Born-Huang

Trajectory approaches within the exact factorization

Exact Factorization

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Alternative representation of the molecular wavefunction: $\Psi(\boldsymbol{r}, \boldsymbol{R}, t) = \Phi(\boldsymbol{r}, t; \boldsymbol{R})\chi(\boldsymbol{R}, t)$

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In the exact factorization, both nuclear and electronic wave functions are time-dependent, so we get a set of coupled equations of motion:

$$i\frac{\partial}{\partial t}\chi(\boldsymbol{R}, t) = \left[\sum_{\nu}^{N_n} \frac{[-i\nabla_{\boldsymbol{R}_\nu} + \boldsymbol{A}_\nu(\boldsymbol{R}, t)]^2}{2M_\nu} + \epsilon(\boldsymbol{R}, t) + v_{\text{int}}(\boldsymbol{R}, t)\right]\chi(\boldsymbol{R}, t)$$

$$i\frac{\partial}{\partial t}\Phi(\boldsymbol{r}, t; \boldsymbol{R}) = \left[\hat{H}_{\text{BO}}(\boldsymbol{r}, \boldsymbol{R}) + \hat{V}(\boldsymbol{r}, \boldsymbol{R}, t) + \hat{U}_{\text{en}}[\Phi, \chi](\boldsymbol{R}, t) - \epsilon(\boldsymbol{R}, t) - v_{\text{int}}(\boldsymbol{R}, t)\right]\Phi(\boldsymbol{r}, t; \boldsymbol{R}),$$

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Two new potentials:
TDVP: $\boldsymbol{A}_\nu(\boldsymbol{R}, t) = \langle\Phi(t; \boldsymbol{R})| - i\nabla_{\boldsymbol{R}_\nu}\Phi(t; \boldsymbol{R})\rangle_{\boldsymbol{r}}$
TDPES: $\epsilon(\boldsymbol{R}, t) = \langle\Phi(t; \boldsymbol{R})|\,[\hat{H}_{\text{BO}}(\boldsymbol{R}) + \hat{U}_{\text{en}}[\Phi, \chi](\boldsymbol{R}, t) - i\partial_t]\,|\Phi(t; \boldsymbol{R})\rangle_{\boldsymbol{r}}$
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$v_{\text{int}}(\boldsymbol{R},t) = \langle\Phi(t;\boldsymbol{R})|\,\hat{V}(\boldsymbol{R},t)\,|\Phi(t;\boldsymbol{R})\rangle_{\boldsymbol{r}}$
Electron-nuclear coupling operator:

$$\hat{U}_{\text{en}}[\Phi,\chi](\boldsymbol{R},t) = \sum_{\nu}\frac{1}{M_\nu}\left(\frac{1}{2}[-i\nabla_{\boldsymbol{R}_\nu} - \boldsymbol{A}_\nu(\boldsymbol{R},t)]^2 + \left(\frac{-i\nabla_{\boldsymbol{R}_\nu}\chi(\boldsymbol{R},t)}{\chi(\boldsymbol{R},t)} + \boldsymbol{A}_\nu(\boldsymbol{R},t)\right)\left(-i\nabla_{\boldsymbol{R}_\nu} - \boldsymbol{A}_\nu(\boldsymbol{R},t)\right)\right)$$

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Single time-dependent scalar and vector potential drive the dynamics – framework for trajectories without hops, spawns, averaging etc.

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BO-picture

Hamiltonian operator:

$$\hat{H} = \sum_{\nu} \frac{(-i\nabla_{\nu})^2}{2M_{\nu}} + \epsilon_{\mathrm{BO}}(\boldsymbol{R})$$

Classical Hamiltonian:

$$H^{\mathrm{cl}} = \sum_{\nu} \frac{\boldsymbol{P}_{\nu}^2(\boldsymbol{R}, t)}{2M_{\nu}} + \epsilon_{\mathrm{BO}}(\boldsymbol{R})$$

For quantum trajectories:

$$H^{\mathrm{q}} = \sum_{\nu} \frac{\boldsymbol{P}_{\nu}^2(\boldsymbol{R}, t)}{2M_{\nu}} + \epsilon_{\mathrm{BO}}(\boldsymbol{R}) + Q_{\mathrm{pot}}$$

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EF-picture

Nuclear Hamiltonian operator:

$$\hat{H}_n = \sum_{\nu} \frac{[-i\nabla_{\nu} + \boldsymbol{A}(\boldsymbol{R}, t)]^2}{2M_{\nu}} + \epsilon(\boldsymbol{R}, t)$$

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Trajectories within EF – proper derivation

We use again the polar form of the nuclear wavefunction[a]

$$\chi(\boldsymbol{R}, t) = \exp[\, iS(\boldsymbol{R}, t)]\,|\chi(\boldsymbol{R}, t)$$

[a] F. Agostini et al., Eur. Phys. J. B (2018), 91, 139; F. Talotta et al., J. Phys. Chem. A (2020), 124, 34, 6764

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Insert it in the TDSE, applying the differential operators, and separating its real and imaginary parts, we derive an evolution equation for the phase:

$$\partial_t S(\boldsymbol{R}, t) = -\sum_\nu \frac{[\nabla_\nu S(\boldsymbol{R}, t) + \boldsymbol{A}_\nu(\boldsymbol{R}, t)]^2}{2M_\nu} - \epsilon(\boldsymbol{R}, t) - \sum_\nu \frac{\nabla_\nu^2 |\chi(\boldsymbol{R}, t)|}{2M_\nu |\chi(\boldsymbol{R}, t)|}$$

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Now, if we take $\boldsymbol{R}, t, S, \nabla S = \boldsymbol{P}, \partial_t S = S_t$ as independent variables, this can be identified with a Hamilton-Jacobi equation with the Hamiltonian:

$$-S_t = H_n^{\mathrm{q}} = \sum_\nu \frac{[\boldsymbol{P}_\nu(\boldsymbol{R}, t) + \boldsymbol{A}_\nu(\boldsymbol{R}, t)]^2}{2M_\nu} + \epsilon(\boldsymbol{R}, t) + v_{\mathrm{int}}(\boldsymbol{R}, t) + Q_{\mathrm{pot}}$$

