Quantum Dynamics Methods for Molecular Excited States: MCTDH and beyond

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The Nuclear Schrödinger Equation

Aim: To solve the Time-dependent Schrödinger Equation for nuclei.

In the **Adiabatic picture** TDSE is:

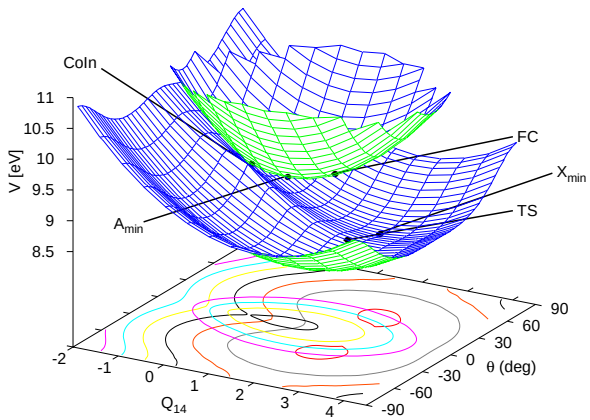
$$(\hat{T}_n + V_j) \mid \psi_j\rangle - \sum_i \hat{\Lambda}_{ji} \mid \psi_i\rangle = i\hbar \frac{\partial}{\partial t} \mid \psi_j\rangle$$

and the wavefunction moves over an *adiabatic* potential energy surface, V, obtained from quantum chemistry calculations. Non-adiabatic couplings $\hat{\Lambda}$ are singular at a conical intersection.

In the **Diabatic picture** TDSE is:

$$\left[\hat{T}_n \mathbf{1} + \mathbf{W}\right] \boldsymbol{\psi} = i\hbar \frac{\partial}{\partial t} \boldsymbol{\psi}$$

where $\mathbf{W}$ is a matrix of potential surfaces and couplings and $\boldsymbol{\psi}$ a vector of wavepackets.



Worth and Cederbaum, Ann. Rev. Phys. Chem., (04) **55**: 127

Propagating wavepacket: The Standard Method

Nuclear wavefunction expanded in primitive basis set:

$$\Psi(q_1, \ldots q_f, t) = \sum_{j_1=1}^{N_1} \cdots \sum_{j_p=1}^{N_f} A_{j_1 \ldots j_f}(t)\, \chi_{j_1}^{(1)}(q_1) \cdots \chi_{j_f}^{(f)}(q_f)$$

Use Dirac-Frenkel Variational Principle:

$$\left\langle \delta\Psi \middle| H - i\frac{\partial}{\partial t} \middle| \Psi \right\rangle = 0$$

to obtain equations of motion for A:

$$i\dot{A}_{j_1 \ldots j_f} = \sum_L \langle \chi_{j_1}^{(1)}(q_1) \cdots \chi_{j_f}^{(f)}(q_f) | H | \chi_{l_1}^{(1)}(q_1) \cdots \chi_{l_f}^{(f)}(q_f) \rangle A_{l_1 \ldots l_f}$$

Kulander “Time-dependent methods for quantum dynamics”, Elsevier, 1991

Kosloff, Ann. Rev. Phys. Chem. (94) **45**: 145

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$$i\dot{\mathbf{A}} = \mathbf{HA}$$

Kulander "Time-dependent methods for quantum dynamics", Elsevier, 1991

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The Hamiltonian matrix elements

Need to evaluate matrix elements (integrals)

$$\begin{aligned} H_{JL} &= \sum_{\ell_1,\ldots\ell_f} \langle \chi^{(1)}_{j_1} \cdots \chi^{(f)}_{j_f} | H | \chi^{(1)}_{\ell_1} \cdots \chi^{(f)}_{\ell_f} \rangle \\ &= \sum_{\ell_1,\ldots\ell_f} \langle \chi^{(1)}_{j_1} \cdots \chi^{(f)}_{j_f} | T + V | \chi^{(1)}_{\ell_1} \cdots \chi^{(f)}_{\ell_f} \rangle \end{aligned}$$

As written an $N^f \times N^f$ matrix of multi-dimensional integrals!

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As written an $N^f \times N^f$ matrix of multi-dimensional integrals!

Use a *Discrete Variable Representation* (DVR) or *collocation* (FFT) to reduce effort

- KEO low dimensional integrals using analytic basis / FFT
- PEO diagonal on spatial grid - N^f points
- DVR equates to Gaussian quadrature of integrals

The Multiconfigurational Time-Dependent Hartree (MCTDH) Method

$$\Psi(q_1,\ldots,q_f,t) = \sum_{j_1=1}^{n_1}\ldots\sum_{j_f=1}^{n_f} A_{j_1\ldots j_f}(t)\prod_{\kappa=1}^{f}\varphi_{j_\kappa}^{(\kappa)}(q_\kappa,t)$$

Variational equations of motion for A and φ.

$$\begin{aligned} i\dot{A}_J &= \sum_L \langle\Phi_J|H|\Phi_L\rangle A_L \\ i\dot{\varphi}^{(\kappa)} &= \left(1-P^{(\kappa)}\right)\left(\rho^{(\kappa)}\right)^{-1}\langle\mathbf{H}\rangle^{(\kappa)}\varphi^{(\kappa)} \end{aligned}$$

- non-linear equations of motion
- Computer memory $n^f + fnN$

SPFs expanded in *primitive grid*

$$\varphi_j = \sum_{i=1}^{N} a_{ij}\chi_i$$

Beck *et al* Phys. Rep. (00) 324:1

Meyer, Gatti and Worth "Multidimensional quantum dynamics", Wiley-VCH, 2009

time-dependent matrix elements

$$H_{JL} = \langle \Phi_J | H | \Phi_L \rangle = \langle \phi_{j_1}^{(1)} \dots \phi_{j_f}^{(f)} | H | \phi_{l_1}^{(1)} \dots \phi_{l_f}^{(f)} \rangle$$

- for efficiency need product potential $V = \sum_s c_s h_s^{(1)} h_s^{(2)} \dots$

$$\langle \Phi_I | H | \Phi_J \rangle = \sum_s c_s \langle \varphi_{i_1}^{(1)} | h^{(1)} | \varphi_{j_1}^{(1)} \rangle \langle \varphi_{i_2}^{(2)} | h^{(2)} | \varphi_{j_2}^{(2)} \rangle \dots$$

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Using *single-hole functions*,

$$\psi_{k_f}^{(f)} = \sum_{j_1=1}^{n_1} \dots \sum_{j_{f-1}=1}^{n_{f-1}} A_{j_1 \dots j_{f-1} k_f}(t) \prod_{\kappa=1}^{f-1} \varphi_{j_\kappa}^{(\kappa)}(q_\kappa, t)$$

mean-field operators

$$\langle H \rangle_{ij}^{(\kappa)} = \langle \psi_{i_\kappa}^{(\kappa)} | H | \psi_{j_\kappa}^{(\kappa)} \rangle$$

and density matrices

$$\rho_{ij}^{(\kappa)} = \langle \psi_{i_\kappa}^{(\kappa)} | \psi_{j_\kappa}^{(\kappa)} \rangle = \sum_J A_{J_i^\kappa}^* A_{J_j^\kappa}$$

Routes to Higher Dimensionality.

First bottleneck to larger systems is no. of configurations n^f

Strategies:

I Combined Mode Particles
II Selected-CI
III Cascading / Multi-layer
IV Parametrized Spfs

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- High-Dimensional Cluster Model
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B GROW
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I. Combined Mode Particles

Re-write MCTDH ansatz

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A “particle” may contain more than one coordinate,
$Q_i = (q_a, q_b, \ldots, q_w)$

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A "particle" may contain more than one coordinate,
$Q_i = (q_a, q_b, \ldots, q_w)$

e.g.

$$\begin{aligned}\Psi(q_1,q_2,q_3,t) &= \sum_{j_1}\sum_{j_2} A_{j_1 j_2}(t)\;\varphi_{j_1}^{(1)}(q_1,t)\;\varphi_{j_2}^{(2)}(q_2,q_3,t)\\ &= \sum_{j_1}\sum_{j_2} A_{j_1 j_2}(t)\;\varphi_{j_1}^{(1)}(Q_1,t)\;\varphi_{j_2}^{(2)}(Q_2,t)\end{aligned}$$

Saving in memory

All 1D functions

$$Mem \sim n^f + fnN$$

Now combine d modes in each particle.
$p = \frac{f}{d}$ particles with grid lengths of N^d
If $\tilde{n} \leq n^d$ save memory.

$$Mem \sim \tilde{n}^p + p\tilde{n}N^d$$

If $d = f$, then full-grid used and $\tilde{n} = 1$

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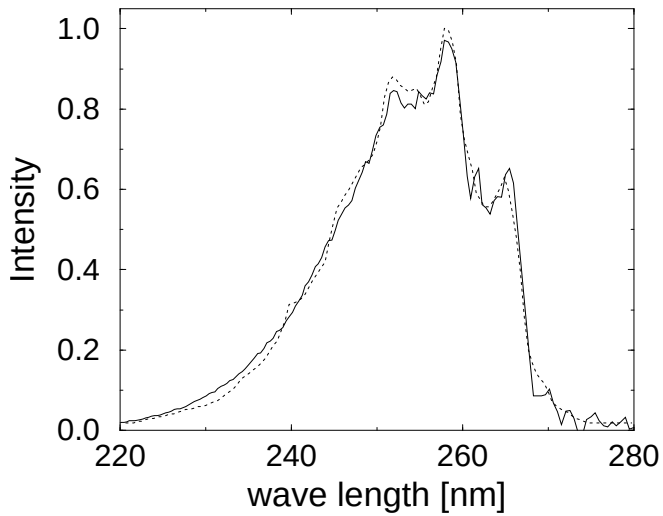
$$Mem \sim N^f$$

Result: MCTDH can treat ca 30 modes

Bench Mark: Pyrazine Spectrum



- full 24D QD
- 650 MB
  (205 MB good result)
- ca 2×10^{22} MB for "standard"

Raab *et al* JCP (99) 110: 936

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Multi-Layer MCTDH (ML-MCTDH)

