Approximation Methods in Multi-Particle Quantum Dynamics
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Time-Dependent Schrödinger Eqn. (TDSE)

\[ \frac{\partial \psi}{\partial t}(x_1, \ldots, x_f, t) = H(t)\psi(x_1, \ldots, x_f, t). \]

- \( f \gg 1 \) electrons; \[ |\psi(x_1, \ldots, x_f, t)|^2 \] probability density for electrons to be located at \( x_1, \ldots, x_f \) at time \( t \).
- The fundamental equation of non-relativistic quantum mechanics. Its solution could answer many questions about the nature of matter.
- But: Exact solution impossible. Direct numerical integration computationally intractable in general for \( f > 2 \Rightarrow \) need for model reduction.

Numerical Solution

Test code for 1D problems — bounded potentials

Method of lines:
- Space discretization (for every \( t \))
- Solution components.
- Evaluating meanfield terms includes inner products of the form

\[ \langle \phi_j | V | \phi_j \rangle = \int \int \langle \phi_j | V(x-y) \phi_j(y) \rangle \; dy \; dx. \]

- ‘Correlation’: The integrals have to be computed for many \( i,j \)!
- Discretization and low rank approximation may be boosted by use of ‘hierarchical matrices’: Linear complexity for “asymptotically smooth” kernels (e.g. Coulomb interaction).

MCTDHF

Multi-configuration time-dependent Hartree-Fock method: Approximate solution of TDSE by
\[ \psi(x_1, \ldots, x_f, t) \approx u := \sum_J a_J(t) \phi_J(x_t, t) \]

Dirac–Frenkel variational principle
\[ \left\langle \delta u | \frac{\partial u}{\partial t} - H u \right\rangle = 0 \quad \forall \; \text{variations} \; \delta u. \]

Additional constraints for uniqueness
\[ \langle \phi_j | \phi_k \rangle = \delta_{j,k}, \quad \langle \phi_j | \frac{\partial \phi_k}{\partial t} \rangle = 0. \]

This yields the equations of motion
\[ \frac{\partial a_J}{\partial t} = \sum_K \langle \phi_J | H | \phi_K \rangle a_K, \quad \frac{\partial \rho_j}{\partial t} = (I-P) \sum_k l \sum_l \rho_{jl} \Pi^{l,k} \phi_k, \]

where
\[ \psi_j := \langle \phi_j | u \rangle, \quad \rho_{jl} := \langle \phi_j | \psi_l \rangle, \quad \Pi^{l,k} := \langle \psi_l | H | \psi_k \rangle, \quad P := \sum_j \langle \phi_j | \langle \phi_j | \rangle. \]

1D model

Electrons in strong, ultrafast laser field:
\[ H(t) := \sum_{k=1}^{f} \left( -\frac{i}{2} \Delta_k - A(t) \right) \]
\[ = U(x_k) + \sum_{l<k} V(x_k - x_l) \]
\[ A(t) := e^{-t^2} \sin(\omega t), \quad U(x) := \frac{-1}{r-a+\sqrt{x^2+ax}+x}, \]
\[ V(x-y) := \frac{1}{\sqrt{1+(x-y)^2}}. \]


Project Aims

- Analytical properties of the solution:
  Extension of results for smooth potential to the singular (Coulomb) case. Domain of existence.
- Convergence of MCTDHF approximations as the number of configurations tends to infinity.
- Invertibility of density matrix \( \rho \). Regularity bounds uniform in the number of configurations. Geometry of the approximation manifold.
- Code for 3D with cylindrical symmetry: Singulart potentials.
- (Adaptive) finite elements for space discretization: Local basis functions favorable for parallelization.
- High order time integrator: Preserve “geometric” properties (e.g. orthogonormality of orbitals \( \phi_j \)). Splitting idea to treat separately fast and slow solution components.

Practical Simulation

- \( f = 4 \) electrons, 15 configurations
- Computations by Runge-Kutta, variable step-size, variable order method, pseudospectral space discretization at 1000 points, 15 optical cycles
- Electron density \( \langle u | u \rangle_{f-1} \)

Collaborations

- Ch. Lubich, Univ. of Tübingen
  Numerical analysis, geometric (time) integration, convergence of the approximation, relationships with low rank approximation of time-dependent matrices.
- N. Mauser, Univ. of Vienna
  Analytical aspects of MCTDHF equations, convergence of the approximation.
- J. M. Melenk, D. Praetorius,
  Vienna Univ. of Technology Computational math., \( \mathcal{H} \)-matrices.
- A. Scrinzi, Vienna Univ. of Technology
  High performance computing, code development, applications.