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Trajectories within EF – proper derivation II

we obtain Hamilton-like evolution equations for the evolution of positions and momenta:

$$\dot{\boldsymbol{R}}_\nu(t) = \frac{\boldsymbol{P}_\nu(t) + \boldsymbol{A}_\nu(\boldsymbol{R}(t), t)}{M_\nu} \quad \text{and} \quad \dot{\boldsymbol{P}}_\nu(t) = -\nabla_{\boldsymbol{R}_\nu} H_n^{\mathrm{q}}(\boldsymbol{P}(t), \boldsymbol{R}(t), t)$$

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Classical trajectories obtained for the limit where the quantum potential is set to zero:

$$\begin{aligned} H_n(\boldsymbol{P}, \boldsymbol{R}, t) =& \sum_\nu \frac{[\boldsymbol{P}_\nu(\boldsymbol{R}, t) + \boldsymbol{A}_\nu(\boldsymbol{R}, t)]^2}{2M_\nu} + \epsilon(\boldsymbol{R}, t) + v_{\mathrm{int}}(\boldsymbol{R}, t) + Q_{\mathrm{pot}}(\boldsymbol{R}, t) \\ =& H_n^{\mathrm{cl}}(\boldsymbol{P}(t), \boldsymbol{R}(t), t) + Q_{\mathrm{pot}}(\boldsymbol{R}, t) \end{aligned}$$

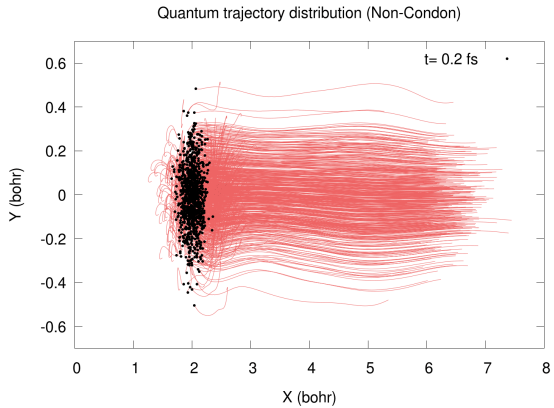
So the evolution equations for the classical trajectories are

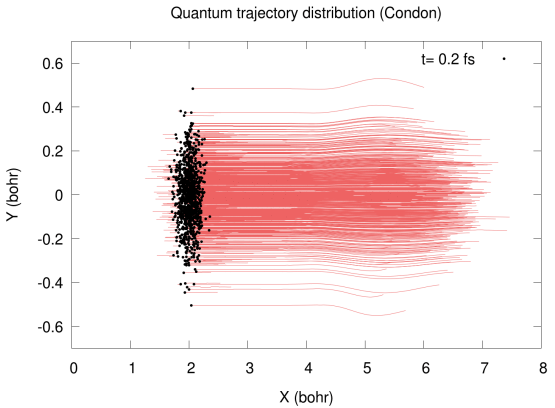
$$\dot{\boldsymbol{R}}_\nu(t) = \frac{\boldsymbol{P}_\nu(t) + \boldsymbol{A}_\nu}{M_\nu} \quad \text{and} \quad \dot{\boldsymbol{P}}_\nu(t) = -\nabla_{\boldsymbol{R}_\nu} H_n^{\mathrm{cl}}(\boldsymbol{P}(t), \boldsymbol{R}(t), t)$$

How to initialize trajectories?

Classical trajectories: Positions and momenta Wigner sampling
Quantum trajectories: Cannot separate positions and momenta. Use Wigner sampled positions, corresponding momenta from $\boldsymbol{A}$.

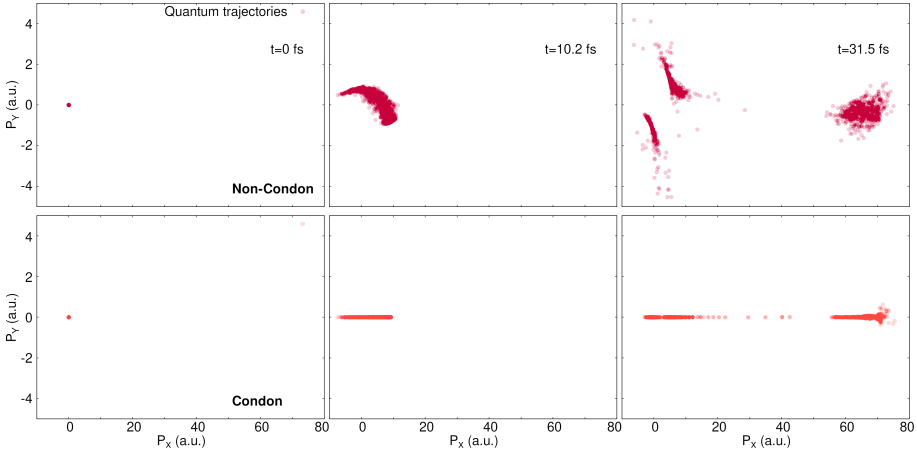
Dynamics of Quantum Trajectories



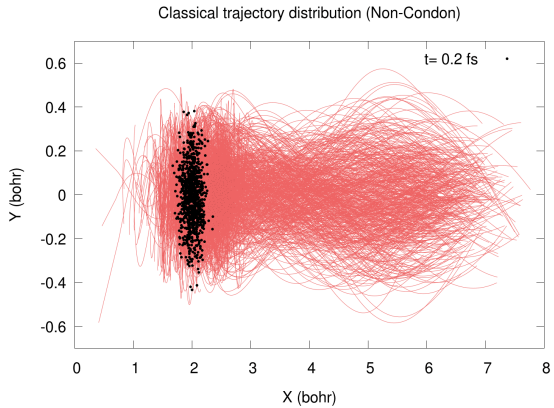


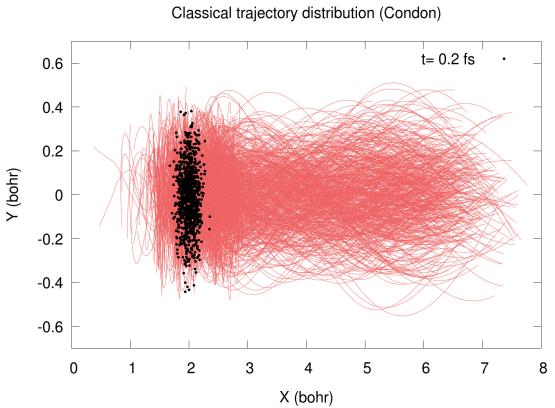
Momentum distribution

Momentum obtained from $\boldsymbol{A}_\nu(\boldsymbol{R}, t)$, drives the dynamics and encodes all the behavior observed in the dynamics.



