ID de Contribution: **37** Type: **Poster**

The connector theory: New approximations for the exchange-correlation potential

In material science we often use model systems to describe real materials. In this talk we are interested in the question of how to import, in principle exactly, a quantity of interest from a model into a real system. The prescription how to do that is what we call "connector theory" [1]. An enormous advantage of this strategy is that model results can be obtained once forever and tabulated. After introducing the theory we will focus on approximating the exchange-correlation (xc) potential of density-functional theory (DFT) [2] including the time-dependent (TD) case, and we use the homogeneous electron gas (HEG) as the model system. Then we discuss the features of the connector theory and explain why it constitutes a better scheme for approximations than an approach that would directly approximate the xc potential. By making use of advanced calculations for the TDDFT xc kernel of the HEG [3], we derive xc potentials that have a non-local density dependence and are non-adiabatic. We consider some examples to discuss qualitative and quantitative differences between the results of our approach and those of the local-density approximation (LDA) and we show why our theory goes beyond the LDA. Finally a generalisation for the efficient calculation of observables will also be discussed.

[1] M. Vanzini, A. Aouina, M. Panholzer, M. Gatti, and L. Reining, arXiv:1903.07930

[2] W. Kohn, Rev. Mod. Phys. 71, 1253 (1999).

[3] M. Panholzer, M. Gatti, and L. Reining, Phys. Rev. Lett. 120, 166402 (2018)

Language

English

Auteur principal: AOUINA, Ayoub (LSI)

Co-auteurs: Dr GATTI, Matteo (LSI); Prof. REINING, Lucia (LSI)

Orateur: AOUINA, Ayoub (LSI)

Classification de Session: Lunch & Posters session

Classification de thématique: Physics