

**Virtual International Seminar on
Theoretical Advancements (VISTA)**
2020/09/10



浙江大学
Zhejiang University

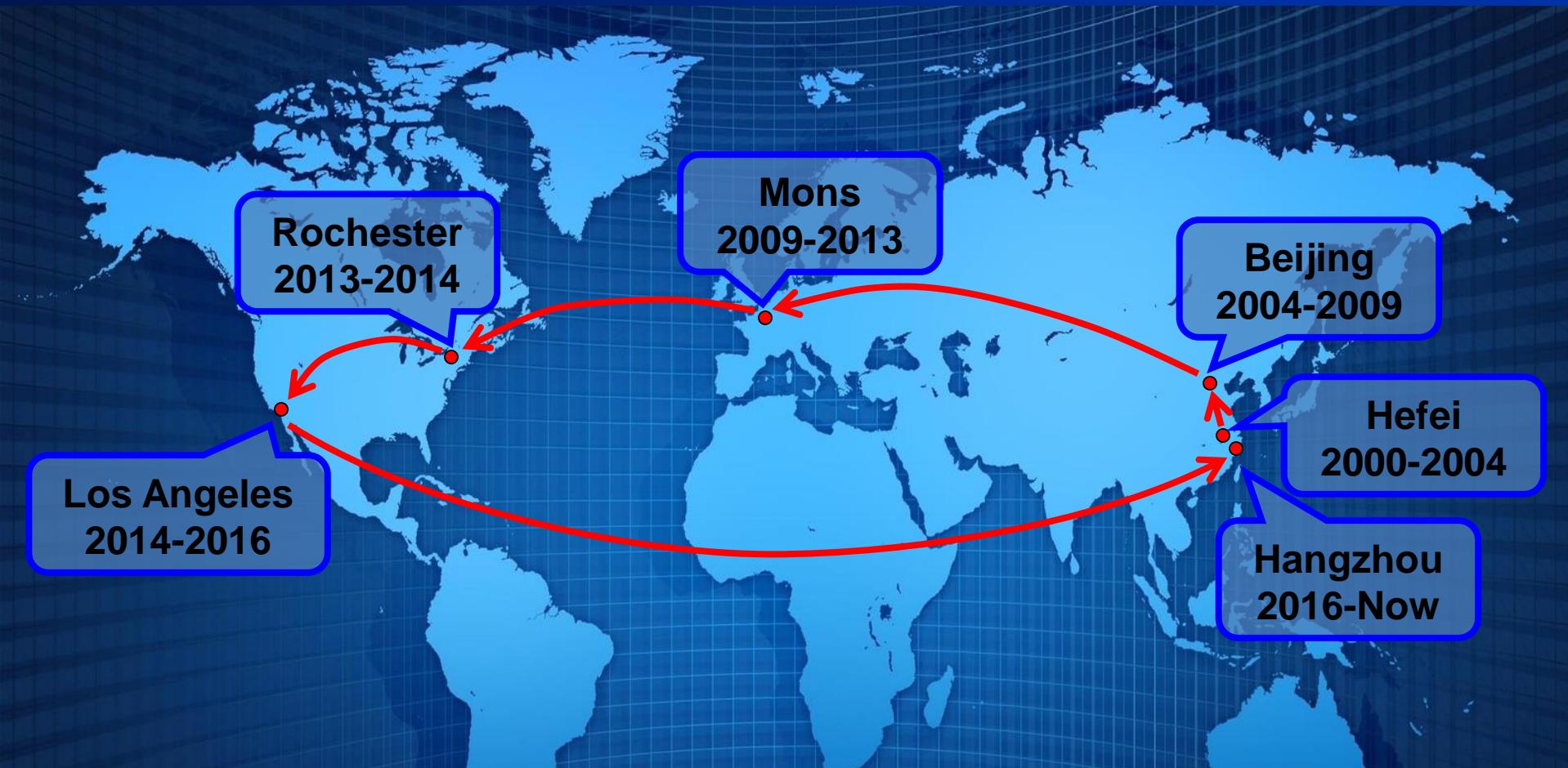
Branching Correction for Mixed Quantum-Classical Dynamics

Linjun Wang

Department of Chemistry, Zhejiang University

Email: ljunwang@zju.edu.cn

Education and Research Experiences



UMONS
Université de Mons





Outline

- Introduction to Mixed Quantum-Classical Dynamics
- Interpretation of Decoherence Correction
- Branching Corrected Surface Hopping
- New Energy-Based Decoherence Time Formulas
- Branching Corrected Mean Field



