Magnons in Vanadium dichalcogenides: spin wave theory and numerical simulations

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Two-dimensional Van der Waals materials are currently of great interest. This is due to unique magnetic and electronic properties of these materials. We have analyzed theoretically and numerically the spectrum of spin waves (magnons) in two-dimensional monolayer and bilayer systems of VX2 (X=S, Se, Te) transition-metal dichalcogenides (TMDs) [1]. The vanadium atoms within individual atomic layers are coupled ferromagnetically, while the exchange coupling between V atoms located in different planes is either ferromagnetic or antiferromagnetic, depending on the stacking type of individual layers. We have analyzed in detail the spin wave spectra as a function of magnetic anisotropy, the Zeeman field, and the proximity effect in the context of Dzyaloshinskii-Moriya interaction (DMI) and in the context of magnon-plasmon hybridization mediated by DMI.

The spin-wave dispersion relations have been derived analytically within the spin-wave theory (SWT), in terms of the Holstein-Primakoff transformation combined with the Bogolubov diagonalization scheme. For numerical discussion, the intra- and interlayer exchange parameters, as well as the magneto-crystalline anisotropy, have been evaluated within the method based on the density functional theory (DFT). The corresponding magnon spectra have been also simulated numerically. From the DFT calculations we have also determined the Curie temperatures of the VS2, VSe2 and VTe2 bilayer systems, which are close to or well above the room temperature, in agreement with the corresponding literature.

We have also verified the spin-wave theory results by means of the atomistic spin dynamics (ASD) numerical simulation method, which can be applied in a first-principles mode, where all interatomic exchange parameters are calculated self-consistently, or it can be applied with fixed parameters estimated from experiments or calculated (e.g. using DFT) for a fixed ground state spin-configuration. We have shown that in the case of vanishing DMI, the ASD technique reproduces with good accuracy the magnon spectra evaluated within the SWT. Second, in case of the system with broken inversion symmetry (e.g. due to strain and/or the proximity effect), the ASD method offers a deeper understanding of the DMI mechanism responsible for the momentum-dependent asymmetry of the spin-wave dispersion. Finally, the ASD allowed for analyzing the temperature and damping effects on the magnon spectra properties.

In the case of antiferromagnetic TMD bilayers, the system undergoes a field-induced transition to the spin-flop phase, which evolves into the saturated ferromagnetic phase for a sufficiently strong magnetic field. The existence of different phases depends on the material parameters, especially on the interlayer exchange and anisotropy parameters. We have analyzed the spin wave spectra in all these phases and showed how these spectra change at the phase transitions and how they evolve with increasing magnetic field. We have taken into account both the in-plane and out-of-plane magnetic anisotropies.

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References

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