A route beyond Ehrenfest: Correlated Electron-Ion Dynamics

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Outline

- Some previous extensions to Ehrenfest:
  - Mixed quantum-classical dynamics
  - ‘Frozen gaussians’ and ‘ab initio quantum molecular dynamics’
- The CEID approach (Coherent Electron-Ion Dynamics):
  - Focusing on correlations
  - Moment CEID
  - polyCEID (motivation and introduction)
  - Details and applications: following talk by Lorenzo Stella
- Outlook and conclusions

Mixed quantum-classical dynamics (1)

Consider Wigner transform of a nuclear density operator ρ

$$\rho_W(\mathbf{R},\mathbf{P}) = h^{-3N}\int \mathrm{d}z \mathrm{e}^{\mathrm{i}\mathbf{P}\cdot\mathbf{z}/\hbar}\langle \mathbf{R}-\mathbf{z}/2|\hat{\rho}|\mathbf{R}+\mathbf{z}/2\rangle$$

and of a nuclear operator O

$$O_W(\mathbf{R},\mathbf{P}) = h^{-3N}\int \mathrm{d}z \mathrm{e}^{-\mathrm{i}\mathbf{P}\cdot\mathbf{z}/\hbar}\langle \mathbf{R}+\mathbf{z}/2|\hat{O}|\mathbf{R}-\mathbf{z}/2\rangle$$

So expectation value is

$$\langle \hat{O}\rangle = \mathrm{Tr}[\hat{\rho}\hat{O}] = \int \mathrm{d}\mathbf{R}\mathrm{d}\mathbf{P} O_W(\mathbf{R},\mathbf{P})\rho_W(\mathbf{R},\mathbf{P})$$

and evolution (Schrödinger picture) is Moyal product

$$\partial_t \rho_W(\mathbf{R},\mathbf{P}) = -\tfrac{1}{\mathrm{i}\hbar}(\overrightarrow{H}_\Lambda \rho_W - \rho_W \overleftarrow{H}_\Lambda) \equiv -\tfrac{1}{\mathrm{i}\hbar} H_W * \rho_W$$

$$\overrightarrow{H}_\Lambda = H_W \mathrm{e}^{\hbar\Lambda/2\mathrm{i}} \quad \overleftarrow{H}_\Lambda = \mathrm{e}^{\hbar\Lambda/2\mathrm{i}} H_W \quad \Lambda = \overleftarrow{\nabla}_{\mathbf{R}}\overrightarrow{\nabla}_{\mathbf{P}} - \overleftarrow{\nabla}_{\mathbf{P}}\overrightarrow{\nabla}_{\mathbf{R}}$$

Mixed quantum-classical dynamics (2)

Key idea: make Wigner transform only with respect to nuclear variables. Keep full quantum equation of motion for 'light' variables **r** and **p**, but for 'heavy' variables **R** and **P** truncate to lowest order in $\hbar$:

$$\overrightarrow{H}_\Lambda \approx H_W(1+\tfrac{\hbar\Lambda}{2\mathrm{i}}) \qquad \overleftarrow{H}_\Lambda \approx (1+\tfrac{\hbar\Lambda}{2\mathrm{i}})H_W$$

$$\partial_t \rho_W(\mathbf{R},\mathbf{P}) \approx \tfrac{1}{\mathrm{i}\hbar}[H_W,\rho_W] + \tfrac{1}{2}\left(\{H_W,\rho_W\} - \{\rho_W,H_W\}\right)$$

Quantum commutator $[H_W,\rho_W] = H_W\rho_W - \rho_W H_W$

Classical Poisson bracket $\{H_W,\rho_W\} = -H_W\Lambda\rho_W$

Nielsen, Kapral and Ciccotti *J Chem Phys* **112** 6543 (2000)
Kapral *Ann Rev Phys Chem* **57** 129 (2006)

Mixed quantum-classical dynamics (3)

In a basis of adiabatic states, equation of motion becomes

$$\partial_t \rho_{nn'} = -\mathrm{i} \sum_{mm'} \mathcal{L}_{nn',mm'} \rho_{mm'}$$

with the Liouvillian super-operator represented as

$$\mathrm{i}\mathcal{L}_{nn',mm'} = (\mathrm{i}\omega_{nn'} + \mathrm{i}L_{nn'})\delta_{nm}\delta_{n'm'} - J_{nn',mm'}$$

$$\mathrm{i}L_{nn'} = \sum_I \left[\frac{\mathbf{P}_I}{M_I} \cdot \nabla_{\mathbf{R}_I} + \frac{1}{2}(\mathbf{F}_{I,n} + \mathbf{F}_{I,n'}) \cdot \nabla_{\mathbf{P}_I} \right]$$

Classical evolution with average force of n and n'

$$J_{nn',mm'} = -\frac{\mathbf{P}_I}{M} \cdot \mathbf{d}_{nm} \left(1 + \frac{1}{2} S_{nm} \nabla_{\mathbf{P}}\right) \delta_{n'm'} - \frac{\mathbf{P}_I}{M} \cdot \mathbf{d}^*_{n'm'} \left(1 + \frac{1}{2} S^*_{n'm'} \nabla_{\mathbf{P}}\right) \delta_{nm}$$