Expand a multi-mode SPF in an MCTDH expansion to create layers:

$$\Psi(q_1,\ldots,q_f,t) = \sum_{j_1=1}^{n_1}\cdots\sum_{j_p=1}^{n_p} A_{j_1\ldots j_p}(t)\prod_{\kappa=1}^{p}\varphi_{j_\kappa}^{(\kappa)}(Q_\kappa,t) \qquad \text{Layer 1}$$

$$\varphi_{j_\kappa}^{(\kappa)}(Q_\kappa,t) = \sum_{k_1=1}^{n_1}\cdots\sum_{k_Q=1}^{n_Q} B_{k_1\ldots k_Q}^{\kappa,j_\kappa}(t)\prod_{\nu=1}^{Q}\nu_{k_\nu}^{(\nu)}(R_\nu,t) \qquad \text{Layer 2}$$

$$\nu_{k_\nu}^{(\nu)}(R_\nu,t) = \sum_{l_1=1}^{n_1}\cdots\sum_{l_R=1}^{n_R} C_{l_1\ldots l_R}^{\nu,k_\nu}(t)\prod_{\xi=1}^{R}\xi_{l_\xi}^{(\xi)}(S_\xi,t) \qquad \text{Layer 3}$$

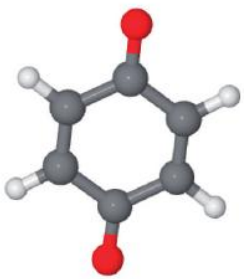
$$\ldots = \ldots$$

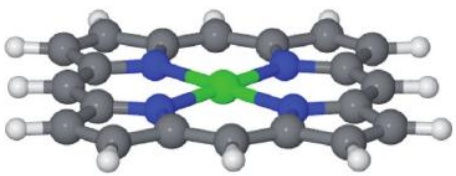
Each layer acts as a set of SPFs for the layer above and a set of coeficients for the layer below.

Leads to a recursive sets of variational equations of motion:

Wang and Thoss JCP (2003) **119**; 1289

$$
\begin{aligned}
i\dot{A}_J &= \sum_L \langle \Phi_J | H | \Phi_L \rangle A_L \\
i\dot{\varphi}^{(\kappa)} &= \left(1 - P^{(\kappa)}\right) \left(\rho^{(\kappa)}\right)^{-1} \langle \mathbf{H} \rangle^{(\kappa)} \varphi^{(\kappa)} \\
i\dot{\nu}^{(\nu)} &= \left(1 - P^{(\nu)}\right) \left(\rho^{(\nu)}\right)^{-1} \langle \mathbf{H} \rangle^{(\nu)} \nu^{(\nu)} \\
\ldots &= \ldots
\end{aligned}
$$

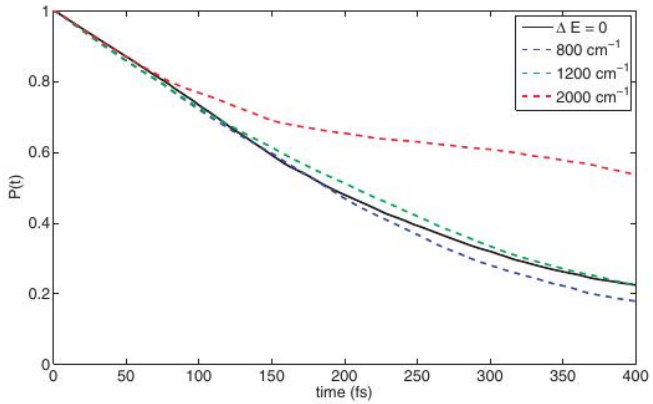




Borelli *et al* Mol. Phys. (2012) 110: 751

135 Mode Quantum Dynamics

Photo-induced ET. Spin-Boson Model.



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A Simple Hamiltonian: The Vibronic Coupling Model

Assume diabatic basis: $\Psi(\mathbf{Q},\mathbf{r}) = \sum_\alpha \phi_\alpha(\mathbf{Q})\psi_\alpha(\mathbf{r};\mathbf{Q})$

$$\mathbf{H}(\mathbf{Q}) = \mathbf{T}(\mathbf{Q}) + \mathbf{W}(\mathbf{Q})$$

$$\hat{T}_\alpha + V^0_\alpha = \frac{\omega_i}{2}\left(\frac{\partial^2}{\partial Q^2} + Q^2\right)$$

$$\begin{aligned} W_{\alpha\beta} &= \langle\psi_\alpha|H_{el}|\psi_\beta\rangle \\ W_{\alpha\beta} &\approx V^0_\alpha\delta_{\alpha\beta} + \varepsilon_\alpha + \sum_i \frac{\partial}{\partial Q_i}\langle\psi_\alpha|H_{el}|\psi_\beta\rangle\, Q_i + \ldots \end{aligned}$$

Köppel *et al* Adv. Chem. Phys. (1984) **57**: 59

Worth *et al*, Int. Rev. Phys. Chem. (08) **27**: 569

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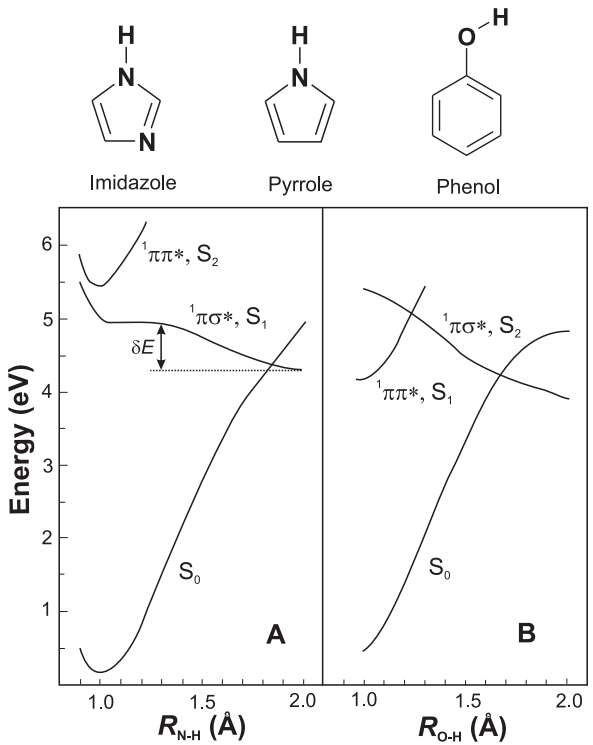
$$\kappa_i, \lambda_i \neq 0 \quad \textit{if} \quad \Gamma_\alpha \times \Gamma_i \times \Gamma_\beta \supseteq A_1$$

Köppel *et al* Adv. Chem. Phys. (1984) **57**: 59

Worth *et al*, Int. Rev. Phys. Chem. (08) **27**: 569

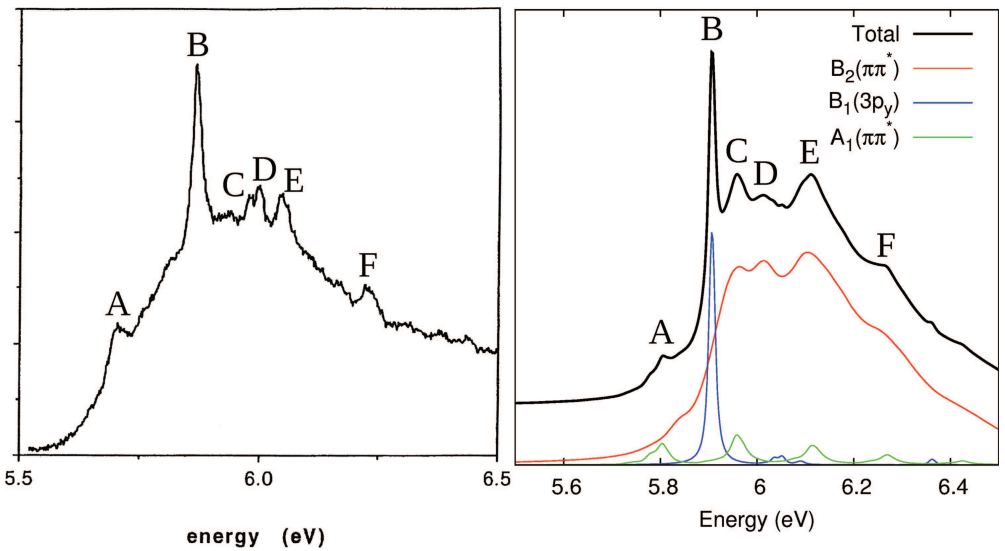
Heteroaromatic Photodissociation

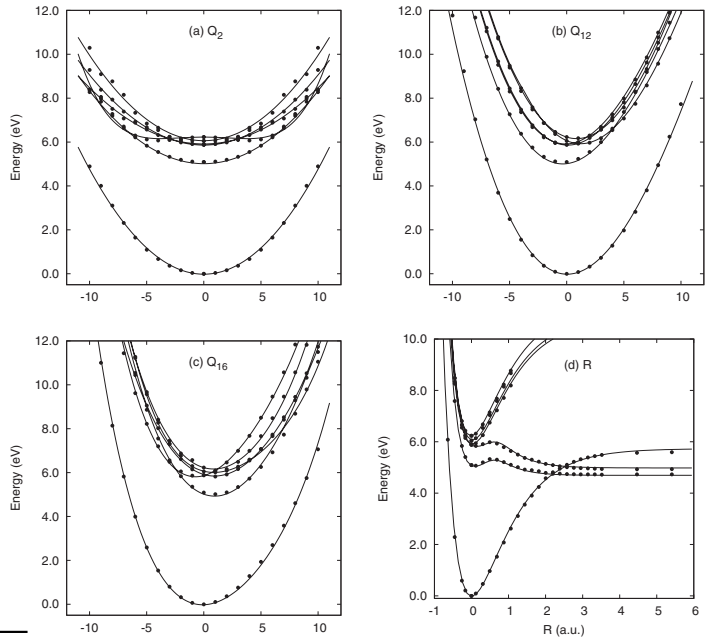


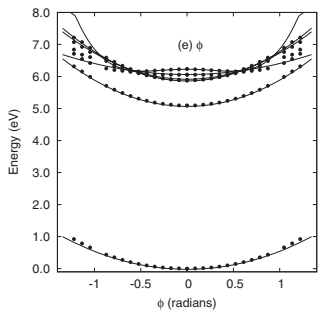
Ashfold *et al* Science (06) **312**: 1637

