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Modeling excitonic effects in the linear and non-linear optical response of transition-metal dichalcogenides

Abstract

We study the excitonic spectrum of a MoS2 monolayer taking into account the anomalous screening in two dimensions and the presence of a substrate by the effective Keldysh interaction. The Bethe-Salpeter equation is solved based on a multi-band tight-binding description of the single particle spectrum and we obtain the system's optical response for the two best tight-binding (TB) models available in the recent literature (Wu et al. [1] and Ridolfi et al.[2]).

We shall analyze the impact of different qualitative features of the underlying TB description in capturing accurately the experimental optical absorption, namely, the contributions of higher energy bands, and the validity of reduced TB models with and without spin-flipping terms in the spin-orbit contribution to the Hamiltonian. Our calculations are extended to the description of the quadratic response where the excitons contribute crucially to the highly resonant nature of the second harmonic spectrum.

References

[1] F. Wu, F. Qu, A.H. MacDonald. Phys. Rev. B (2015), 91, 075310
[2] E. Ridolfi, D. Le, T.S. Rahman, E.R. Mucciolo, C.H. Lewenkopf. Phys.: Condens. Matter (2015) 27, 365501