Effect of transitions between quantum states

Commonly implemented by surface hopping (again): evolve forward through Δt using L and consider transitions $n \rightarrow m$ or $n' \rightarrow m'$ with probability

$$\pi_{n\to m} = \left| \frac{\mathbf{P}}{M} \cdot \mathbf{d}_{nm} \right| \Delta t \left(1 + \left| \frac{\mathbf{P}}{M} \cdot \mathbf{d}_{nm} \right| \Delta t \right)^{-1}$$

Advantages and disadvantages

- Advantages
  - Makes contact with surface hopping approach
  - Natural recovery of separate quantum and classical evolution
- Disadvantages
  - Systematic improvement difficult
  - Representation of coupled electron-ion system not available
  - Large number of trajectories required

Wavefunction propagation: ab initio multiple spawning (AIMS) technique

Represent full wavefunction as

$$\Psi(\mathbf{r},\mathbf{R}) = \sum_n \psi_n(\mathbf{r};\mathbf{R})\chi_n(\mathbf{R},t)$$

with each χ expanded as a sum of Gaussians:

Expansion coefficients

Phases

Exponents (fixed)

$$\chi_n(\mathbf{R},t) = \sum_{j=1}^{N_n(t)} C_{nj}(t)\chi_{nj}(\mathbf{R};\overline{\mathbf{R}}_{nj},\overline{\mathbf{P}}_{nj},\gamma_{nj},\alpha_{nj})$$

$$\chi_{nj}(\mathbf{R};\overline{\mathbf{R}}_{nj},\overline{\mathbf{P}}_{nj},\gamma_{nj},\alpha_{nj}) \sim \mathrm{e}^{\mathrm{i}\gamma_{nj}}\exp[-\alpha_{nj}(\mathbf{R}-\overline{\mathbf{R}}_{nj})^2+\mathrm{i}\overline{\mathbf{P}}_{nj}\cdot(\mathbf{R}-\overline{\mathbf{R}}_{nj})/\hbar]$$

Basis function position centres and momenta initially chosen from Wigner distribution and then propagated classically along with phases:

$$\partial_t\overline{\mathbf{R}}_{nj,I} = \frac{\overline{\mathbf{P}}_{nj,I}}{M_I}$$

$$\partial_t\overline{\mathbf{P}}_{nj,I} = \langle\psi_n(\mathbf{R})|\hat{\mathbf{F}}_{I,e}|\psi_n(\mathbf{R})\rangle + \mathbf{F}_{\mathrm{nuc},I}$$

$$\partial_t\gamma_{nj} = \sum_I \frac{\mathbf{P}_I^2}{2M_I} - [E_n(\overline{\mathbf{R}}_{nj}) + V_{\mathrm{ion}}(\overline{\mathbf{R}}_{nj})]$$

AIMS (2)

Propagate nuclear wavefunction expansion coefficients quantum mechanically from the Schrödinger equation:

$$\partial_t \mathbf{C}_n = -\mathrm{i}(S_n)^{-1}[(H_n - \mathrm{i}\dot{S}_n)\mathbf{C}_n + \sum_{m \neq n} H_{nm}\mathbf{C}_m]$$

$$S_{n,ij} = \langle \chi_{ni} | \chi_{nj} \rangle$$

$$\dot{S}_{n,ij} = \langle \chi_{ni} | \partial_t \chi_{nj} \rangle$$

$$H_{nm,ij} = \langle \chi_{ni} | \langle \psi_n | \hat{H} | \psi_m \rangle | \chi_{mj} \rangle$$

'Spawn' additional nuclear basis functions in order to represent new branches of the total wavefunction whenever

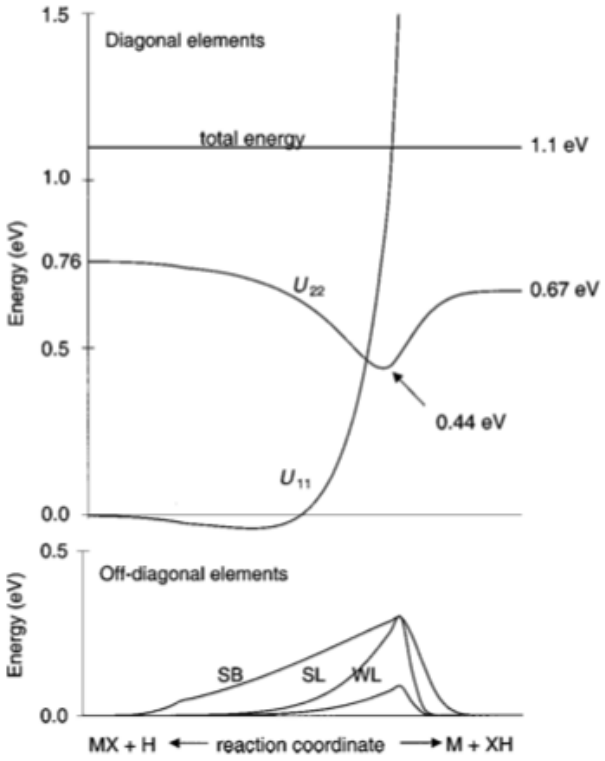
$$|\dot{\mathbf{R}} \cdot \mathbf{d}_{nm}|$$