Excitation to $\pi\pi^*$ states
Dissociation after crossing to $\pi\sigma^*$ states

Electronic Absorption Spectrum of Pyrrole







Symmetry	Character	CASSCF	CASPT2
A_1		0.00	0.00
A_2	$3s/\pi\sigma^*$	4.17	5.06
B_1	$3s/\pi\sigma^*$	4.87	5.86
A_2	$3p_z$	4.91	5.87
A_1	$\pi\pi^*$	6.47	6.01
B_2	$\pi\pi^*$	7.83	6.24
B_1	$3p_z$	5.67	6.69

S.P. Neville & G.A. Worth, JCP, 2014, **140**, 034317

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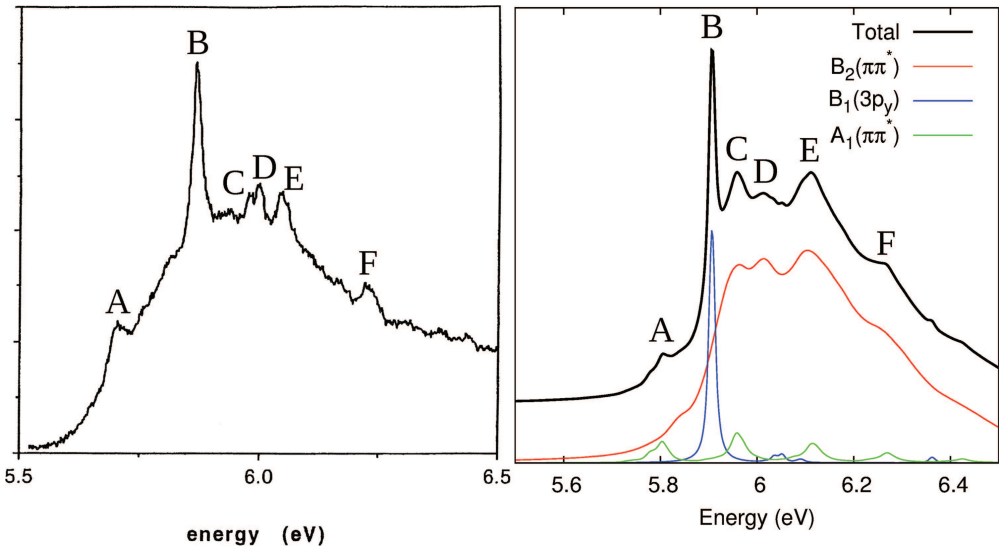
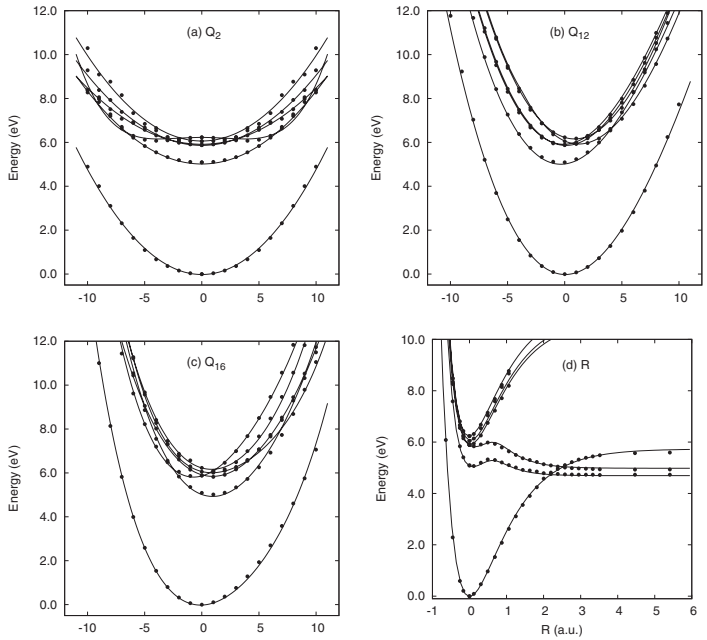
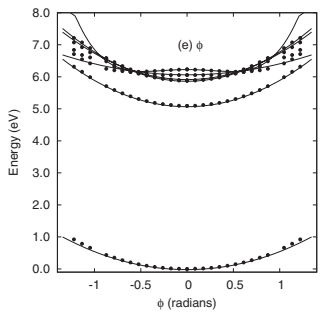






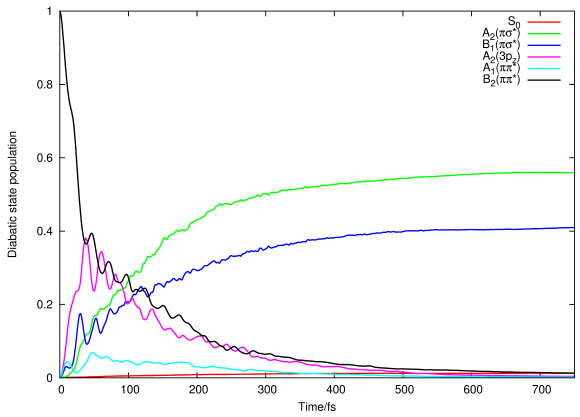
- 6-state, 9-mode model.
- Strong vibronic coupling between states.
- Contribution from excitation to three states.
- Intensity borrowing allows excitation to lower lying Rydberg states.

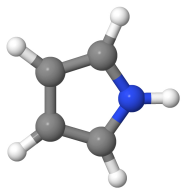
S.P. Neville & G.A. Worth, JCP, 2014, **140**, 034317

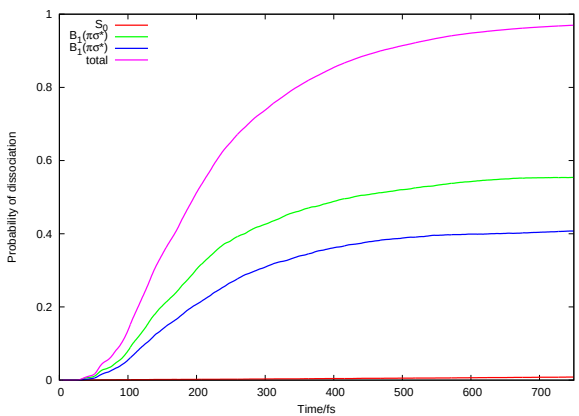
Pyrrole: 6-State 9(10)-Mode Model

Ignoring ν_2

State populations







Flux

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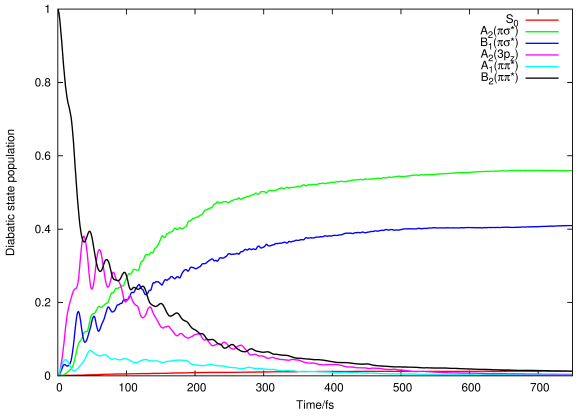
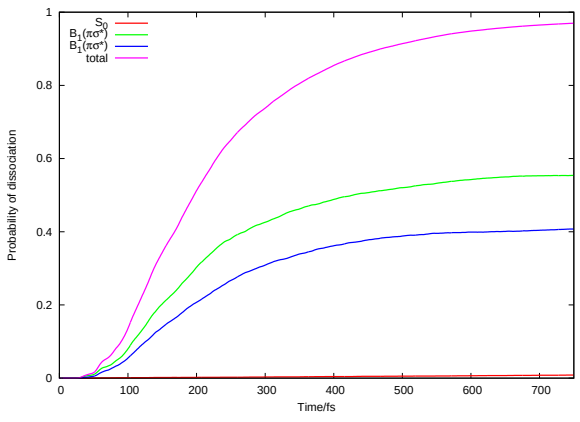
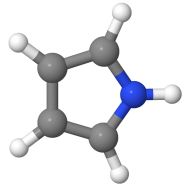
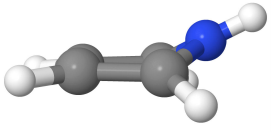
State populations





Flux

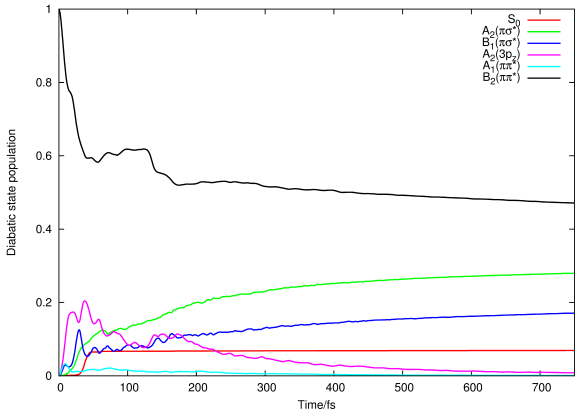


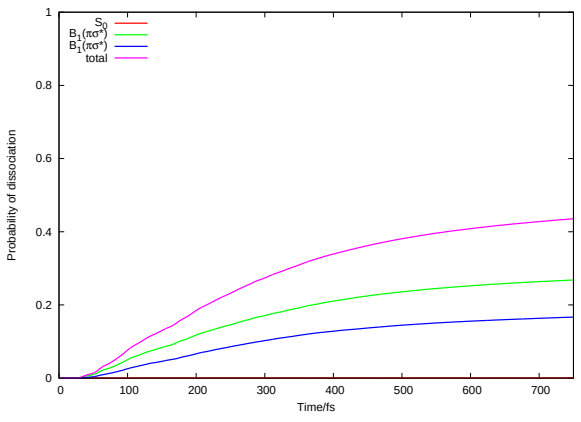


"Trapped"
"Geometry"

