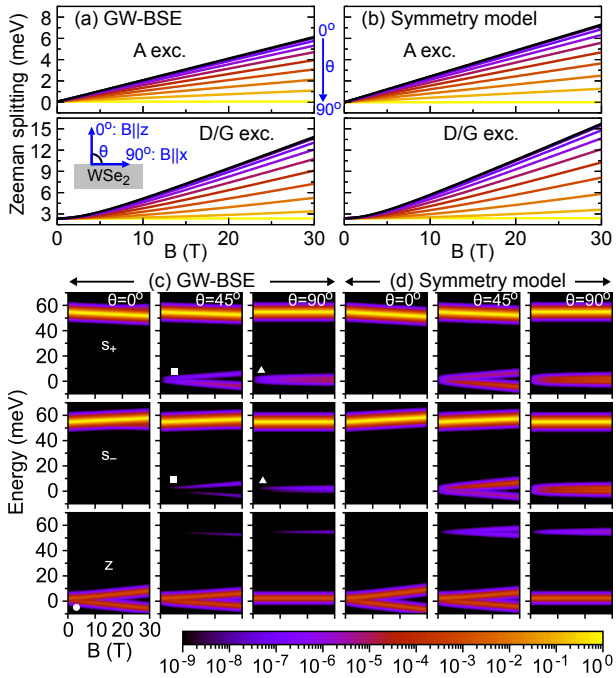

Figure 2. Zeeman splitting of the low-energy excitons under applied magnetic field at different angles, θ, for (a) the GW-BSE and (b) the symmetry-adapted model. The top (bottom) panels correspond to the A (D/G) excitons. Calculated absorption via the (c) GW-BSE and (d) symmetry-adapted model under applied magnetic field oriented at different angles ($\theta = 0°, 45°, 90°$) for s_+ (top row), s_- (middle row), and z (bottom row) polarizations. The spectra are normalized to the maximum value of the s_+ emission. For each transition, a broadening was applied using a sech function with 1 meV full-width at half-maximum. The closed circle, squares, and triangles highlight important brightening signatures.

To validate our approach, we show in Figs. 2(a-b) the Zeeman splitting of A and D/G excitons for different orientations of the magnetic field. In the symmetry model we assume δ-like exciton wavefunctions fully localized at

±K points, as in previous works [51]. Besides the difference in the Zeeman splitting (∼1.2 meV at 30 T, due to the **k**-space exciton wavefunction spread [46, 56, 57]), all the dependencies match accordingly, revealing that the exciton couplings are properly captured by our general *ab initio* formalism.

The magneto-optical signature of exciton mixing is observed in the intensity of the photoluminescence spectra [33, 50, 51]. In Figs. 2(c-d) we present the calculated absorption spectra in logarithmic scale [70] for different magnetic field orientations ($\theta = 0°, 45°, 90°$). Our calculations reproduce all the relevant mixing-induced brightening mechanisms observed experimentally: (1) brightening of the D exciton due to the D-G mixing for out-of-plane fields [33] (closed circle); (2) brightening of both G and D excitons in tilted magnetic fields [50] (squares); and (3) brightening of both D and G excitons for in-plane fields [51] (triangles). The mixing-induced exciton brightening under magnetic fields is a direct consequence of the off-diagonal elements of the spin and orbital angular momenta matrices, correctly incorporated in the general expression, Eq. (1), of the exciton g-factor.

Magnetic-hybridization of high-energy excitons. While low-energy excitons are easily described by effective models, high-energy excitons (often called *excited* excitons) pose a greater challenge due to the increasingly denser excitonic manifold of available states with enhanced intervalley exchange and spin-orbital mixing. To emphasize the significance of the exciton hybridization at higher energies, we present in Fig. 3(a-b) the absolute values of the out-of-plane and in-plane g-factors for the lowest 20 excitons(see Sec. V of the SM [59] for a larger exciton subset). Notably, both g-factor components display significant presence of off-diagonal elements responsible for hybridizing states that belong to different exciton subspaces, completely absent in previous studies [56, 57]. Moreover, g-factors of p-like excitons (indices 5-12 and 17-20) have similar magnitude of their s-like counterparts (indices 1-4 and 12-16). In Sec. V of the SM [59] we present the exciton wavefunctions.

In Fig. 3(c-e) we display the calculated absorption for $s_\pm$ and z polarization for the exciton subset shown in Fig. 3(a-b). For $s_\pm$ polarizations, external magnetic fields lead to the brightening of several optically inactive excitonic states. In particular, we reveal a clear signature of the mixing of s-p excitons, recently observed by external in-plane electric fields in monolayer WSe_2 [71]. For z-polarized light, we recover the brightening of the excited D/G states, see Fig. 2(c). Similar to the recently proposed s–p mixing of excitons in van der Waals heterostructures [72], this brightening cannot be captured by purely (Wannier or symmetry-based) effective models, underscoring the importance of including the full complexity of the excitonic spectrum using the generalized GW-BSE treatment.

Rydberg series of g-factors. To showcase the robust capabilities of our approach, we address the long-standing puzzle and conflicting experimental reports of the Rydberg series of the A exciton g-factors for the so-called 1s–4s states. Fig. 4(a) compiles the available experimental g-factors in hBN-encapsulated monolayer WSe_2 from Refs. [36–39]. These experiments reveal an overall decreasing trend together with clear non-monotonic signatures, varying slightly due to environmental and sample-dependent factors [73–75].