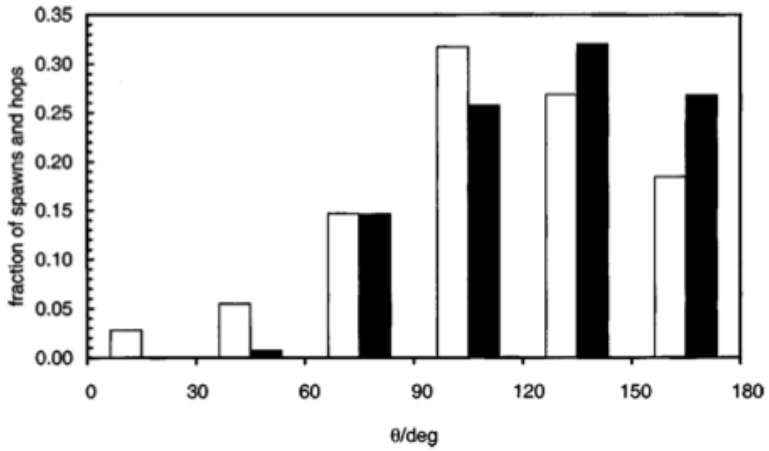
exceeds a chosen critical value

Ben-Nun and Martinez *Adv Chem Phys* **121** 439 (2002)

Example

Six-dimensional (three-atom, excluding COM) test calculation with two electronic states



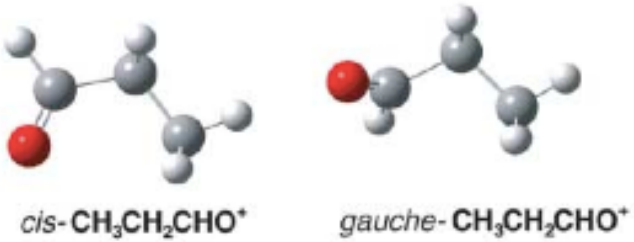


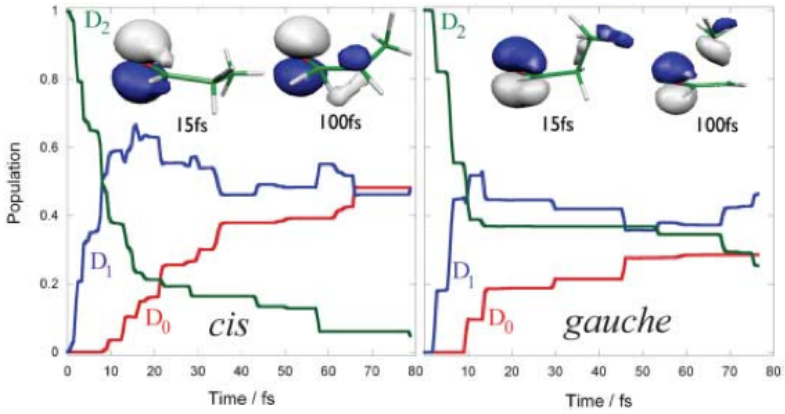
Trajectory spawnings occur in same region as surface hops

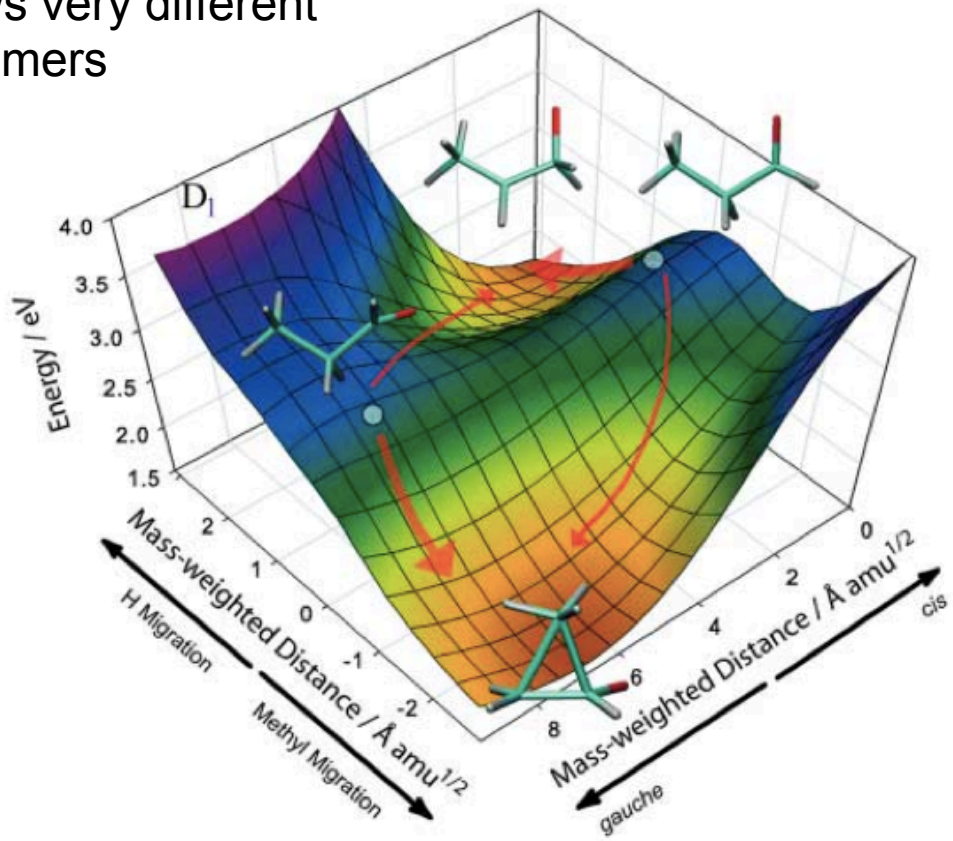
Hack *et al. J Chem Phys* **115** 1172 (2001)