Including ν_2

State populations





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C Direct Dynamics

IV. Parametrized Spfs (G-MCTDH)

$$\Psi(Q_1,\ldots,Q_f,t)=\sum_{j_1=1}^{n_1}\ldots\sum_{j_p=1}^{n_f}A_{j_1\ldots j_p}(t)\prod_{\kappa=1}^{p-n}\varphi_{j_\kappa}^{(\kappa)}\prod_{\kappa=n+1}^{p}g_{j_\kappa}^{(\kappa)}$$

Replace single-particle functions with Gaussian functions

$$g_j(\mathbf{Q},t)=\exp\left(\mathbf{Q}^T\zeta_j\mathbf{Q}+\mathbf{Q}^T\xi_j+\eta_j\right)$$

Propagate parameters $\lambda=\{\zeta,\xi,\eta\}$

$$\begin{aligned}
i\dot{A}_j &= \sum_{lk}\mathcal{S}^{-1}_{jk}\langle\Phi_k|H|\Phi_l\rangle A_l-\sum_{\kappa=1}^{p}\sum_{l=1}^{n_\kappa}iS^{-1}_{jk}\langle g_k|\frac{\partial}{\partial t}g_l\rangle A_{J_l^\kappa}\\
&= \sum_{lk}\mathcal{S}^{-1}_{jk}H_{kl}A_l-\sum_{\kappa=1}^{p}\sum_{l=1}^{n_\kappa}iS^{-1}_{jk}\tau_{kl}A_{J_l^\kappa}\\
i\dot{\boldsymbol{\lambda}} &= \mathbf{C}^{-1}\boldsymbol{\Upsilon}
\end{aligned}$$

Burghardt *et al* JCP (99) 99:2927

Burghardt *et al* JCP (08) 129:174104

ADVANTAGES

- Need more GFs than SPFs,
- **BUT** set of parameters smaller than no. of grid points
- spatially unrestricted

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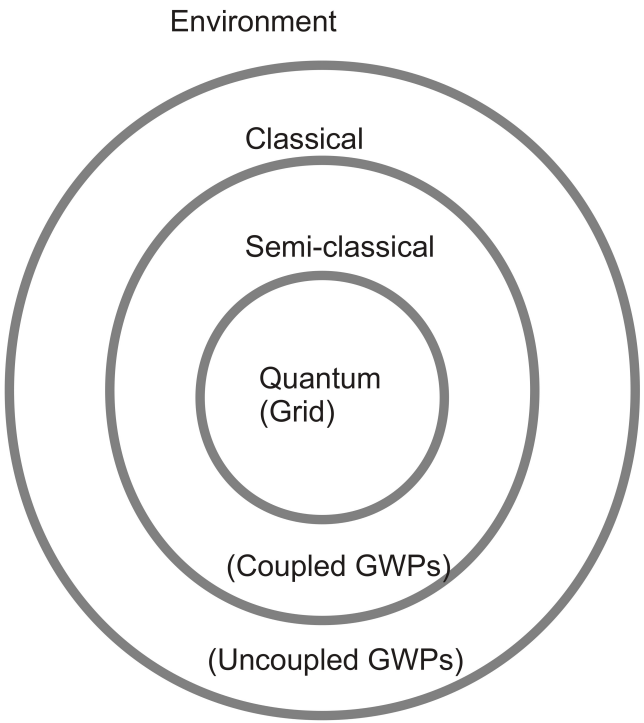
DISADVANTAGES

- Non-orthogonal basis set - numerically difficult
- Efficiency requires approximate integral evaluation
  LHA $V = V(x_0) + V'(x - x_0) + V''(x - x_0)^2$
  - convergence on exact result depends on accuraccy of integrals

General Scheme

G-MCTDH gives general framework for Quantum — semi-classical — classical dynamics. Can also treat open systems using density matrix formalism.



Grid-based QD $\longrightarrow$ Gaussian Wavepackets

In limit of only GWP basis functions G-MCTDH becomes the Variational Multi-configurational GWP Method: vMCG

$$\Psi(\mathbf{x}, t) = \sum_J A_J g_J(\mathbf{x}, t)$$

GWPs long-tradition in time-dependent QD.

- Conceptually simple
- Can be related to semi-classical dynamics
- possible to use for *direct dynamics*

BUT

- numerically unstable
- convergence properties not clear - no “natural population”
- limited to rectilinear coordinates

vMCG Equations of Motion

$$\Psi(Q_1, \ldots, Q_f, t) = \sum_{j=1}^{n_1} A_j(t) g_j$$

Replace single-particle functions with Gaussian functions

$$g_j(\mathbf{Q}, t) = \exp\left(\mathbf{Q}^T \zeta_j \mathbf{Q} + \mathbf{Q}^T \boldsymbol{\xi}_j + \eta_j\right)$$

Propagate parameters. For expansion coefficients $\lambda = \{\boldsymbol{\zeta}, \boldsymbol{\xi}, \eta\}$

$$i\dot{A}_j = \sum_{lk} \mathcal{S}^{-1}_{jk} \left[H_{kl} - i\tau_{kl}\right] A_l$$

and for the linear parameters, $\xi_{l\beta} = -2\zeta_{l\beta\beta} q_{l\beta} - p_{l\beta}$ can be written

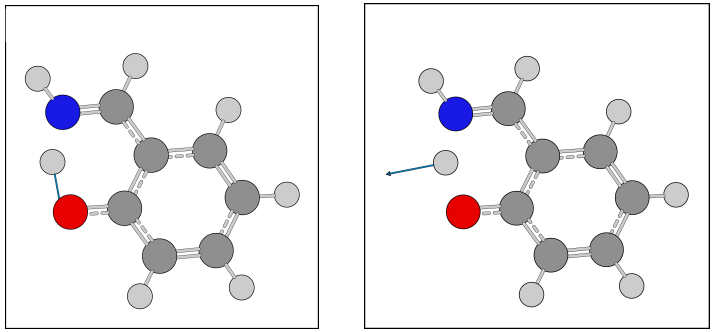
$$\begin{aligned} \dot{q}_{l\beta} &= \frac{p_{l\beta}}{m_\beta} + \frac{1}{2\zeta_{l\beta}} \mathrm{Im} \sum_{m\alpha} C^{-1}_{l\beta m\alpha} \tilde{Y}_{m\alpha} \\ \dot{p}_{l\beta} &= -V'_{l\beta} + \mathrm{Re} \sum_{m\alpha} C^{-1}_{l\beta m\alpha} \tilde{Y}_{m\alpha} \end{aligned}$$

Burghardt *et al* JCP (99) 99:2927 Burghardt *et al* JCP (08) 129:174104

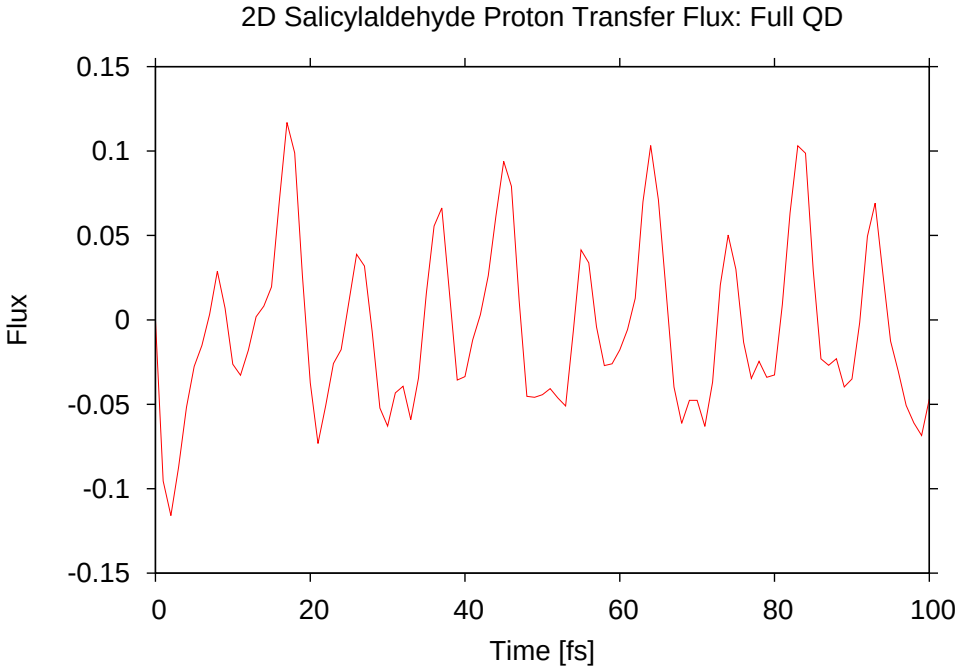
Salicylaldimine Test Case: 2D Proton transfer

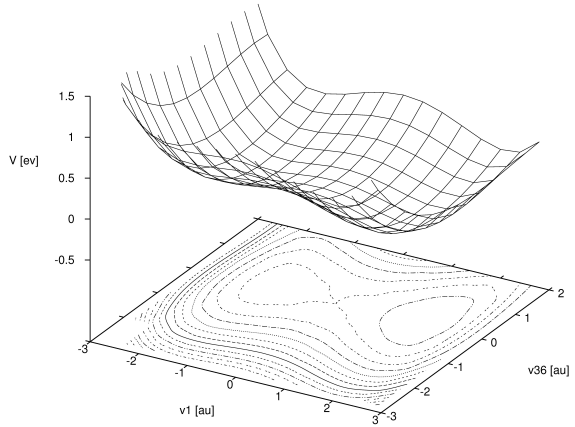
Hamiltonian in normal modes fitted to RHF/3-21G*

$$H = \sum_{\kappa=1,18} \frac{\omega_\kappa}{2}\left(\frac{\partial^2}{\partial q_\kappa^2} + q_\kappa^2\right) + \sum_{n=1}^{4} A_n q_1^n + B_{11} q_1 q_{18} + B_{22} q_1^2 q_{18}^2 + B_{31} q_1^3 q_{18} + B_{13} q_1 q_{18}^3$$