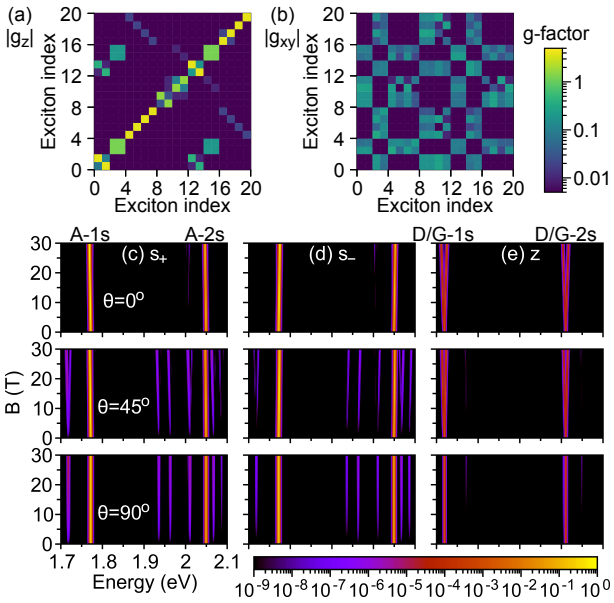

Figure 3. Absolute value of the (a) out-of-plane g-factor matrix, g_z, and (b) in-plane g-factor matrix, $|g_{xy}| = \sqrt{g_x^2 + g_y^2}$, via Eq. (1), as a function of the exciton index, demonstrating the significance of the off-diagonal terms. Calculated absorption for high-energy excitons as a function of the magnetic field oriented at different angles ($\theta = 0°, 45°, 90°$) using the GW-BSE approach for (c) s_+, (e) s_-, and (e) z polarizations. The values are normalized to the maximum value of the s_+ emission. We apply the same broadening as in Fig. 2. Several exciton peaks emerge around 1.95 eV, visible for $\theta = 45°, 90°$. We consider the nonzero oscillator strengths only for s-like exciton states.

In Fig. 4(b), we present our calculated g-factors via the full *ab initio* GW-BSE approach, revealing that non-monotonic features naturally emerge from our formalism (see Sec. V of the SM [59] the wavefunctions of 1s–4s states). Notably, the g-factors for D/G Rydberg excitons also exhibit non-monotonic dependencies, see inset of Fig. 4(b). We also evaluate the g-factors using an effective (parabolic) two-band model incorporating the dielectric screening of vacuum and hBN-encapsulation (see Sec. I of the SM [59]). The effective model systematically yields a monotonic behavior and fails to reproduce the oscillations obtained in the GW-BSE g-factor calculations via Eq. (1). These non-monotonic features cannot be explained by simplified models but naturally emerge from

our generalized GW-BSE formalism, which incorporates orbital and spin mixing induced by external magnetic fields. Our results firmly indicate that the interplay between the excitonic fine structure and magnetic response is highly nontrivial and strongly dependent on the exciton state, emphasizing the need for first-principles-based approaches when interpreting high-resolution magneto-optical measurements.

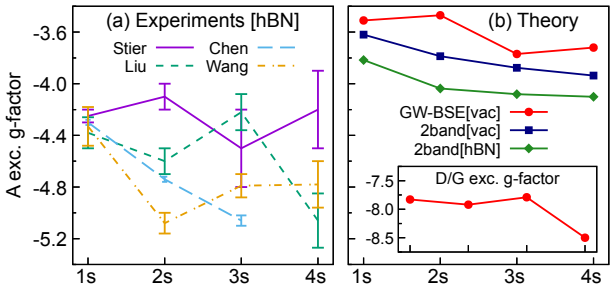

Figure 4. (a) Experimental g-factors of the Rydberg series (1s–4s) of the A exciton by Stier *et al.* [36], Liu *et al.* [37], Chen *et al.* [38], and Wang *et al.* [39]. (a) Calculated g-factors via the GW-BSE approach (circles), using an effective two-band model (squares), and via the two-band model considering hBN encapsulation (diamonds). Notably, the observed non-monotonic trends can only be accurately reproduced using our *ab initio* GW-BSE generalized g-factor theory. Inset: g-factors of D/G Rydberg excitons, also exhibiting non-monotonic features.

Conclusions. In this paper, we developed a robust and general framework based on *ab initio* many-body GW-BSE formalism that incorporates the interplay of the spin and orbital angular momenta via the exciton g-factors. This approach takes into account the hybridization of single-particle bands and many-body states through off-diagonal matrix elements of spin and orbital angular momenta. Moreover, we establish a previously-unexplored synergy between GW-BSE and group theory models of excitonic subspaces. We validate our approach for the archetypal TMDC monolayer WSe_2, capturing and rationalizing the observed results of the exciton Zeeman splitting as well as brightening of the optically dark/grey excitons by in-plane/tilted magnetic fields. We also explore the brightening of high-energy excitons, a challenging task for pure symmetry-based models, emphasizing that many-body off-diagonal components of the g-factor are crucial to capture the magnetic mixing of exciton states. These results imply that interpreting high-energy features in magneto-optics requires caution, as nominally distinct excitonic subspaces can strongly hybridize. Furthermore, the robustness of our approach allows us to unveil the non-monotonic behavior of the Rydberg series of exciton g-factors, a long-standing puzzle observed by several experimental groups [36–39]. Our novel approach provides a robust foundation to study many-body effects of multidirectional magneto-excitons in other complex two-dimensional materials and van der Waals heterostructures. It is particularly relevant to study nontrivial spin-valley dynamics [76] and unusual topological and chiral excitons [77, 78] as well as many-body effects in the emergent field of orbitronics [79].

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