Variational Gaussian wavepacket methods for quantum propagation

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These lectures address time-dependent Gaussian wavepacket methods, which have a long history in the theoretical chemistry community. We will discuss these methods in the context of the time-dependent variational principle and show how efficient wavefunction propagation in many dimensions can be carried out using Gaussian-based variants of the Multi-Configuration Time-Dependent Hartree (MCTDH) approach. Various applications illustrate the flexibility of these methods in conjunction with model Hamiltonians, precomputed potential energy surfaces, and on-the-fly schemes.

The lectures will be of interest for PhD students of the École Doctorale SIE of the Université Paris-Est. They are also suitable for the Label de Chimie Théorique for Master and PhD students from the area around Paris, or for PhD students from the GDR Dynamique Quantique who are interested in the connection between mathematical and computational aspects of quantum dynamics.

These lectures are the first part of a course whose second part is planned for 2021.

Format :

- ◊ Virtual conference
- ◊ Zoom videoconference link will be sent to registered participants

Timing :

- ◊ Wednesday, September 2nd, 16:00 - 18:00
- ◊ Thursday, September 3rd, 16:00 - 18:00
- ◊ Friday, September 4th, 16:00 - 18:00

Program :

(1) Time-dependent variational principle
(2) Introduction to numerical methods in quantum dynamics
(3) Semiclassical and Gaussian wave-packet methods
(4) Gaussian-based Multi-Configuration Time-Dependent Hartree: G-MCTDH and vMCG

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