ν_{18}





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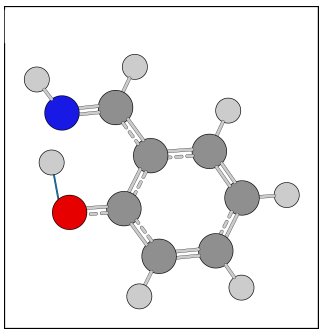

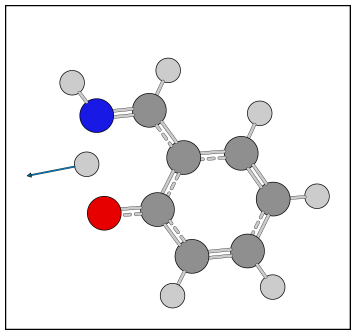

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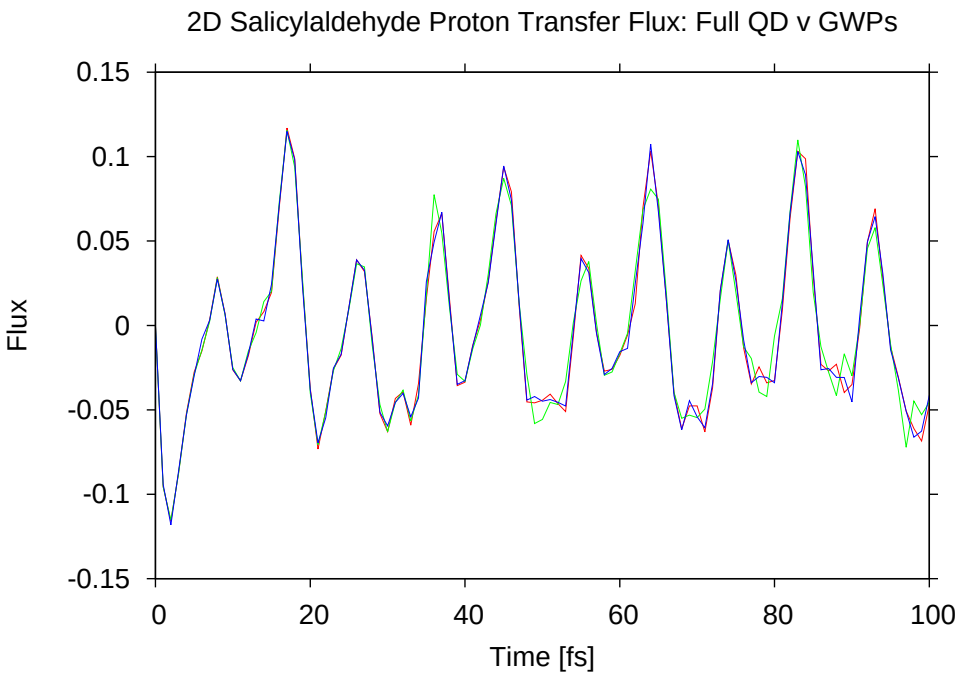
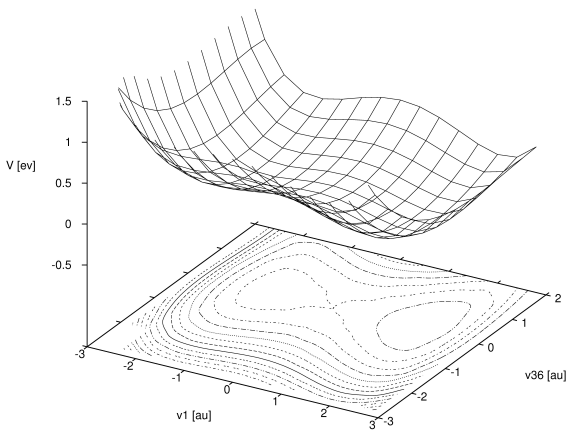
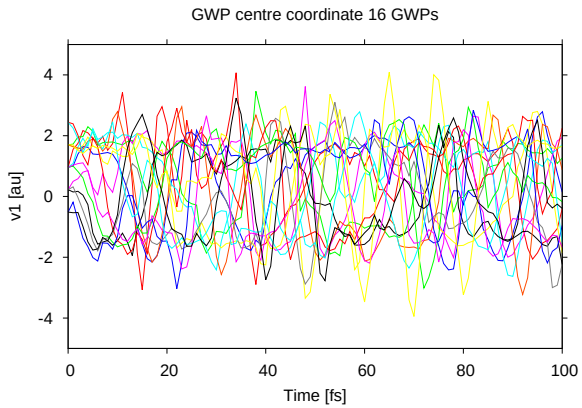


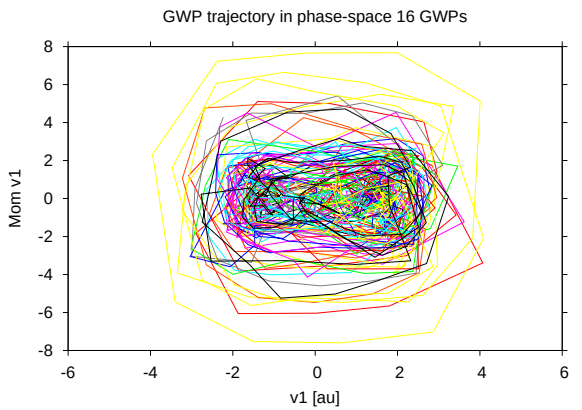


16 / 32 GWPs

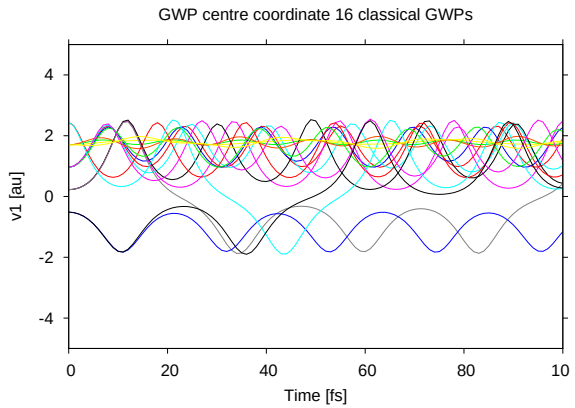
Trajectories with 16 GWPs

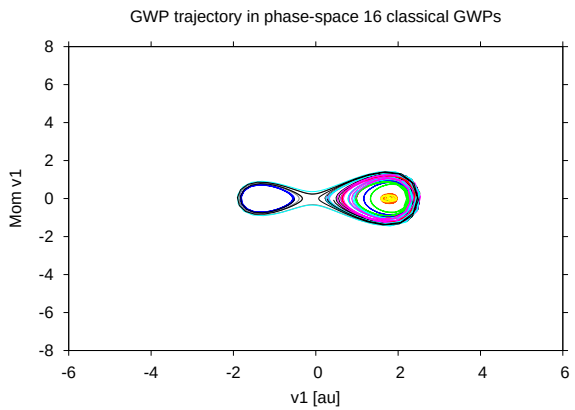
vMCG

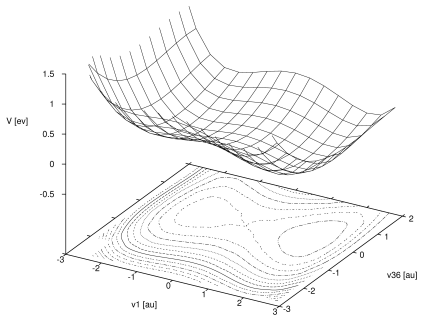




Classical



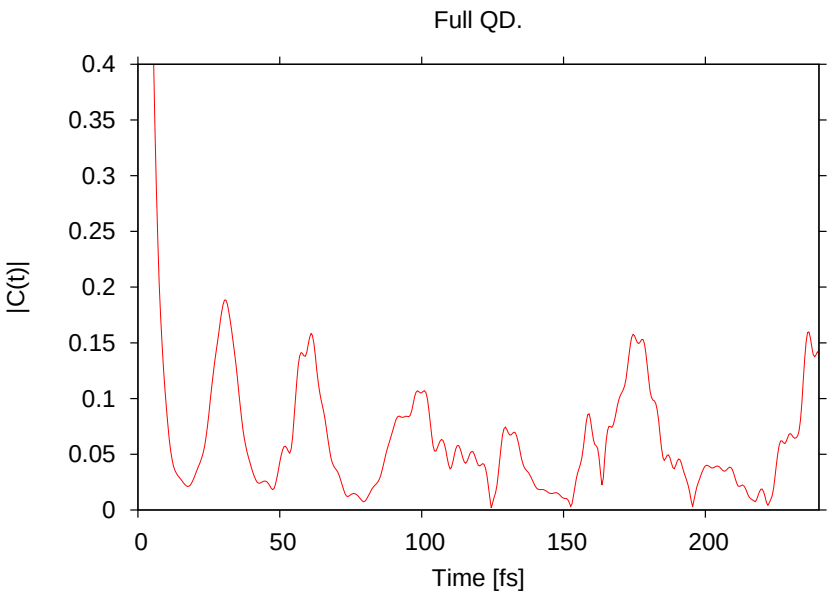




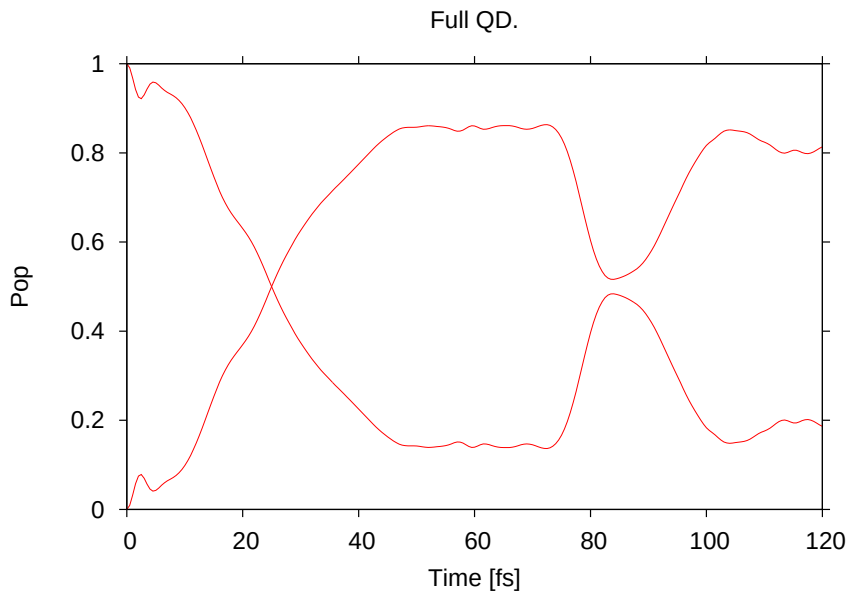
Richings *et al* Int. Rev. Phys. Chem. (15) **34**: 269

