Seminar Announcement

Thursday, January 30, 2025
1:00 pm

Room CH 63214, TUM Chemistry Building (6 floor, yellow staircase)

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From semi–classical swings to tad–poles: the Electron–Phonon problem as the *devil in the details* of Many–Body Theory

Electrons and phonons are basic concepts, considered as the most elemental and well defined example of fermions and bosons. So it may appear that their formal properties are clear and well established. In reality, despite books and reviews the theory of electron-phonon interaction(EPI) is still very much debated. The reason is mostly historical. Indeed the state-of-the art theoretical and numerical approach to the EPI has been built on top of two popular methods: model Hamiltonians and Density Functional Perturbation Theory (DFPT). These popular approaches have instilled two basic assumptions that are widely used in the literature and even coded in public Ab–Initio codes.
The first assumption is that the elemental EPI Hamiltonian is well approximated by

$$\hat{H}_{EPI} \sim \sum_{ij\nu} g^{\nu}_{ij}\big|_{SCR}\, \hat{c}^{\dagger}_{i}\hat{c}_{j}\left(\hat{b}_{\nu}+\hat{b}^{\dagger}_{\nu}\right)$$

with $g^{\nu}_{ij}|_{SCR}$ the adiabatically screened EPI interaction as obtained from DFPT.

The second assumption is clearly written in a recent Review of Modern Physics of F. Giustino[1] where he writes that "*the MBPT phonon self-energy is in agreement with the expression derived starting from time-dependent density-functional perturbation theory*".

In this talk I will disassemble $\hat{H}_{EPI}$ to demonstrate its stringent limitations. I will also introduce a time-dependent formulation of DFPT showing how it can be *exactly* rewritten as the problem of a classical pendulum immersed in a quantistic liquid (semi-classical swing)[2]. I will discuss the countless implications of such a problem linked the very basic foundations of MBPT.

I will then move to present a formal an accurate derivation[3] of the dynamical screening of the EPI. I will, in particular, demonstrate that it is possible to derive an effective vertex correction function that can be easily defined using simple ingredients and used to amend calculations based on the statically screened approximation.

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1 Giustino, F. *Electron-phonon interactions from first principles*. Rev. Mod. Phys. **89** (Feb 2017), 015003.

2 Marini, A. *Nonadiabatic effects lead to the breakdown of the semiclassical phonon picture*. Phys. Rev. B **110** (2024).

3 Marini, A. *Dynamical electron-phonon vertex correction, arXiv:2501.01866 (2025)*