Exploring the Role of Indirect Excitons in Spectroscopic Properties of Materials: Insights from MBPT and Yambo Code

Many-Body Perturbation Theory (MBPT) is a powerful approach for predicting the spectroscopic properties of materials such as quasiparticle energies and optical spectra. In particular, the Bethe-Salpeter equation has demonstrated exceptional results in describing excitonic features in the optical absorption of semiconductors. In this talk, we present a recent implementation in the Yambo code [1,2] for the description of finite-momentum indirect excitons. These excited states are characterized by electrons and holes occupying different regions of the Brillouin zone and can be detected via electron energy loss experiments (EELS). We present recent results obtained by our group, demonstrating the essential role of electron-hole interaction in obtaining EELS spectra that are in qualitative and quantitative agreement with high-resolution experiments in free-standing graphene [3] . Additionally, we discuss the role of indirect excitons in the exciton instability and the realization of the excitonic insulator phase in bulk MoS_2 under high pressure and below a critical temperature [4]. Finally, we demonstrate how considering radiative emission from "indirect" excitons via coupling to finite-momentum phonons enables the description of phonon-assisted luminescence spectra and the discrimination between different polytypes of bulk boron nitride.

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[4] S. S. Ataei, D. Varsano, E. Molinari and M. Rontani Proc. Natl. Acad. Sci. 118 , 13 (2021)