4D model: Linear Coupling

Autocorrelation function:



State Populations:



QD basis size: 4060 SPFs, 355,000 primitives

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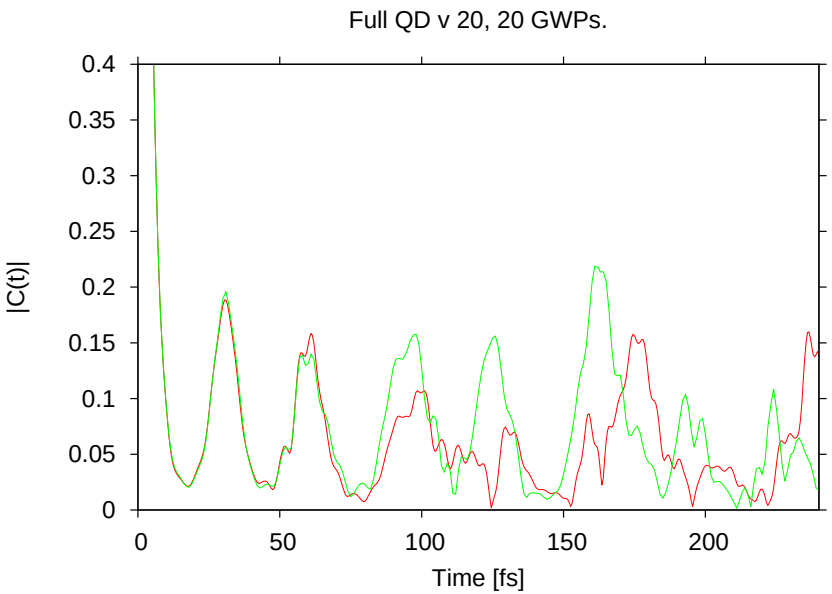

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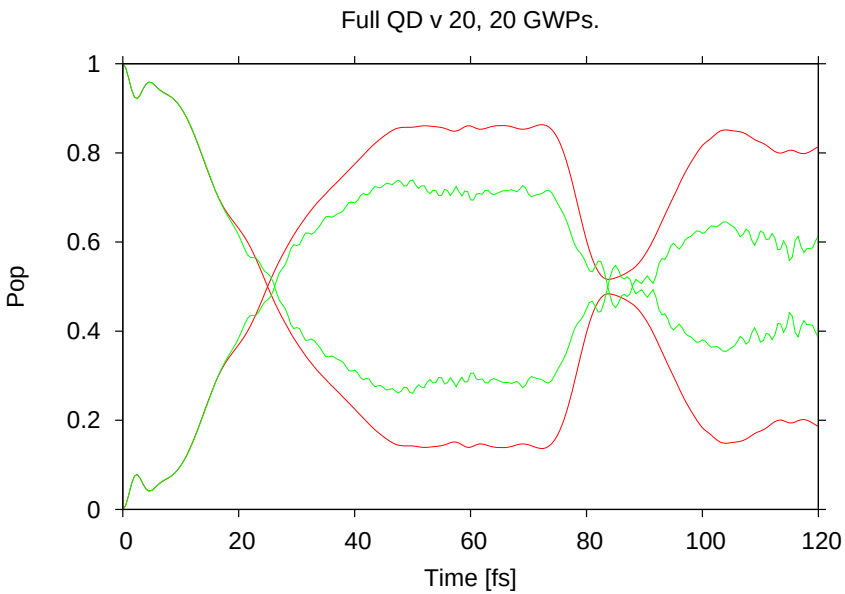

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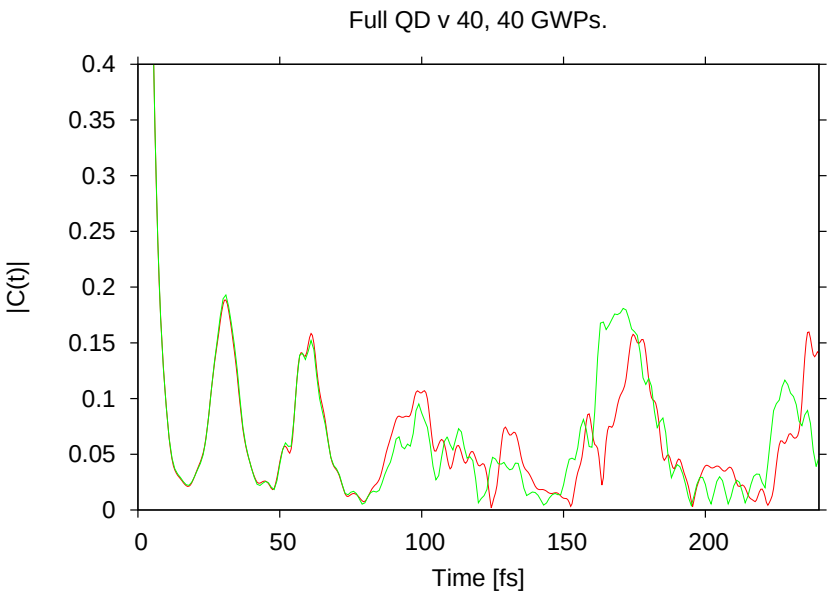

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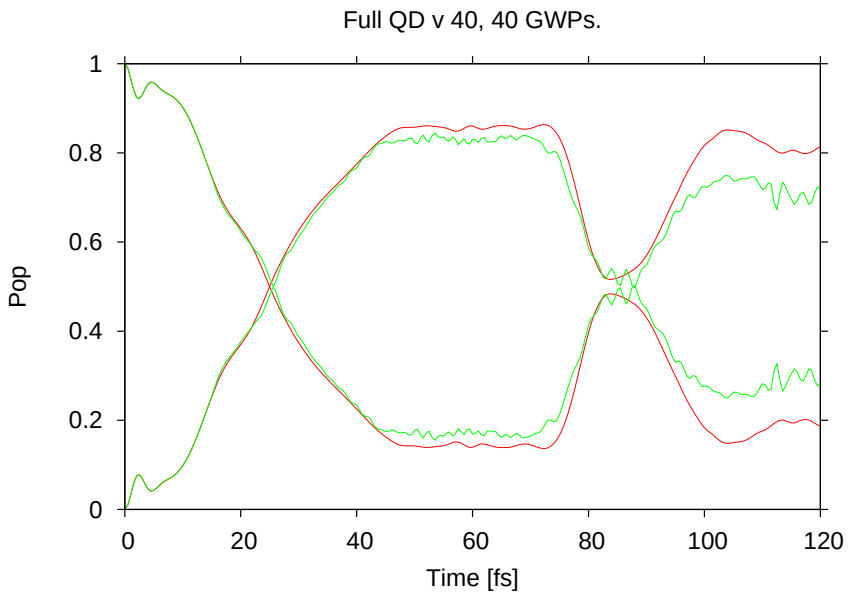

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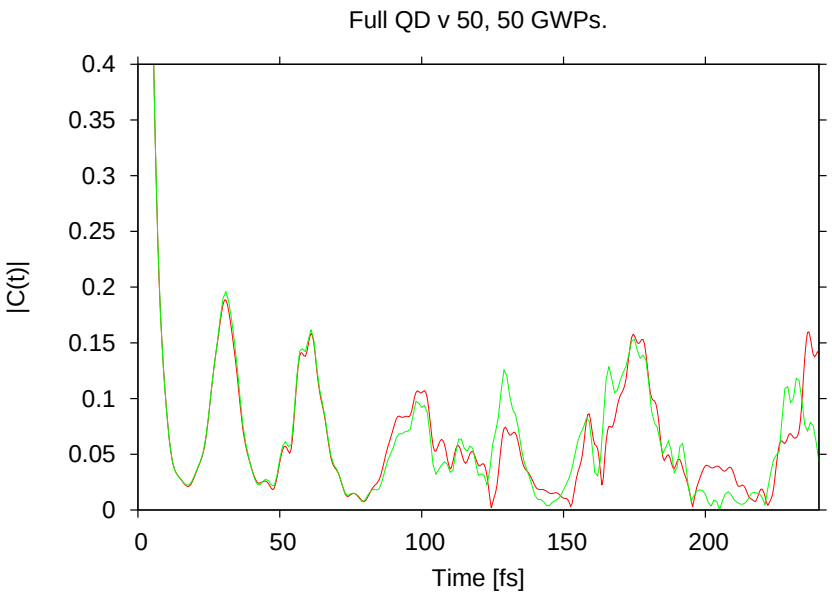