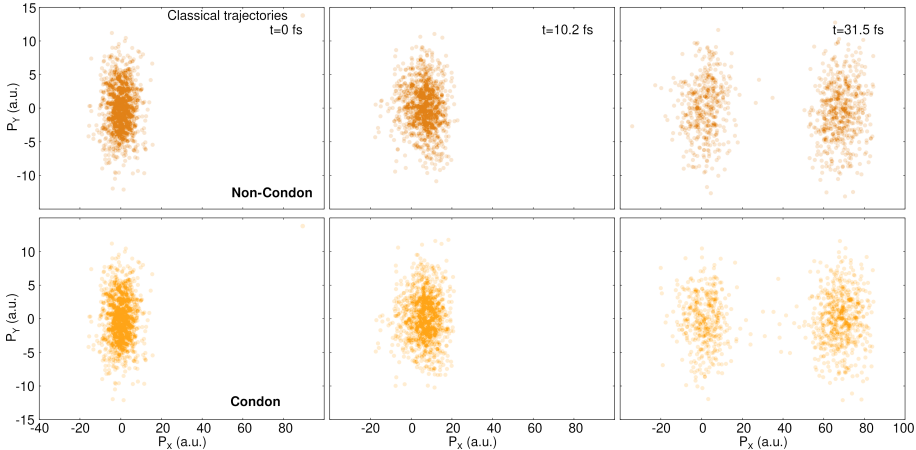
Dynamics of Classical Trajectories



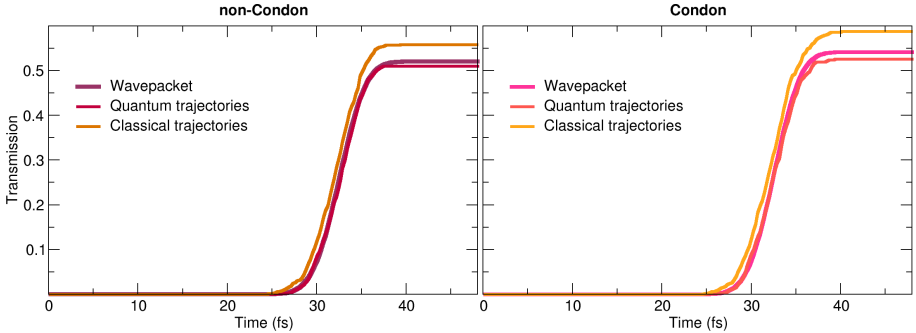


Momentum distribution

Momentum obtained from $\boldsymbol{A}_\nu(\boldsymbol{R}, t)$, initialized from Wigner distribution.



Trajectories in EF



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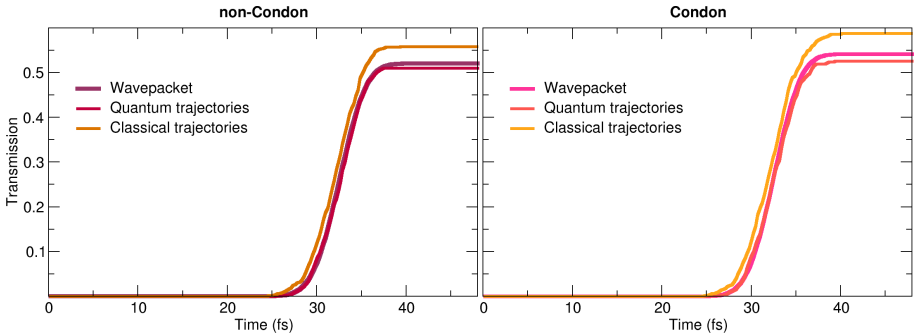

Dynamics of trajectories on single surface incorporates all nonadiabatic effects. But need to know full TDPES and TDVP, derived within 2D Gauge of $S = 0$. How can we move to EF based trajectories for molecules?

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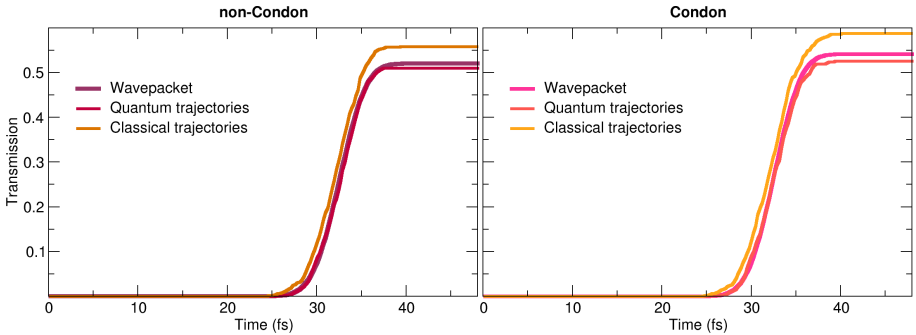

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1. Get TDVP and TDPES on-the-fly
2. Calculate TDVP and TDPES from adiabatic quanities
3. Use generally applicable gauge (for any number of degrees of freedom).

Classical trajectory methods from EF for molecules

As before, the nuclear wavefunction is written in the polar form, and we get evolution equations from the nuclear time-dependent Schrödinger equation (we already neglect Q_{pot}):

$$-\partial_t S(\boldsymbol{R},t) = \sum_\nu \frac{\nabla_\nu S(\boldsymbol{R},t) + \boldsymbol{A}_\nu(\boldsymbol{R},t)]^2}{2M_\nu} + \epsilon(\boldsymbol{R},t)$$

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S.K. Min et al., Phys. Rev. Lett. 2015, 115, 7, 073001

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We can again solve with characteristics, to get to

$$\dot{\boldsymbol{R}}_\nu(t) = \frac{\boldsymbol{P}_\nu(t)}{M_\nu} \qquad \dot{\boldsymbol{P}}_\nu(t) = -\nabla_\nu \left[\epsilon(\boldsymbol{R}(t),t) + \sum_{\nu'} \dot{\boldsymbol{R}}_{\nu'}(t) \cdot \boldsymbol{A}_{\nu'}(\boldsymbol{R}(t),t) \right] + \dot{\boldsymbol{A}}_\nu(\boldsymbol{R}(t),t)$$

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$$\epsilon(\boldsymbol{R}(t),t) + \sum_\nu \dot{\boldsymbol{R}}_\nu(t) \cdot \boldsymbol{A}_\nu(\boldsymbol{R}(t),t) = 0$$

