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Resonance Raman intensities including excitonic effects from first-principles: application to 2D materials

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Resonance Raman spectroscopy of 2D semiconductors such as monolayer MoS_2 and ReS_2 contains rich information such as sample thickness and electron-phonon couplings [1]. Although the theory for calculating Resonance Raman intensities has been well developed for graphene, strong excitonic effects in 2D semiconductors call for further scrutiny on the computation of Raman intensities from first-principles. Compared to existing methods of calculating Resonance Raman intensities using finite differences where the Bethe-Salpeter equation (BSE) was solved twice for each degree of freedom, we develop a computational framework based on a perturbational approach in which the BSE is only solved once statically [2]. Comparisons with experimental results are discussed, as well as the extension to model second-order Raman scattering processes [3].

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[2] In preparation.

[3] B. R. Carvalho, Y. Wang, S. Mignuzzi, D. Roy, M. Terrones, C. Fantini, V. H. Crespi, L. M. Malard, and M. A. Pimenta, Nat. Commun. 8, 14670 (2017).