Example (2)

Propanal cation CH_3-CH_2-CHO^+ shows very different dissociation dynamics for different isomers







Kim *et al.* Science **315** 1561 (2007)

Advantages and disadvantages

- Advantages
  - Explicit treatment of electron/nuclear correlations
  - Spawning focuses computational effort in regions of large non-adiabatic coupling
- Disadvantages
  - Large number of nonorthogonal nuclear basis functions required, separate solution of electronic problem along each trajectory
  - Many parameters to tune/set

Beyond Ehrenfest? Two classes of method

- Methods based on Born-Oppenheimer surfaces
  - Surface hopping
  - ‘Frozen gaussians’ and ‘ab initio quantum molecular dynamics’
- Methods based on semiclassical expansions for equations of motion or correlation functions
  - Mixed quantum-classical dynamics
  - (Ring polymer dynamics)

Aims of method – the CEID idea

- Retain
  - Correlations between electrons and nuclei
  - The idea of making expansion about the Ehrenfest trajectory
- Avoid
  - Giving preferred role to adiabatic (Born-Oppenheimer) states
  - Making assumptions about loss of phase coherence with time

Aside – two types of decoherence

A superposition such as

$$|\Psi\rangle = \sum_n c_n(t)|\psi_n(\overline{\mathbf{R}}_n)\rangle \otimes |\chi(\overline{\mathbf{R}}_n)\rangle$$

does not correspond to a pure state of either ions or electrons; e.g. if different χ states are orthogonal,

$$\hat{\rho}_\mathrm{e} = \mathrm{Tr}_\mathrm{e}|\Psi\rangle\langle\Psi| = \sum_n |c_n(t)|^2 |\psi_n(\overline{\mathbf{R}}_n)\rangle\langle\psi_n(\overline{\mathbf{R}}_n)|$$

Decoherence of electron system through its interaction with the ions

In addition the entire density operator

$$|\Psi\rangle\langle\Psi| = \left[\sum_n c_n(t)|\psi_n(\overline{\mathbf{R}}_n)\rangle \otimes |\chi(\overline{\mathbf{R}}_n)\rangle\right]\left[\sum_m c_m^*(t)\langle\psi_m(\overline{\mathbf{R}}_m)| \otimes \langle\chi(\overline{\mathbf{R}}_m)|\right]$$

will tend to decay as a result of interactions with the wider environment:

$$|\Psi\rangle\langle\Psi| \rightarrow \sum_n |c_n(t)|^2 |\psi_n(\overline{\mathbf{R}}_n)\rangle\langle\psi_n(\overline{\mathbf{R}}_n)| \otimes |\chi(\overline{\mathbf{R}}_n)\rangle\langle\chi(\overline{\mathbf{R}}_n)|$$

Decoherence of entire simulation system through interactions with the rest of the world

CEID moments – concepts and equations

Expand the full Hamiltonian to second order in the nuclear displacements about the instantaneous **R** and **P**:

$$\hat{H} \approx \hat{H}_{\mathrm{e,eff}}(\overline{\mathbf{R}}) + \sum_I \frac{1}{2M_I}\left[\overline{\mathbf{P}}_I^2 + 2\overline{\mathbf{P}}_I \cdot \Delta\hat{\mathbf{P}}_I + (\Delta\hat{\mathbf{P}}_I)^2\right] - \sum_I \hat{\mathbf{F}}_I(\overline{\mathbf{R}}) \cdot \Delta\hat{\mathbf{R}}_I + \sum_{IJ} \hat{K}_{IJ}(\overline{\mathbf{R}})\Delta\hat{\mathbf{R}}_I\Delta\hat{\mathbf{R}}_J$$

NOT a usual harmonic approximation because **F** and *K* depend on **R** and **P**