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Classical trajectory methods from EF for molecules

Evolution of the nuclear density can be described by the continuity equation, coupled to the evolution of the phase.
But replace by trajectories, reconstruct a classical like nuclear density from the trajectories (see later), assuming that for short enough times, ensemble of classical trajectories will sample nuclear configuration space with high probability density.
How about electronic evolution?

$$i\frac{\partial}{\partial t}\Phi(\boldsymbol{r},t;\boldsymbol{R}) = \left[\hat{H}_{\mathrm{BO}}(\boldsymbol{r},\boldsymbol{R}) + \hat{U}_{\mathrm{en}}[\Phi,\chi](\boldsymbol{R},t) - \epsilon(\boldsymbol{R},t)(\boldsymbol{R},t)\right]\Phi(\boldsymbol{r},t;\boldsymbol{R})$$

Important property to look at: $\hat{U}_{\mathrm{en}}[\Phi,\chi]$ electron-nuclear coupling operator!

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Classical trajectory methods from EF for molecules

The electron-nuclear coupling operator

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is then approximated and simplified:

$$\hat{U}_{\text{en}}\approx\sum_{\nu}\left(\dot{\boldsymbol{R}}_\nu(t)+i\frac{\mathcal{P}_\nu(\boldsymbol{R}(t),t)}{M_\nu}\right)\left(-i\nabla_\nu-\boldsymbol{A}_\nu(\boldsymbol{R}(t),t)\right)$$

[b] F. Eich and F. Agostini, J. Chem. Phys. 2016, 145, 054110

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We neglect the first term, that was shown to be smaller[b] and with the characteristic definitions the rest simplifies and we introduce the *quantum momentum* as $\mathcal{P}_\nu(\boldsymbol{R}(t),t) = \frac{-\nabla_\nu|\chi(\boldsymbol{R}(t),t)|^2}{2|\chi(\boldsymbol{R}(t),t)|^2}$

Quantum momentum: purely imaginary correction, introduces quantum decoherence effects, needs nuclear density — *coupled trajectories*

We'll talk later in detail how we get to this quantity!

[b] F. Eich and F. Agostini, J. Chem. Phys. 2016, 145, 054110

Evolution of coefficients in CT-MQC

We reconstrunct the nuclear density from N_{traj} trajectories, labelled with α. Let's express nuclear wavefunction in terms of eigenfunctions of $\hat{H}_{\text{BO}}$:

$$\Phi(\boldsymbol{r}, t; \boldsymbol{R}^{\alpha}(t)) = \sum_{J} C_J(\boldsymbol{R}^{\alpha}(t), t) \phi^{(J)}_{\boldsymbol{R}^{\alpha}(t)}(\boldsymbol{r})$$

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we can derive evolution equations for the expansion coefficients

$$\dot{C}^{\alpha}_{J} = \dot{C}^{\alpha}_{J,\text{TSH}}(t) + \dot{C}^{\alpha}_{J,\text{qm}}(t)$$

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with the two contributions

$$\dot{C}^{\alpha}_{J,\text{TSH}}(t) = -iE^{\alpha}_J C^{\alpha}_J(t) - \sum_K \sum_{\nu}^{N_n} \dot{\boldsymbol{R}}^{\alpha}_{\nu}(t) \cdot \boldsymbol{d}^{\alpha}_{\nu,JK} C^{\alpha}_K(t) \qquad \dot{C}^{\alpha}_{J,\text{qm}}(t) = \sum_{\nu}^{N_n} \frac{\mathcal{P}^{\alpha}_{\nu}(t)}{M_{\nu}} \cdot (\boldsymbol{f}^{\alpha}_{\nu,J} - \boldsymbol{A}^{\alpha}_{\nu}(t)) C^{\alpha}_J(t)$$

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$$\boldsymbol{A}^{\alpha}_{\nu}(t) = \sum_{J,K} \Im[\bar{C}^{\alpha}_{J}(t)C^{\alpha}_{K}(t)]\boldsymbol{d}^{\alpha}_{\nu,JK} + \sum_{J}|C^{\alpha}_{J}(t)|^2\boldsymbol{f}^{\alpha}_{\nu,J} \approx \sum_{J}|C^{\alpha}_{J}(t)|^2\boldsymbol{f}^{\alpha}_{\nu,J}$$

Nuclear evolution in CT-MQC

The nuclear trajectory $\boldsymbol{R}_\nu^\alpha(t)$ is propagtated according to the CT-MQC force given by

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with a mean-field contribution, a contribution from the nonadiabatic coupling vectors (those make up a standard Ehrenfest term) and an additional contribution, dependent on quantum momentum and accumulated force

$$\boldsymbol{F}_{\nu,\mathrm{MF}}^\alpha(t) = \sum_J |C_J^\alpha(t)|^2(-\nabla_\nu E_J^\alpha)$$

$$\boldsymbol{F}_{\nu,\mathrm{NAC}}^\alpha(t) = \sum_{J,K} \bar{C}_J^\alpha(t) C_K^\alpha(t)(E_J^\alpha - E_K^\alpha)\boldsymbol{d}_{\nu,JK}^\alpha$$

$$\boldsymbol{F}_{\nu,\mathrm{qm}}^\alpha(t) = 2\sum_J |C_J^\alpha(t)|^2 \left[\sum_\mu^{N_n} \boldsymbol{\mathcal{P}}_\mu^\alpha(t)\cdot \boldsymbol{f}_{\mu,J}^\alpha\right](\boldsymbol{f}_{\mu,J}^\alpha - \boldsymbol{A}_\nu^\alpha(t))$$

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Quantum decoherence: trajectory-based algorithms rely on ad-hoc corrections.
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The crucial quantity is the quantum momentum,

$$\mathcal{P}_\nu^\alpha(\boldsymbol{R}^\alpha(t),t) = \frac{-\nabla_\nu|\chi(\boldsymbol{R}^\alpha(t),t)|^2}{2|\chi(\boldsymbol{R}^\alpha(t),t)|^2}$$

Requires information of the full nuclear density. Therefore, to be able to approximate this for trajectories, we need to have a set of coupled trajectories, that allow us to reconstruct the nuclear density.

