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Phonons and vibrons as markers of the composite nature of excitons in solids and nanostructures

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The Ab-Initio description of the excitonic states, obtained by solving the Bethe-Salpeter (BS) equation of Many-Body Perturbation Theory, constitutes a well-established approach to interpret the photoexcited properties of bulk materials, surfaces, nanostructures and organic/bio-molecules[1].
Although absorption and photoluminescence experiments are usually performed at room temperature, in the standard approach the BS equation is solved assuming the atoms frozen in their crystallographic positions, thus neglecting the effect of lattice vibrations. As a consequence excitons turn out to be insensitive to the temperature T and to have an infinite lifetime, in stark contrast with the experimental results[2].

In this talk I show how to extend, in a fully Ab-Initio manner, the Bethe-Salpeter equation in order to take in account the coupling with phonons and vibrons[3]. The picture of the excitons obtained within a frozen-atom approximation turns out to be deeply modified, both at zero and finite temperature. Excitons acquire a non-radiative lifetime, otherwise infinite in the frozen-atom approximation.
I will show that the proposed polaronic BS equation correctly describes, in the T->0 limit, the effect of zero-point vibrations, and it induces bright-to-dark (and viceversa) transitions in layered materials.

The results showed in this talk will point out that phonons act on the excitons by, mainly, disentangling the internal, composite, structure of the excitonic packet. This will rule out the simplified interpretation of the exciton-phonon scattering in terms of bosonic only degrees of freedom.
I will conclude the talk by proposing a method to rewrite the exciton-phonon scattering process as as simplified Dyson equation, without requiring the explicit introduction of bosonized excitons.

[1] G.Onida, L.Reining and A.Rubio, Rev. Mod. Phys. 74, 601 (2002).
[2] For a review, see M. Cardona, Solid State Comm. 133,3 (2005).
[3] A. Marini, Phys. Rev. Lett. 101, 106405 (2008).