Retain correlations between electrons and ions by evolving moments of the fluctuations Δ**R** and Δ**P** along the Ehrenfest trajectory:

$$\overline{F} = \mathrm{Tr}_e\left[\hat{\rho}_e \hat{F}_{el}(\overline{R})\right] - \sum_J \mathrm{Tr}_e\left[\hat{K}_{IJ}\hat{\mu}_J\right]$$

$$\mathrm{i}\hbar\frac{\partial\hat{\rho}_e}{\partial t} = \left[\hat{H}_e(\overline{R}), \hat{\rho}_e\right] - \sum_I \left[F_{el}(\overline{R}), \hat{\mu}_I\right]$$

$$\mathrm{i}\hbar\frac{\mathrm{d}\hat{\mu}_I}{\mathrm{d}t} = \left[\hat{H}_e\left(\overline{R}\right), \hat{\mu}_I\right] + \mathrm{i}\hbar\frac{\hat{\lambda}_I}{M_I}$$

$$\mathrm{i}\hbar\frac{\mathrm{d}\hat{\lambda}_I}{\mathrm{d}t} = \left[\hat{H}_e\left(\overline{R}\right), \hat{\lambda}_I\right] + \frac{\mathrm{i}\hbar}{2}\left\{\Delta\hat{F}, \hat{\rho}_e\right\} - \frac{\mathrm{i}\hbar}{2}\sum_J\left\{\hat{K}_{IJ}, \hat{\mu}_J\right\}$$

with $\hat{\rho}_e \equiv \mathrm{Tr}_I\left[\hat{\rho}(t)\right]$ and

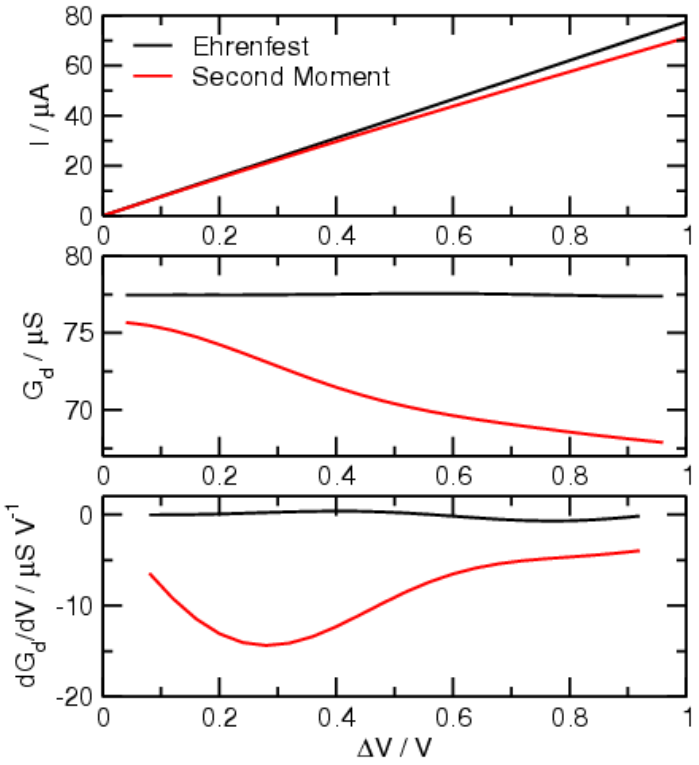
$$\hat{\mu}_I \equiv \mathrm{Tr}_I\left[\hat{X}_I\hat{\rho}\right]$$

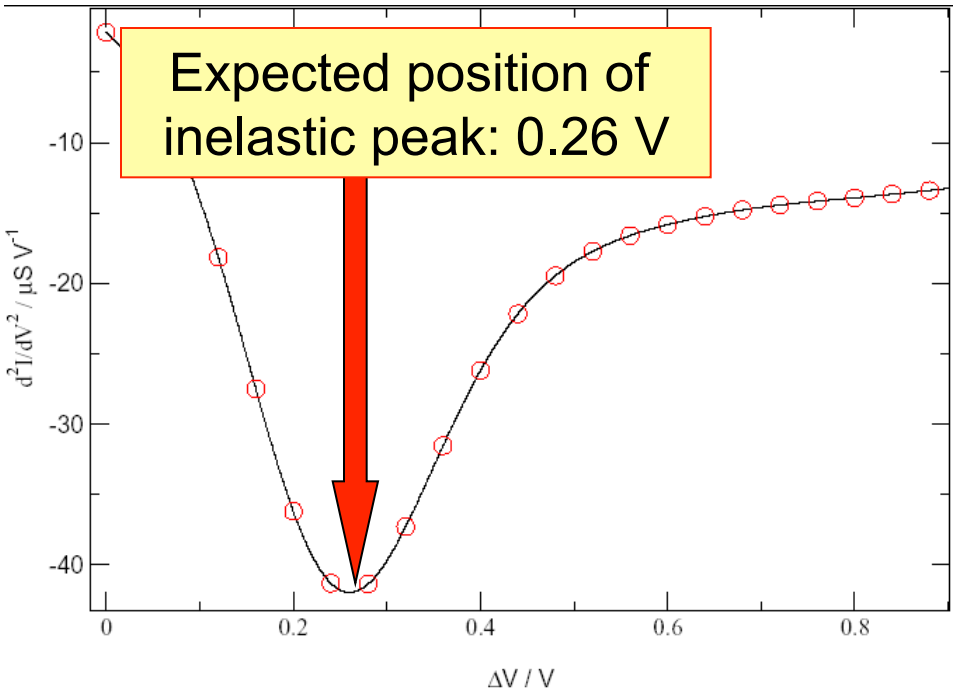
$$\hat{\lambda}_I \equiv \mathrm{Tr}_I\left[\hat{P}_I\hat{\rho}\right]$$

$$\Delta\hat{F}_I \equiv \hat{F}_I - \overline{F}$$

Example – inelastic Spectroscopy

Even though it starts from a *classical* path, CEID (at first moment level) already contains the standard selection rules for electron-phonon scattering and hence enough information to describe IETS