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$$\chi(\boldsymbol{R}^\alpha(t),t) = \frac{1}{N_{\text{traj}}}\sum_\beta^{\text{traj}} \sqrt{G_\sigma^{\alpha\beta}}\exp[iS_\beta(t)]$$

Approximations to the quantum momentum

Only taking the diagonal parts of $|\chi(\boldsymbol{R}^{\alpha}(t),t)|^2$:

$$\mathcal{P}_{\nu}^{\alpha}(t) = \Gamma_{\nu}^{\alpha}(t)\boldsymbol{R}_{\nu}^{\alpha}(t) - \mathcal{R}_{\nu}^{\alpha}(t) = \frac{1}{\sigma_{\nu}}\left(\boldsymbol{R}_{\nu}^{\alpha}(t) - \sum_{\beta}^{N_{\text{traj}}} \boldsymbol{R}^{\beta}(t)\frac{G_{\sigma}^{\alpha\beta}}{\sum_{\gamma}^{N_{\text{traj}}} G_{\sigma}^{\alpha\gamma}}\right)$$

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However, when looking at the change of population over time, it can change even when the nonadiabatic couplings are zero. In the average over all trajectories is needs to yield zero population transfer from state J to K if the corresponding nonadiabatic couplings are zero. To ensure this, we impose a condition on the quantum momentum, that the change of population is zero if the nonadiabatic couplings are zero, for each nuclear degree of freedom, ν

$$\sum_\alpha^{N_{\text{traj}}} \mathcal{P}_{\nu,KJ}^\alpha(t)(f_{\nu,K}^\alpha - f_{\nu,J}^\alpha)|C_J^\alpha|^2|C_K^\alpha|^2 = 0 \forall J,\nu$$

Short summary of CT-MQC

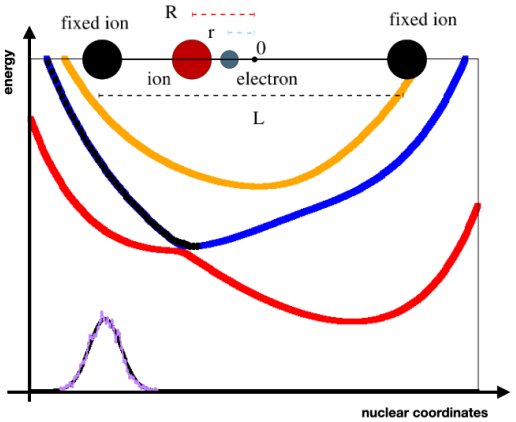
CT-MQC is an algorithm to propagate classical trajectories based on the TDPES and TDVP, but constructs them on-the-fly from adiabatic quantities. Trajectories propagated with an Ehrenfest-like force (that contains mean-field and NAC) and a coupled-trajectory term:

$$\boldsymbol{F}^{\alpha}_{\nu}(t) = \boldsymbol{F}^{\alpha}_{\nu,\mathrm{MF}}(t) + \boldsymbol{F}^{\alpha}_{\nu,\mathrm{NAC}}(t) + \boldsymbol{F}^{\alpha}_{\nu,\mathrm{CT}}(t)$$

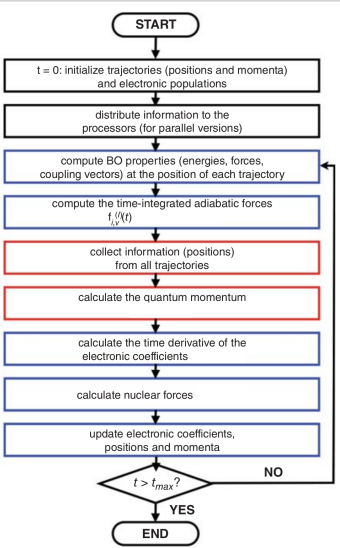
Also evolution of electronic coefficients includes an Ehrenfest-like term and a term depending on the quantum momentum:

$$\dot{C}^{\alpha}_{J}(t) = \dot{C}^{\alpha}_{J,\mathrm{TSH}}(t) + \dot{C}^{\alpha}_{J,\mathrm{qm}}(t)$$

The quantum momentum induces decoherence and requires information of the nuclear density — approximated through coupled trajectories.



Workflow CT-MQC



G-CTMQC:
https://gitlab.com/agostini.work/g-ctmqc.git

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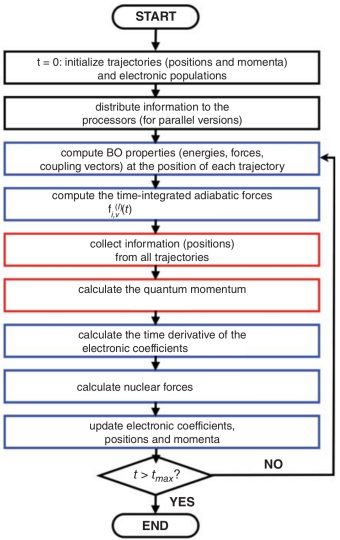

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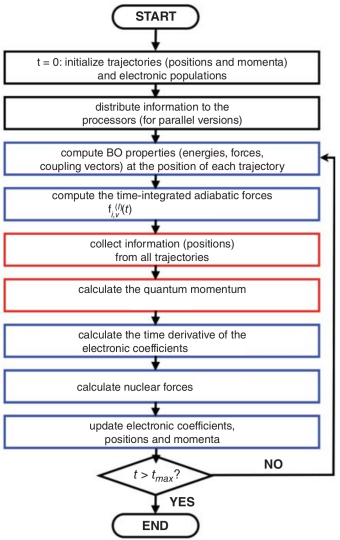

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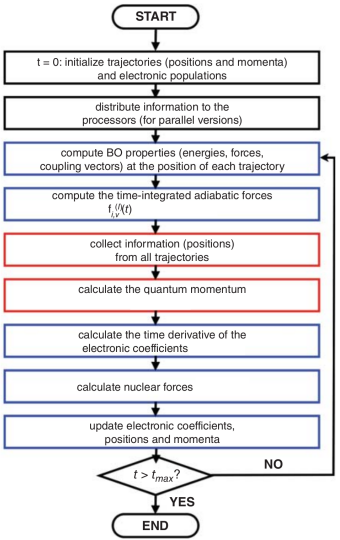

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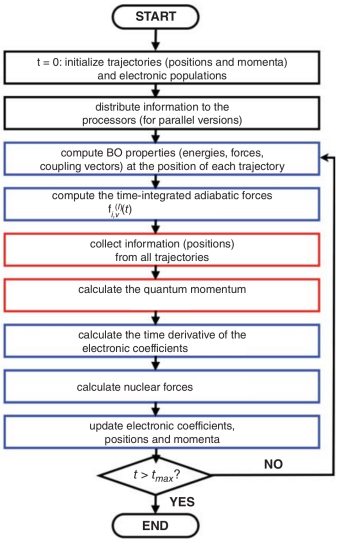

