

VISTA Seminar

Seminar 46

November 30, 2022

**10:00 am – 11:30 am EST / 3:00 – 4:30 pm GMT London / 4:00 pm –
5:30 pm CET Paris / 11 pm CST Beijing**

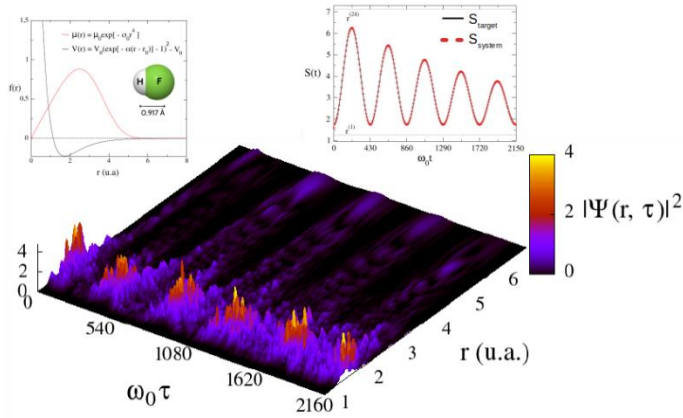
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Piece-wise time-independent method for tracking quantum control and its relevant features for applications

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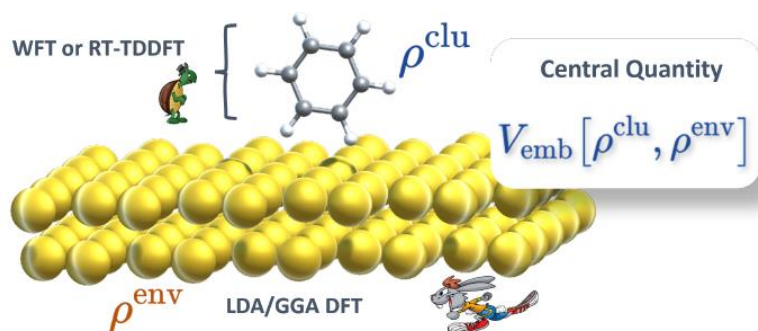
There are different powerful approaches to implement quantum control (QC), some being more appropriate at distinct applications. For the so-called tracking QC, a particularly simple scheme is the piece-wise time-independent QC method (PTIM). Its relative generality allows the PTIM to be used both for closed and open quantum systems. For instance, due to its construction straightforwardness, the PTIM has been recently employed in the context of quantum information, e.g., for driving coupled qubits, qutrits, etc, under the influence of Markovian and non-Markovian noise. Moreover, the PTIM is very suitable for the assessment and selection of the multiple possible solutions typically arising in tracking QC problems. This is a feature particularly useful if one wishes to control a system by imposing special constraints on the sought evolution. For example, one shall have a specified tracking trajectory for a physical observable, but further demand a minimal dispersion for this same observable. In the present talk, I will highlight the main aspects of the PTIM and also discuss some relevant usages.

Density Functional Theory Based Embedding for Molecular and Periodic Systems Using Gaussian Basis Functions

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The high computational demand for modeling hybrid systems, such as solvated molecules or molecules adsorbed on a surface, has led to the development of many embedding methods, especially since the region of interest is usually smaller. An implementation of density functional theory-based embedding coupled with wavefunction theory (WFT) methods and real time-time dependent density functional theory (RT-TDDFT) is presented. Its key feature is that it allows treating both periodic and aperiodic systems on an equal footing using an all-electron direct-space representation, by employing Gaussian basis functions. The three flavors of embedding: molecule-in-molecule, molecule-in-periodic, and periodic-in-periodic are implemented using embedding potentials based on non-additive kinetic energy density functionals (approximate) and level-shift projection operator (exact). The applicability of (i) WFT-in-DFT embedding, in predicting the ground and excited state properties of the embedded clusters, and (ii) RT-TDDFT-in-DFT, in predicting the absorption spectra, is explored for various test systems.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 46

Time: Nov 30, 2022 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting

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149.137.40.110 (Singapore)

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