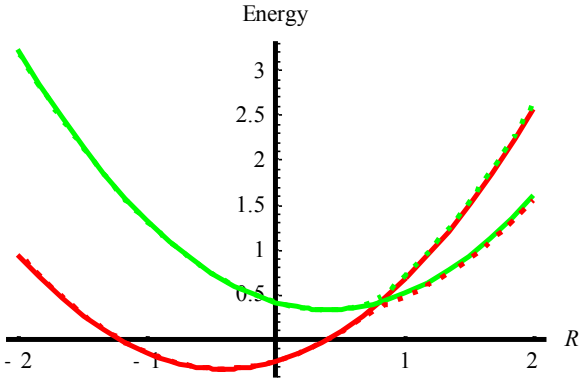
Sanchez, Todorov, Horsfield

When moments are not enough

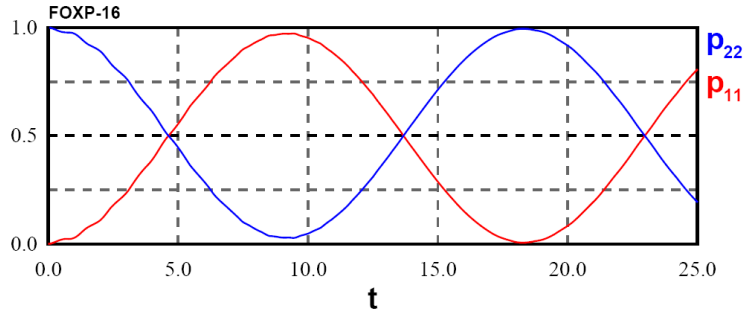
- Problem: difficult to describe situations in which electron state is strongly coupled to a small number of vibrational degrees of freedom
  - Manifests itself in poor convergence
- Reason: a broad probability distribution is not necessarily well described by its moments:

A simple strongly coupled system - example

Occupation probabilities for ground and excited states in case where potential surfaces have an avoided crossing:

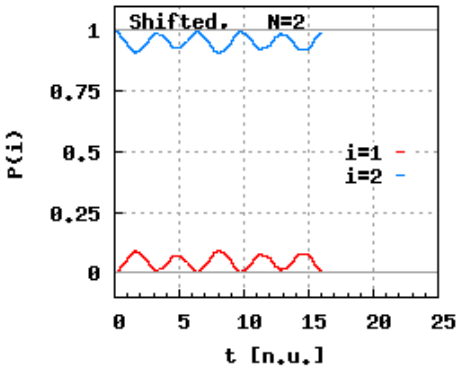


Exact results for occupation probabilities:

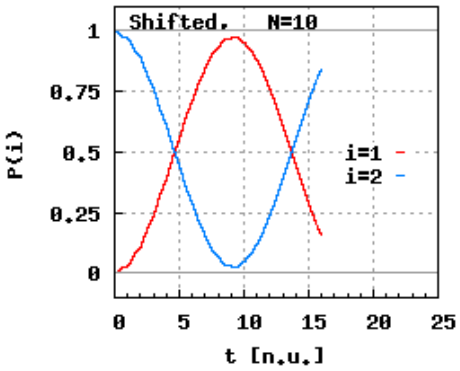


CEID results:

N=2



N=10



CEID with a basis

Alternative idea: construct an explicit representation of the full density operator in an orthonormal nuclear basis

$$\hat{\rho} = \sum_{m,n} |m\rangle \hat{\rho}_{mn} \langle n|$$

where

$$\hat{\rho}_{mn} = \langle m|\hat{\rho}|n\rangle$$

is still an operator on the electronic degrees of freedom

Similarly for operators:

$$\hat{O} = \sum_{m,n} |m\rangle \hat{O}_{mn} \langle n|$$

For electronic operators: $\hat{O}_{mn} = \hat{O}_{\mathrm{e}} \delta_{mn}$

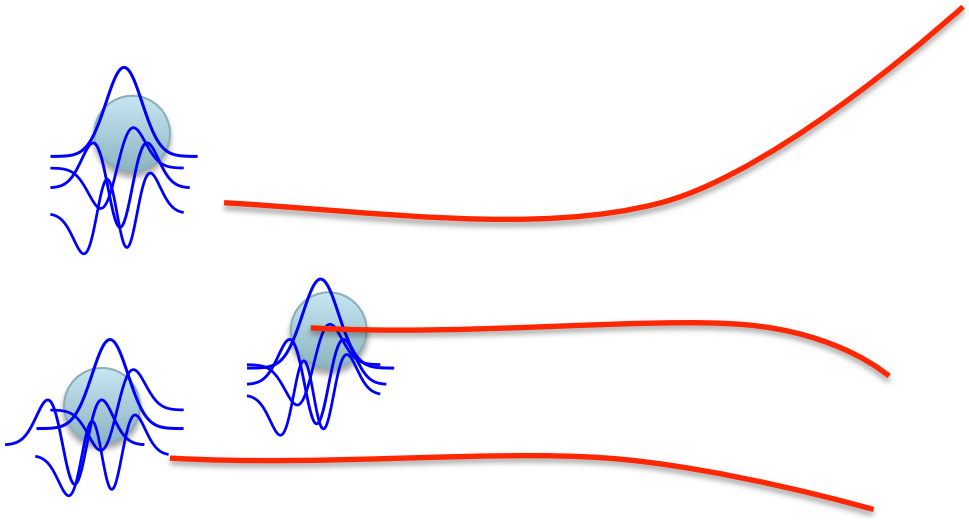
For nuclear operators: $\hat{O}_{mn} \propto \hat{1}_{\mathrm{e}}$

Choosing the basis set

In the full basis-set limit corresponds to an exact solution of the coupled electron-nuclear problem, and is therefore exponentially hard.

Q: How can we avoid exponential scaling and make use of the semi-classical nature of the nuclei?

A: Move the basis with the Ehrenfest trajectory, in order to represent the fluctuations about it



$$|n\rangle = |n(\overline{\mathbf{R}})\rangle$$

$$\hat{\rho}_{mn} = \hat{\rho}_{mn}(\overline{\mathbf{R}})$$

Transforming to the co-moving frame

Corresponds to transformation to an effective Lagrangian coordinate system

$$\Delta\hat{\mathbf{R}}(t) = \hat{\mathbf{R}} - \overline{\mathbf{R}}(t)$$
$$\Delta\hat{\mathbf{P}}(t) = \hat{\mathbf{P}} - \overline{\mathbf{P}}(t)$$

Transformation defined by the unitary operation

$$\hat{U}(\overline{\mathbf{R}}, \overline{\mathbf{P}}) = \exp[(\overline{\mathbf{R}}\hat{\mathbf{P}} - \overline{\mathbf{P}}\hat{\mathbf{R}})/\mathrm{i}\hbar]$$

So for a general operator

$$\hat{O}_L(\overline{\mathbf{R}}, \overline{\mathbf{P}}) = \hat{U}^\dagger(\overline{\mathbf{R}}, \overline{\mathbf{P}})\hat{O}\hat{U}(\overline{\mathbf{R}}, \overline{\mathbf{P}})$$

Position and spatial components commute, so a classical transformation

Constructing the basis

Begin with a Gaussian wavepacket of width α centered at each atomic site:

$$|0\rangle = C \prod_{i=1}^{3N} \exp\left[-\alpha_i^2 (R_i - \overline{R}_i)^2/4\right]$$

Define a set of modes (in principle arbitrary but in practice normal modes of a reference geometry are often the best choice)

$$\Delta\hat{\eta}_\alpha(t) = \sum_\beta U_{\alpha\beta} \Delta\hat{R}_\beta(t) \qquad \Delta\hat{\zeta}_\alpha(t) = \sum_\beta U^*_{\alpha\beta} \Delta\hat{P}_\beta(t)$$

and define annihilation and creation operator algebra

$$\Delta\hat{\eta}_\alpha(t) = \frac{\mathrm{i}}{\sqrt{2}} b_\alpha (\hat{a}_\alpha - \hat{a}^\dagger_\alpha) \qquad \Delta\hat{\zeta}_\alpha(t) = \frac{1}{\sqrt{2}} a_\alpha (\hat{a}_\alpha + \hat{a}^\dagger_\alpha)$$

Length and momentum scales obeying

$$a_\alpha b_\alpha = \hbar$$

Constructing the basis (2)

Then construct the CEID basis as

$$|n_1, n_2, \ldots n_{3N}\rangle = \prod_{i=1}^{3N} \frac{(\hat{a}^\dagger_{\alpha_i})^{n_i}}{\sqrt{n_i!}} |0\rangle$$

truncating at a maximum number of excitations

$$\sum_i n_i = N_{\mathrm{CEID}}$$

Exact in the limit $N_{\mathrm{CEID}} \to \infty$

In practice optimize by choosing *a* and *b* to minimize the quadratic energy and choosing a finite *N*

Equations of motion

Nuclear kinetic energy (Δn, Δm=0 or 2)