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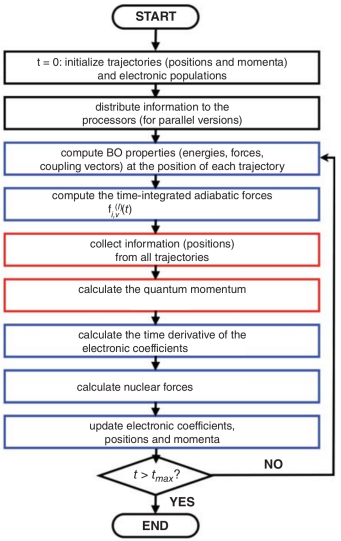

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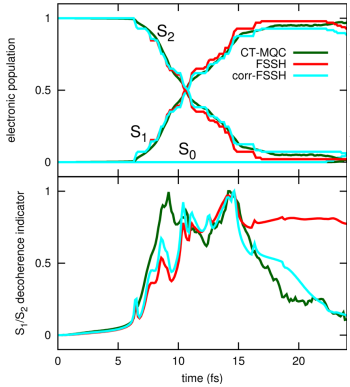
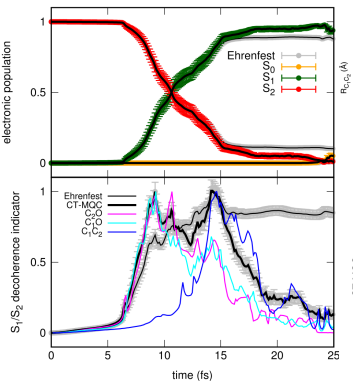
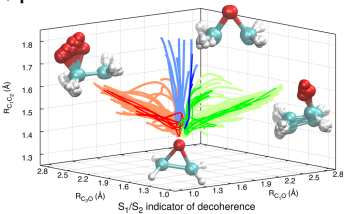
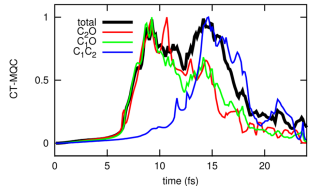
Example CT-MQC for molecules: oxirane

CT-MQC was interfaced with CPMD, 100 trajectories, TD-PBE, plane wave basis set. [a]









[a] S.K. Min et al., J. Phys. Chem. Lett. 2017, 8, 13, 3048−3055; B.F.E. Curchod et al., Eur. Phys. J. B 2018 91, 168

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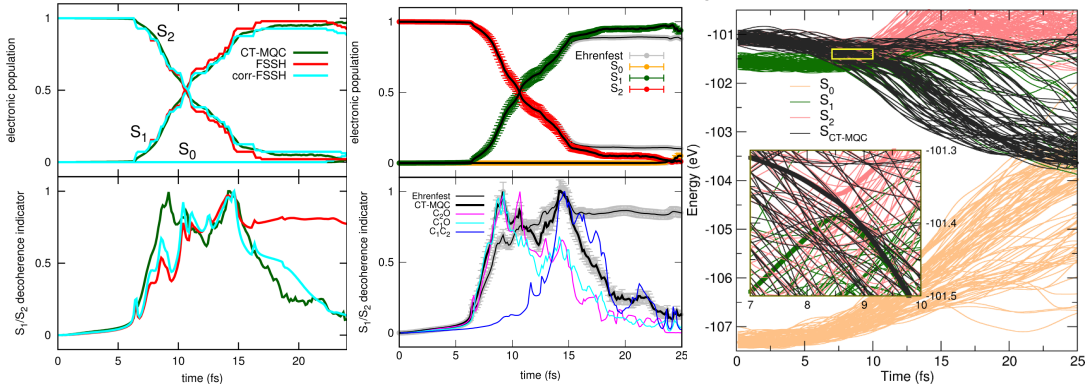

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Extensions of CT-MQC: Triplets

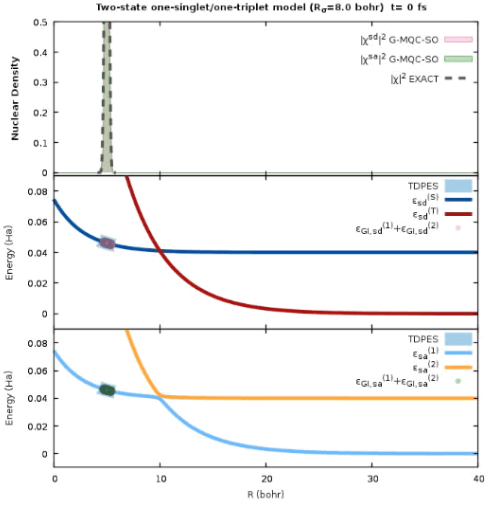
Including spin-orbit couplings in G-CT-MQC. [a]

$$i\partial_t \chi(\boldsymbol{R}, t)\Phi(\boldsymbol{x}, t; \boldsymbol{R}) =$$
$$\left(\hat{T}_{\text{el}} + \hat{H}_{\text{BO}} + \hat{H}_{\text{SOC}}\right)\chi(\boldsymbol{R}, t)\Phi(\boldsymbol{x}, t; \boldsymbol{R})$$

spin-diabatic basis (eigenstates of $\hat{H}_{\text{BO}}$) vs. spin-adiabatic basis (eigenstates of $\hat{H}_{\text{BO}} + \hat{H}_{\text{SOC}}$)

Here is a new link for visio mode, we hope this one will work better : https://eu.bbcollab.com/guest/d22947d971214

Sorry for the inconvenience,



[a] F. Talotta et al., Phys. Rev. Lett. 2020, 124, 033001; F. Talotta et al., J. Chem. Theory Comput. 2020, 16, 8, 4833-4848

Extensions of CT-MQC: Time-periodic fields

Including time-periodic fields ($\hat{V}(t) = -\hat{\mu}E_0\cos(\Omega t)$) with Floquet formalism, F-CT-MQC: [c]

$$i\partial_t \chi(\boldsymbol{R}, t)\Phi(\boldsymbol{r}, t; \boldsymbol{R}) = \left(\hat{T}_{\text{el}} + \hat{H}_{\text{BO}} + \hat{V}(t)\right)\chi(\boldsymbol{R}, t)\Phi(\boldsymbol{r}, t; \boldsymbol{R})$$

Floquet theorem for the TDSE

A complete set of solutions of a time-periodic TDSE with period T takes the form $e^{i\mathcal{E}_m t}\phi_m(t)$ where the eigenvalues of the Floquet Hamiltonian $\hat{H}_{\text{Fl}}(t) = \hat{H}_{\text{BO}} + \hat{V}(t) - i\partial_t$ are called Floquet quasi-energies

$$\hat{H}_{\text{Fl}}(t)\phi_m(t) = \mathcal{E}_m\phi_m(t)$$

and Floquet eigenmodes are periodic in time: $\phi_m(t) = \phi_m(t+T)$.

