Numerical analysis of high-dimensional quantum dynamics

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The lecture aims at presenting mathematical analysis of successful numerical methods for high-dimensional quantum dynamics.

The lecture will address PhD students of the *École Doctorale MSTIC* of the University Paris-Est or for PhD students from the GDR Dynamique Quantique. It could also suit for students from the *École Doctorale SIE* of the University Paris-Est that would be interested in numerical analysis.

Where? Lama, Copernic's building, Room 4B 125, 4th floor, cité Descartes.
Access map: http://www.enpc.fr/en/getting-school

When?

- ◊ Wednesday, March 4th, 14:00 - 16:00
- ◊ Thursday, March 5th, 13:30 - 17:45 with a 15 mn break
- ◊ Friday, March 6th, 10:00 - 12:00 & 14:00 - 16:00
- ◊ Thursday, March 12th, 13:30 - 17:45 with a 15 mn break
- ◊ Friday, March 13th, 10:00 - 12:00 & 14:00 - 16:00

Program

1. Time-dependent Born-Oppenheimer approximation: time-dependent Galerkin approximation, semiclassical approximation, role of potential energy surface crossings.

2. Numerical methods for low dimensions: time-splitting and pseudospectral methods in the semiclassical regime, Hermite-Galerkin methods, Lanczos method.

3. Gaussian variational wave packets: Dirac-Frenkel time-dependent variational principle, manifold of Gaussian wave packets, determination of the equations of motion.

4. Hagedorn's semiclassical wave packets: parametrization of complex-valued Gaussian functions by the Siegel half space, parametrized raising and lowering operators, time-splitting and Galerkin approximation with Hagedorn wave packets.

5. Semiclassical initial value representations and Gaussian beams: continuous superpositions of Gaussian wave packets, frozen versus thawed Gaussian approximations, derivation of the Hermann-Kluk prefactor, random sampling of Gaussian wave packet transforms.

6. Wigner function methods: Wigner functions and expectation values, random sampling of Wigner functions, Egorov's theorem.

7. Surface hopping algorithms: non-adiabatic coupling of potential energy surfaces, surface hopping of the fewest switches, Landau-Zener (single switch) surface hopping.

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