Ehrenfest Hamiltonian

$$\dot{\rho}_{n,m} = -\frac{1}{4M_0\imath\hbar}\sum_\alpha b_\alpha^2\left[\sqrt{(n_\alpha+2)(n_\alpha+1)}\rho_{n+2_\alpha,m} - (2n_\alpha+1)\rho_{n,m} + \sqrt{n_\alpha(n_\alpha-1)}\rho_{n-2_\alpha,m}\right.$$

$$\left. -\sqrt{m_\alpha(m_\alpha-1)}\rho_{n,m-2_\alpha} + (2m_\alpha+1)\rho_{n,m} - \sqrt{(m_\alpha+2)(m_\alpha+1)}\rho_{n,m+2_\alpha}\right] + \frac{1}{\imath\hbar}[H_e(\bar{\zeta}),\rho_{n,m}]$$

$$-\frac{1}{\sqrt{2}\imath\hbar}\sum_\alpha a_\alpha[\Delta\tilde{F}_\alpha(\bar{\zeta})(\sqrt{n_\alpha+1}\rho_{n+1_\alpha,m} + \sqrt{n_\alpha}\rho_{n-1_\alpha,m}) - (\sqrt{m_\alpha}\rho_{n,m-1_\alpha} + \sqrt{m_\alpha+1}\rho_{n,m+1_\alpha})\Delta\tilde{F}_\alpha(\bar{\zeta})]$$

Fluctuations producing nuclear forces (gradient of Hamiltonian)

$$,m + (2n_\alpha+1)\rho_{n,m} + \sqrt{n_\alpha(n_\alpha-1)}\rho_{n-2_\alpha,m})$$

$$-(\sqrt{m_\alpha(m_\alpha-1}\quad\quad \bar{\zeta})]$$

Note presence of *electronic* operators (i.e. changing the electronic evolution) arising from coupling to the dynamics of the *nuclei*

Quadratic flu ,m

mode

$$+\sqrt{n_\alpha(n_\beta+1)}\rho_{n-1_\alpha+1_\beta,m} + \sqrt{n_\alpha n_\beta}\rho_{n-1_\alpha-1_\beta,m}) - (\sqrt{m_\alpha m_\beta}\rho_{n,m-1_\alpha-1_\beta} + \sqrt{m_\alpha(m_\beta+1)}\rho_{n,m-1_\alpha+1_\beta}$$

$$+\sqrt{(m_\alpha+1)m_\beta}\rho_{n,m+1_\alpha-1_\beta} + \sqrt{(m_\alpha+1)(m_\beta+1)}\rho_{n,m+1_\alpha+1_\beta})\tilde{K}_{\alpha,\beta}(\bar{\zeta})],$$

Quadratic fluctuations in different modes

Notes

(a) In the limit $N_{\mathrm{CEID}} \to \infty$

get an exact solution of the coupled electron-nuclear problem

(b) In the case $N_{\mathrm{CEID}} = 0$

recover an Ehrenfest-like calculation

Relation to moment expansion

Can recover a simple relation to the previous (moment expansion) version of CEID:

$$\hat{\mu}_{n,m}(t) = \frac{1}{2\pi\hbar}\int \mathrm{d}\mathbf{P}\mathrm{d}\mathbf{R}\Delta R^n \Delta P^m \hat{\rho}_W(R,P) = \sum_{kl} A_{kl}^{n,m}\hat{\rho}_{kl}$$

where $$A_{kl}^{n,m} \equiv \frac{1}{2^n}\sum_{r=0}^{n}\binom{n}{r}\langle k|(\Delta\hat{R})^r(\Delta\hat{P})^m\Delta\hat{R}^{(n-r)}|l\rangle$$

These quantities can be simply evaluated via recurrence relations to give, for example

$$\hat{\mu}_{1,0} = a_0\sum_n \sqrt{\frac{n}{2}}[\hat{\rho}_{n,n-1} + \hat{\rho}_{n-1,n}]$$

$$\hat{\mu}_{0,1} = -\mathrm{i}b_0\sum_n \sqrt{\frac{n}{2}}[\hat{\rho}_{n,n-1} + \hat{\rho}_{n-1,n}]$$

Scaling of CEID

Dimension of the Hilbert space needed to describe the ions:

$$D_I = \sum_{i=0}^{N_{\mathrm{CEID}}} \begin{pmatrix} i + N_C - 1 \\ i \end{pmatrix} = \begin{pmatrix} N_C + N_{\mathrm{CEID}} \\ N_C \end{pmatrix}$$

In the highly quantum limit for all modes $N_{\mathrm{CEID}} \gg N_C$

Effort is $$\frac{1}{N_C} \left(\frac{N_{\mathrm{CEID}}}{N_C} \right)^{2N_C}$$

Exponential scaling

For a minority of highly quantum modes $N_C \gg N_{\mathrm{CEID}}$

Effort is $$\frac{1}{N_{\mathrm{CEID}}} \left(\frac{N_C}{N_{\mathrm{CEID}}} \right)^{2N_{\mathrm{CEID}}}$$

Polynomial scaling of degree $2N_{\mathrm{CEID}}$

Advantages and disadvantages

- Advantages
  - Representation of full coupled electron-nuclear state
  - No special status to B-O states
  - Systematically improvable
  - Does not rely on decoherence from outside
  - Possible to treat different degrees of freedom to different accuracy

- Disadvantages
  - Not compatible with TDDFT in its present form
  - No thermostat yet
  - Scaling becomes worse as accuracy increased

Thanks to…

- Imperial
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  - Euan McInery
- UCL
  - David Bowler
  - Rafael Miranda
  - Lorenzo Stella
- EPSRC (£s)

Tchavdar Todorov (Belfast)

Andrew Horsfield (formerly UCL, now Imperial College)