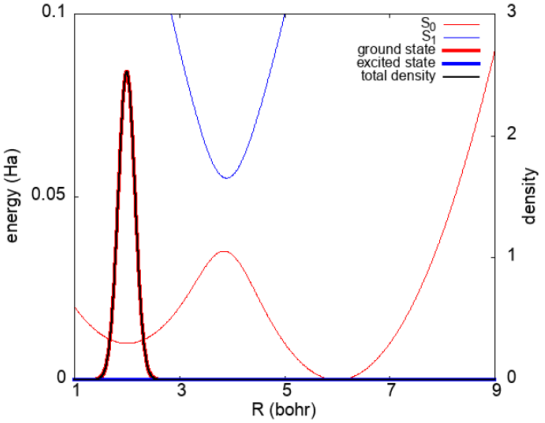
The eigenmodes are expanded in harmonics of the external drive with $\omega_n = n\Omega$

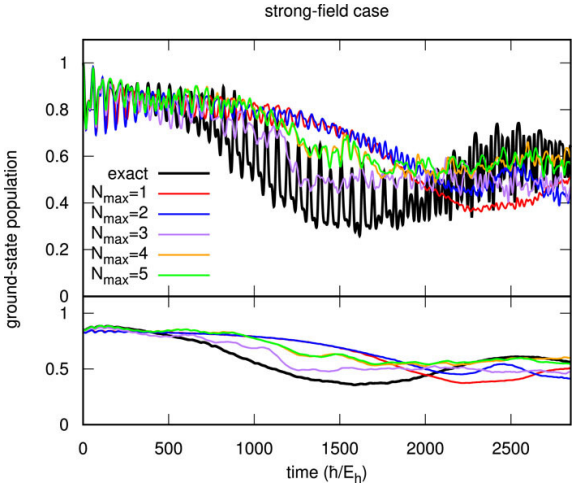
$$\phi_m(t) = \sum_{n=-\infty}^{n=+\infty} e^{i\omega_n t}\phi_m^{(n)}$$

an eigenvalue problem can be solved for the Fourier components $\phi_m^{(n)}$ and the problem becomes essentially stationary. States 'dressed' with the harmonics

[c] M. Schiró et al., J. Chem. Phys. 2021, 154, 114101

Extensions of CT-MQC: Time-periodic fields





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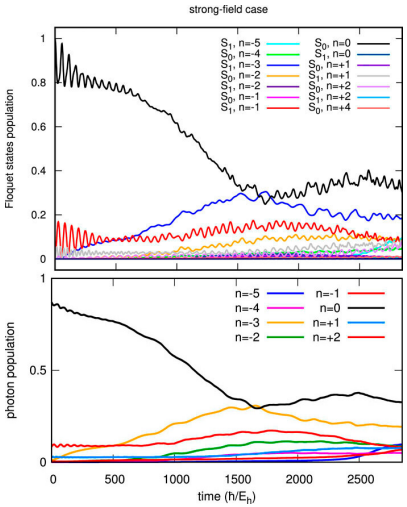

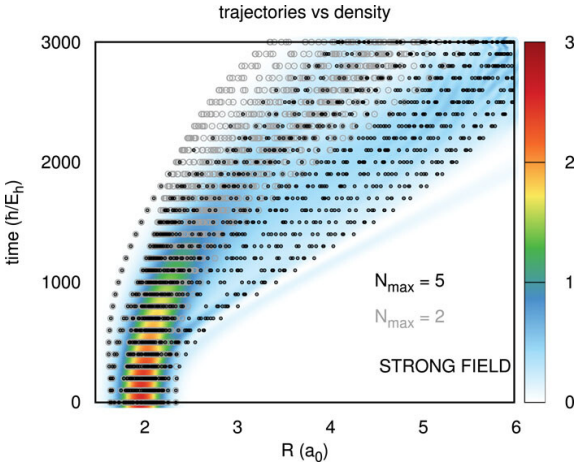

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Initial conditions and approximations of CT-MQC

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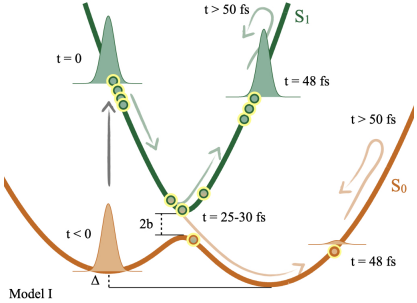

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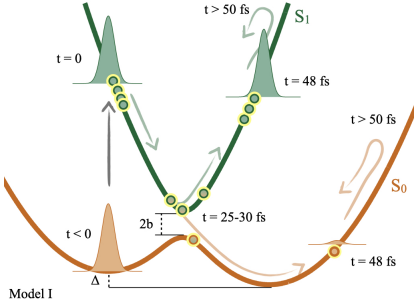
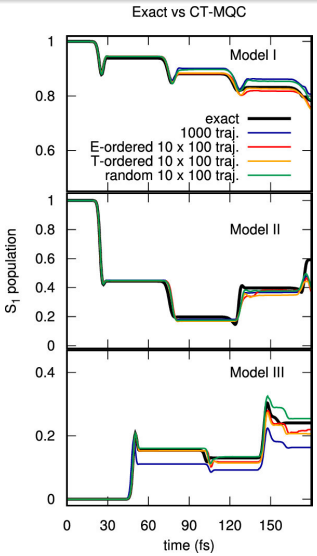


