Exciton g-factors of van der Waals heterostructures from first principles calculations

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External fields are a powerful tool to probe optical excitations in materials. The linear energy shift of an excitation in a magnetic field is quantified by its effective g-factor. Here we show how exciton g-factors and their sign can be determined by converged first principles calculations. We apply the method to monolayer (1L) excitons in semiconducting transition metal dichalcogenides (TMDs) and to interlayer excitons in $MoSe_2/WSe_2$ heterobilayers and obtain excellent agreement with recent experimental data. The precision of our method allows to assign measured g-factors of optical peaks to specific transitions in the band structure and also to specific regions of the samples. This revealed the nature of various, previously measured interlayer exciton peaks. We further show that, due to specific optical selection rules, g-factors in van der Waals heterostructures are strongly spin and stacking-dependent. The presented approach can potentially be applied to a wide variety of semiconductors [1].

The method was successfully applied to bigger excitonic complexes: trions, their phonon replicas and biexcitons in 1L WS_2. It also overcomes the currently used simple models, yielding g-factors of individual electrons and holes in perfect agreement with their experimental values [2].

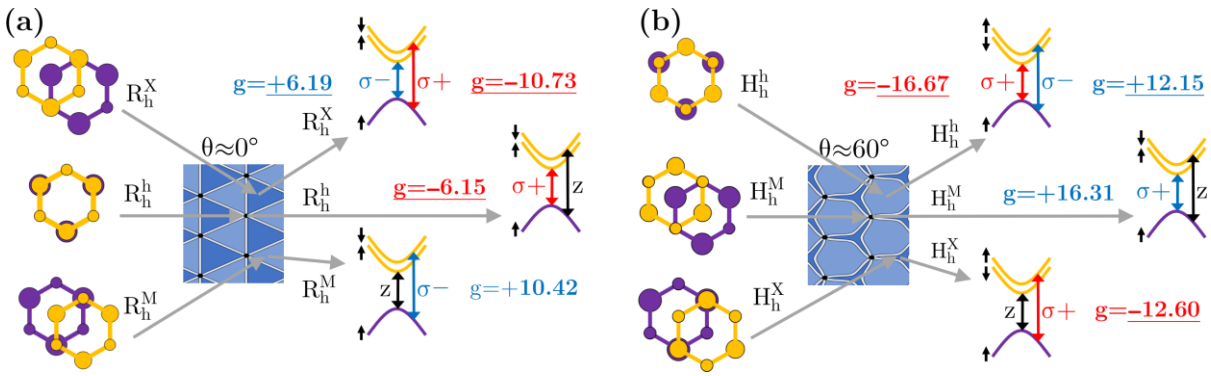

Figure 1: Exciton g-factors for high-symmetry stacking configurations in (a) 0° and (b) 60° $MoSe_2/WSe_2$ heterobilayer.

[1] T. Woźniak, P. E. Faria Junior, G. Seifert, A. Chaves, J. Kunstmann, *Phys. Rev. B* **101**, 235408 (2020).
[2] M. Zinkiewicz, T. Woźniak, T. Kazimierczuk, P. Kapuściński, K. Oreszczuk, M. Grzeszczyk, M. Bartoš, K. Nogajewski, K. Watanabe, T. Taniguchi, C. Faugeras, P. Kossacki, M. Potemski, A. Babiński, M. R. Molas, *Nano Lett.* **21**, 6, 2519–2525 (2021).