Excitons with the yambo code: from the Bethe-Salpeter equation to nonequilibrium excitons and exciton-phonon coupling

D. Sangalli[1]

[1] *Istituto di Struttura della Materia-CNR (ISM-CNR), Division of Ultrafast Processes in Materials (FLASHit), Area della Ricerca di Roma 1, Monterotondo Scalo, Italy*

I discuss the modelling of the physics of the exciton with the yambo code [1].

Starting from the standard linear response approach to the Bethe-Salpeter Equation (BSE), I move to the real-time version. The latter describes coherent excitons generation due to the action of laser pulses [2, 3]. The real-time BSE is obtained via the propagation of the density matrix projected in the Kohn-Sham basis set, within the time–dependent Hartree plus Screened EXchange (TD-HSEX) approaximation [4].

Using LiF as a prototype material, I show that the scheme is able to model the exciton signature both in time-resolved angle-resolved photoemission spectroscopy and transient absorption experiments [2, 5]. Moreover, I show how similar results can be obtained assuming a non-coherent excitonic state, constructed taking advantage of the BSE eigenvectors.

In the last part I focus on the concept of exciton-phonon lifetimes [6], and on the idea of interfacing yambo and abinit to compute the exciton-phonon matrix elements.

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