[a] C. Pieroni and F. Agostini, J. Chem. Theory Comput. 2021, 17, 10, 5969–5991



Initial conditions and approximations of CT-MQC

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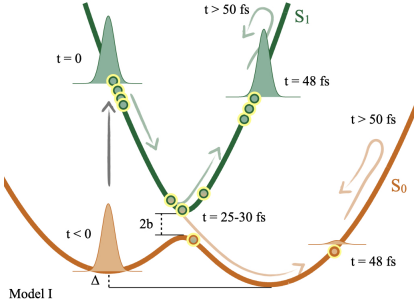

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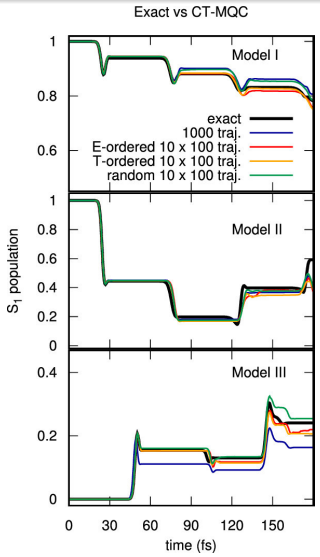

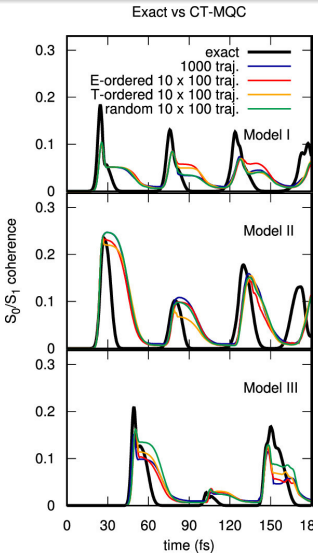

CT-TSH

In CT-MQC trajectories propagated with an Ehrenfest-like force (that contains mean-field and NAC) and a coupled-trajectory term:

$$\boldsymbol{F}_{\nu}^{\alpha}(t) = \boldsymbol{F}_{\nu,\mathrm{MF}}^{\alpha}(t) + \boldsymbol{F}_{\nu,\mathrm{NAC}}^{\alpha}(t) + \boldsymbol{F}_{\nu,\mathrm{CT}}^{\alpha}(t)$$

Also evolution of electronic coefficients includes an Ehrenfest-like term and a term depending on the quantum momentum:

$$\dot{C}_{J}^{\alpha}(t) = \dot{C}_{J,\mathrm{TSH}}^{\alpha}(t) + \dot{C}_{J,\mathrm{qm}}^{\alpha}(t)$$

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CT-TSH propagates following the adiabatic forces, but still includes the quantum momentum in the evolution of the coefficients — increases stability, reduces cost (no more explicit NAC) [d]

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method	trajectory	nuclear foreces	electronic evolution	hopping	decoherence
CT-MQC	coupled	TDPES and TDVP	$\dot{C}_{\mathrm{TSH}}(t) + \dot{C}_{\mathrm{qm}}(t)$	none	QM
FS-CT-TSH	coupled	BOPES	$\dot{C}_{\mathrm{TSH}}(t) + \dot{C}_{\mathrm{qm}}(t)$	FS	QM
LZ-CT-TSH	coupled	BOPES	$\dot{C}_{\mathrm{TSH}}(t) + \dot{C}_{\mathrm{qm}}(t)$	LZ	QM
FS-TSH	ITA	BOPES	$\dot{C}_{\mathrm{TSH}}(t)$	FS	none
FS-TSH-EDC	ITA	BOPES	$\dot{C}_{\mathrm{TSH}}(t)$	FS	EDC

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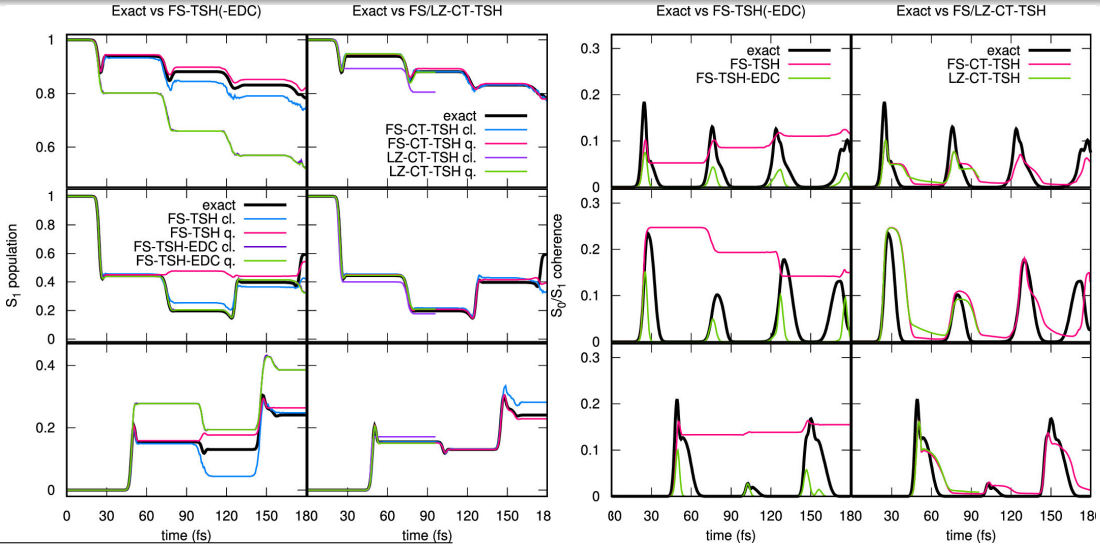
CT-TSH



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Overview

- CT-MQC and CT-TSH allow to run trajectories in an algorithm derived from the exact factorization.
- Decoherence included derived from QM
- Extensions for triplets and time-periodic fields
- Much more room for developments in the future!

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- Much more room for developments in the future!

Hands-On:

- G-CTMQC: `https://gitlab.com/agostini.work/g-ctmqc.git`:
  VERY easy to compile and run (only needs gfortran, lapack and blas to run on your laptops).
  At the moment interface with QuantumModelLib
  (`https://github.com/lauvergn/QuantumModelLib.git`) for a large number of model Hamiltonians.
- Today: 1D (NaI) and 2D (conical intersection) model systems
- compare CT-MQC, CT-TSH, Ehrenfest, TSH, TSH-EDC with exact calculations.
- Highlight differences between methods, decohrence etc.
- Lots of possibilities to play with the code and get understandings of trajectory based dynamics!

Acknowledgments

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Carlotta Pieroni

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