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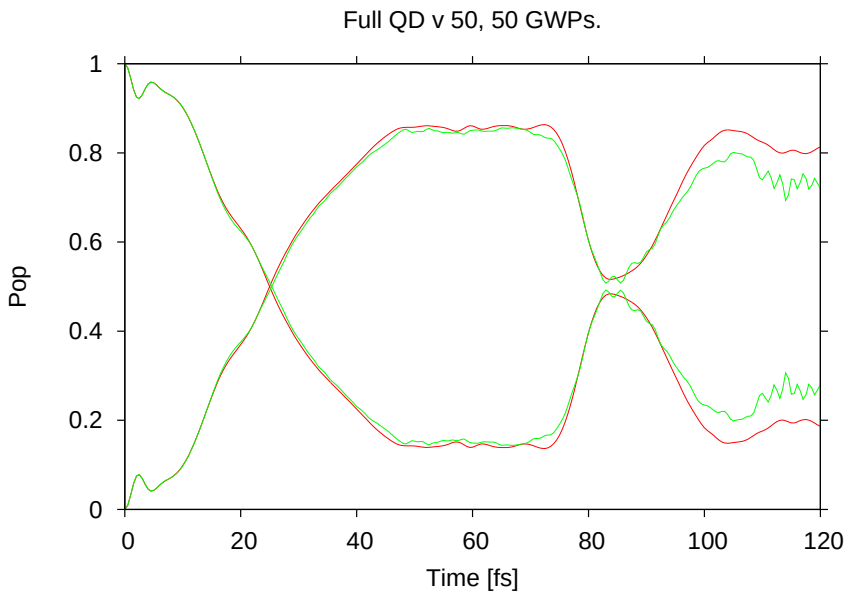

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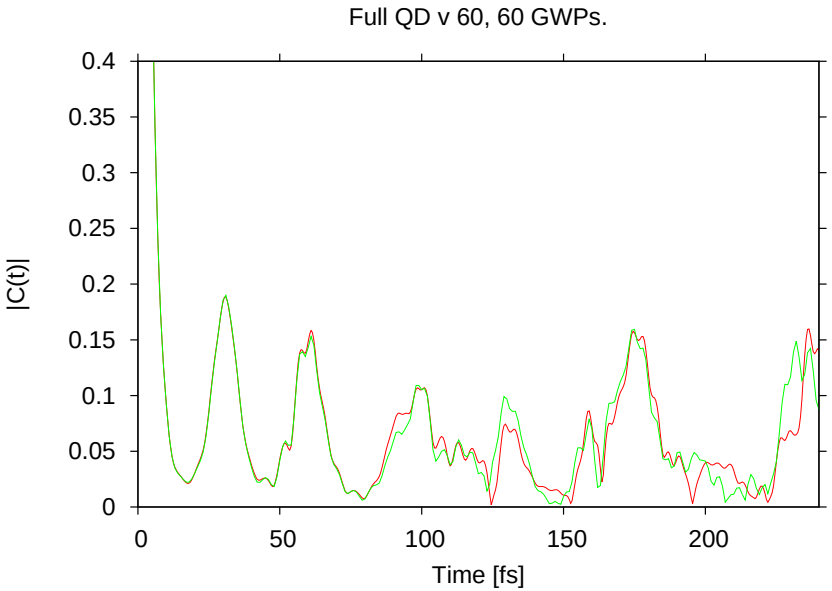

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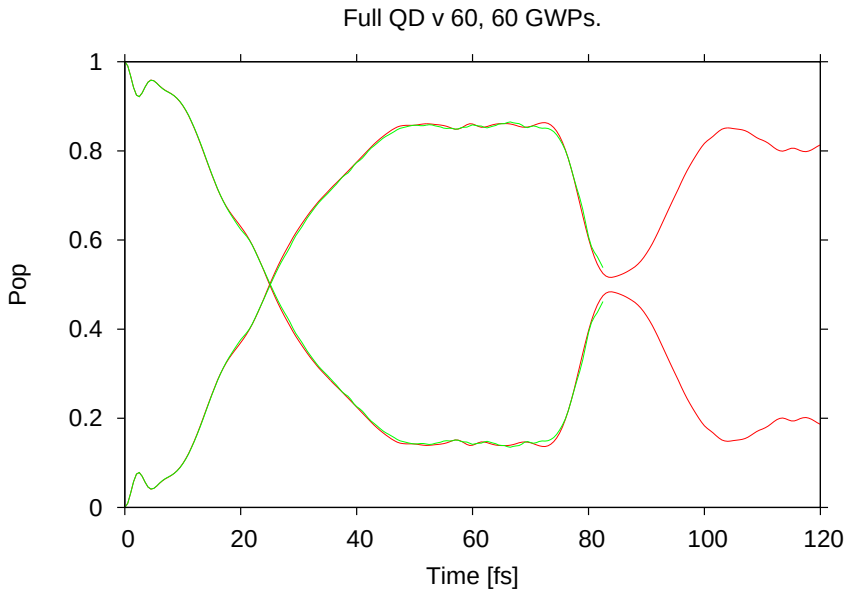

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Routes to Higher Dimensionality.

First bottleneck to larger systems is no. of configurations n^f

Strategies:

I Combined Mode Particles
II Selected-CI
III Cascading / Multi-layer
IV Parametrized Spfs

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Second bottleneck is calculating potential

Strategies:

A Parametrized Hamiltonian
- Reaction Path Model
- High-Dimensional Cluster Model
- Vibronic Coupling Model

B GROW

C Direct Dynamics

Direct Dynamics

- For integrals $\langle g_j|H|g_k\rangle$, Quantum chemistry to second order.
- Gradients and Hessians directly from quantum chemistry.
- Store results in a database (energy, gradient, Hessian)

Ideally use adiabatic PES in direct dynamics as they are readily available from quantum chemistry packages.

- States interact *via* the non-adiabatic coupling terms (NACT)

$$\mathbf{F}_{ab} = \frac{\langle \psi_a|\nabla \hat{H}_{\mathrm{el}}|\psi_b\rangle}{V_b - V_a}$$

- NACTs go to infinity at a conical intersection and adiabatic PES become non-differentiable at such points.

Problem for LHA. Avoid these problems by transforming to the diabatic picture.

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Problem for LHA. Avoid these problems by transforming to the diabatic picture. How can we define diabatic states on-the-fly?

Diabatisation by Propagation

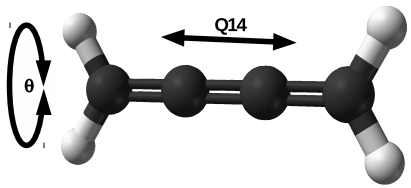
Adiabatic - Diabatic transformation, **S**, defined by

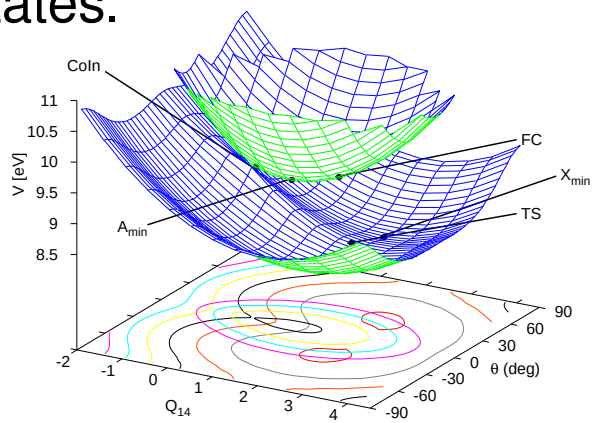
$$\nabla \mathbf{S} = -\mathbf{F}\mathbf{S}$$

where **F** is NACT. Exact for complete set of states.

- Choose $\mathbf{S} = \mathbf{1}$ at the initial point of the propagation.
- Solve for **S** by propagating from the nearest point.
- Applicable to any number of states.

First test: Butatriene ionisation

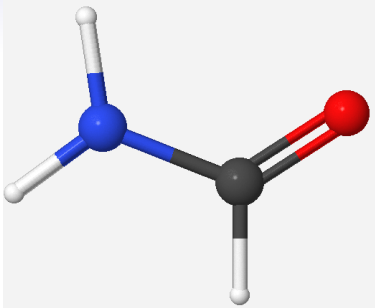




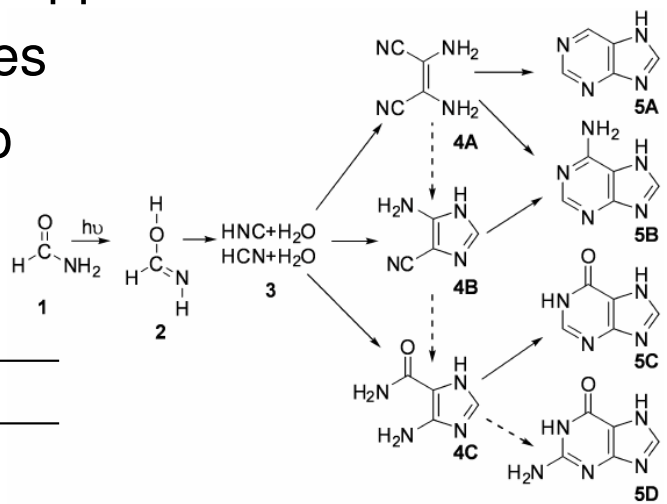
- Dynamics run on first-excited ion states.
  - DD-vMCG using 25 GWPs with propagated diabatisation.
  - Powell updated Hessian

Richings and Worth J. Phys. Chem. A (2015) 119: 12457

Formamide



- Smallest stable molecule consisting of HCNO
- Prebiotic Earth
- Found, by spectral molecular survey, on Hale-Bopp
- Tentatively found in IR-spectra of interstellar ices
- Decomposition pathways studied but as yet, no excited state studies



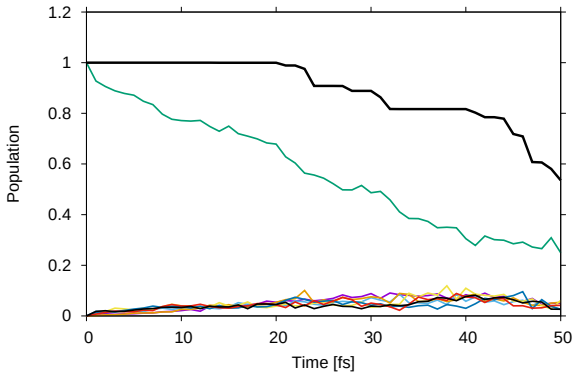
SA-CAS(10,8)/6-31G*

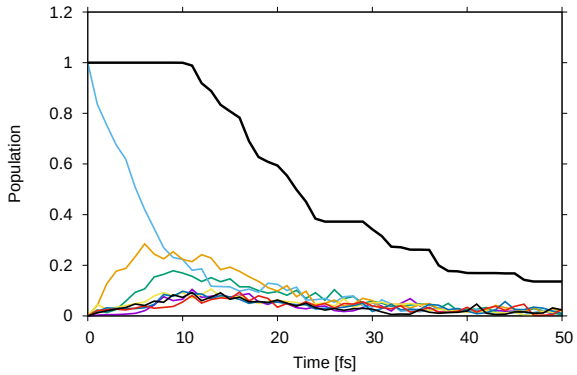
State	VEE/eV	T Dipole/au	Character
S_1	5.607	0.000	Olp-π^*
S_2	8.015	0.000	π-NH_2^*
S_3	8.159	0.022	Olp-NH_2^* + $\pi\pi^*$
S_4	9.118	0.000	π-NH_2^*
S_5	10.033	0.071	Olp-NH_2^*
S_6	10.574	0.726	$\pi\pi^*$ + Olp-NH_2^*
S_7	11.450	0.001	π-NH_2^* + $\pi\pi^*$

Formamide: Direct Dynamics 48GWP

Diabatic Populations

$S_1(\mathrm{Olp}\pi^*)$



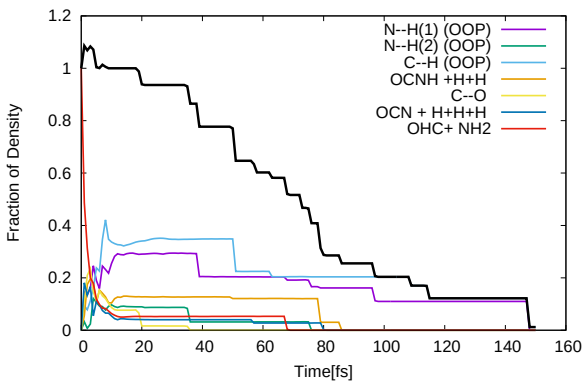


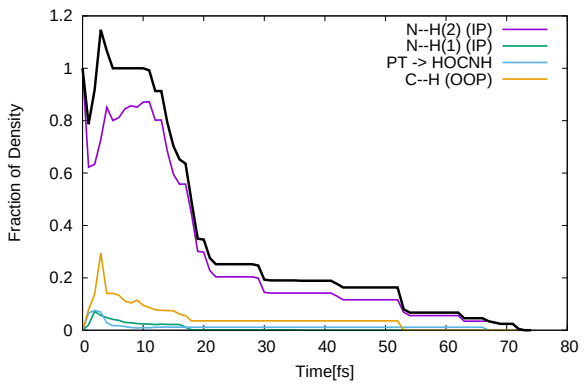
$S_2(\pi\pi^*)$

Product Analysis: Weight GWP trajectories ending in a particular channel by Gross Gaussian Population

$$\mathrm{GGP}_i = \sum_j Re\left(A_i^* S_{ij} A_j\right)$$

$S_1(\mathrm{Olp}\pi^*)$





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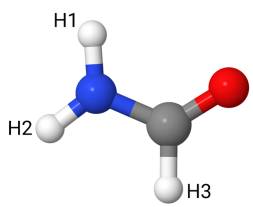
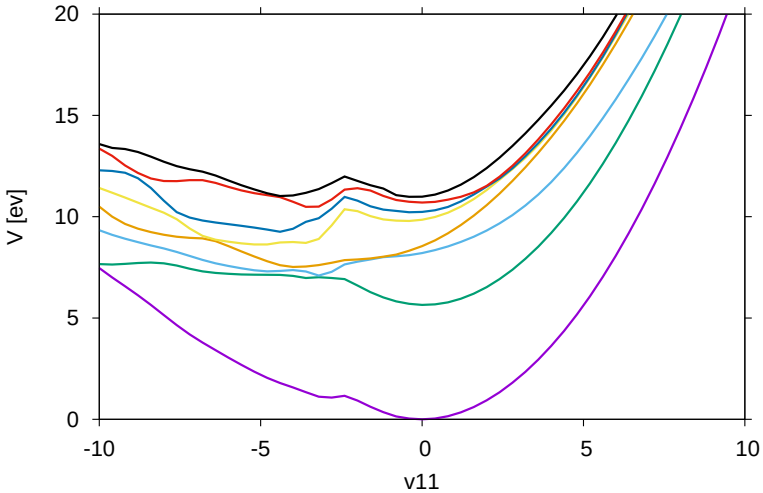


Spinlove *et al.* (18) In Preparation

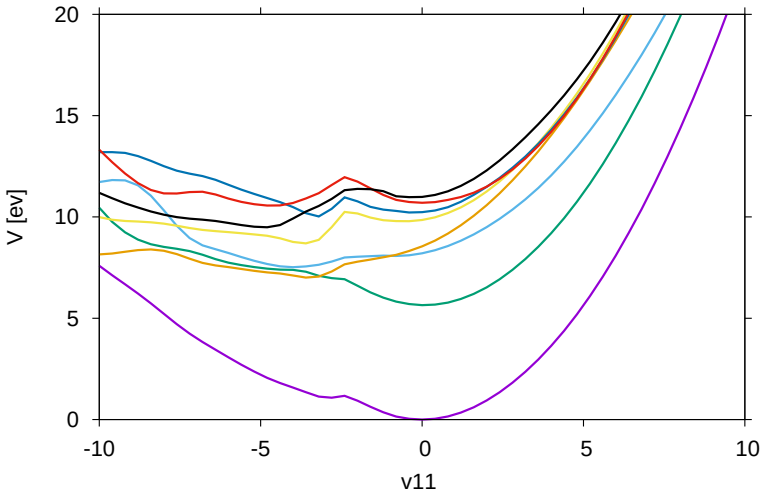
Formamide Potential Surfaces

Along NH_2 Symm Stretch

Adiabatic

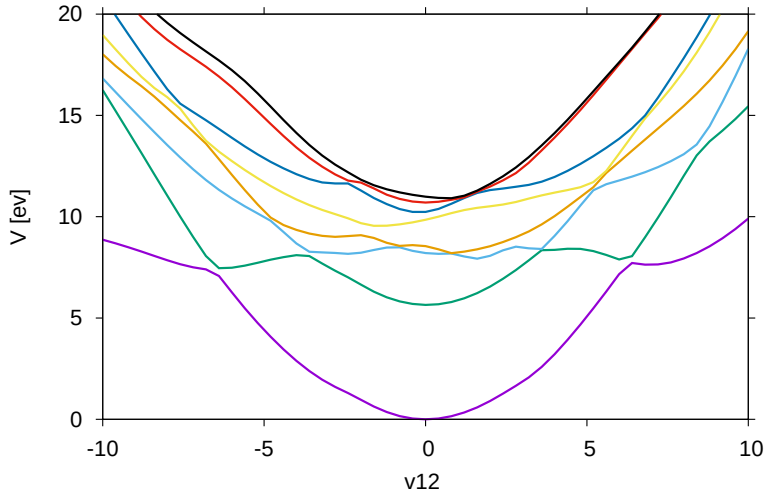


Diabatic

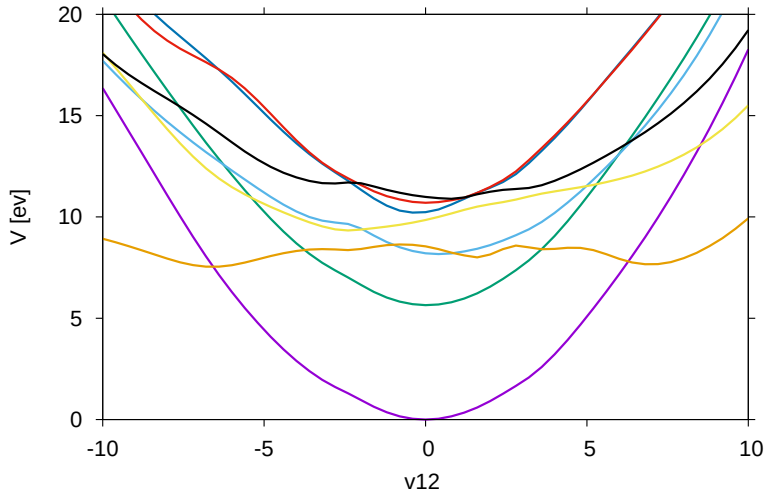


Along NH_2 Anti-symm Stretch

Adiabatic



Diabatic



Conclusions

Variational time-dependent basis sets are a powerful way of obtaining the full solution to the TDSE.

- MCTDH provides a complete framework for quantum dynamics.
  - ML-MCTDH grid-based for truly large systems - simple PES
  - G-MCTDH flexible route to approximate dynamics - any PES but restricted coordinates
- G-MCTDH $\longrightarrow$ vMCG $\longrightarrow$ GWP methods
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Present bottleneck: Electronic Structure theory!

Acknowledgments

Main Collaborators:

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Irene Burghardt, Frankfurt
Mike Robb and Mike Bearpark, Imperial
Benjamin Lasorne, Montpellier

Birmingham / UCL:

Mariana Assmann
Angelo Giussani
Eryn Spinlove
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QUANTICS Documentation

QUANTICS

A suite of programs for molecular QUANTum dynamICS simulations.
Capabilities

User Manual

- Installation and Compilation
- User's Guide (PostScript)
- Troubleshooting
- The Quantics Program
  - Usage
  - Input Documentation
  - Output Documentation
  - Hamiltonian/Liouvillian Documentation
  - Density Operator Propagation
  - Optimal Control Documentation
- The Potfit Program
  - Program Documentation
  - Input Documentation
  - Output Documentation
  - PES Projection
- Cluster-Expansion
- The Analyse Programs
- The Filter Program
- The VCHam Program
- The Real Wavepacket Program
- How To....

Developers's Manual

- Guidelines for Developers
- Automatic Program Test *(Elk Test)*
- Code Description
- Notes on implementation
- Operator Details
- Libraries Description
- Developing New Analysis Programs
- To Be Done

Caution: this documentation is in part out of date and does not apply to the QUANTICS package.

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