Outline

■ Introduction to Mixed Quantum-Classical Dynamics

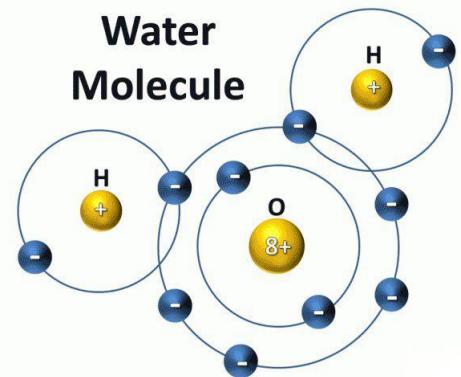
- Interpretation of Decoherence Correction
- Branching Corrected Surface Hopping
- New Energy-Based Decoherence Time Formulas
- Branching Corrected Mean Field

Born-Oppenheimer Approximation

■ Schrödinger equation:

$$\mathbf{H}\psi_n(\{\vec{R}_\alpha, \vec{r}_i\}) = E_n\psi_n(\{\vec{R}_\alpha, \vec{r}_i\})$$

$$\mathbf{H} = \sum_{\alpha} \frac{-\nabla_{\alpha}^2}{2M_{\alpha}} + \sum_i \frac{-\nabla_i^2}{2} + \sum_{\alpha < \beta} \frac{Z_{\alpha}Z_{\beta}}{|\vec{R}_{\alpha} - \vec{R}_{\beta}|} + \sum_{i < j} \frac{1}{|\vec{r}_i - \vec{r}_j|} + \sum_{\alpha, i} \frac{-Z_{\alpha}}{|\vec{r}_i - \vec{R}_{\alpha}|}$$

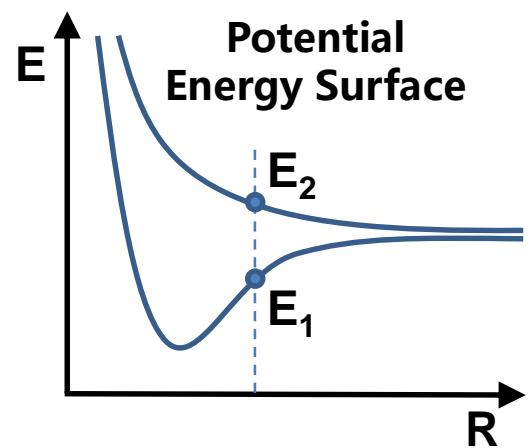


■ Born-Oppenheimer approximation:

$$\mathbf{H} = \sum_{\alpha} \frac{-\nabla_{\alpha}^2}{2M_{\alpha}} + \mathbf{H}_e$$

$$\mathbf{H}_e = \sum_i \frac{-\nabla_i^2}{2} + \sum_{\alpha < \beta} \frac{Z_{\alpha}Z_{\beta}}{|\vec{R}_{\alpha} - \vec{R}_{\beta}|} + \sum_{i < j} \frac{1}{|\vec{r}_i - \vec{r}_j|} + \sum_{\alpha, i} \frac{-Z_{\alpha}}{|\vec{r}_i - \vec{R}_{\alpha}|}$$

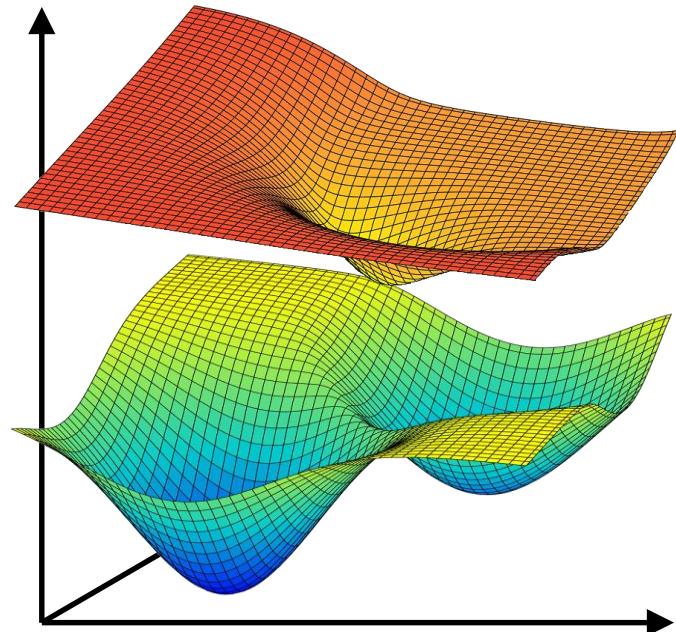
$$\mathbf{H}_e(\{\vec{R}_{\alpha}\})\psi_n(\{\vec{r}_i; \vec{R}_{\alpha}\}) = E_n(\{\vec{R}_{\alpha}\})\psi_n(\{\vec{r}_i; \vec{R}_{\alpha}\})$$



Adiabatic and Nonadiabatic Dynamics

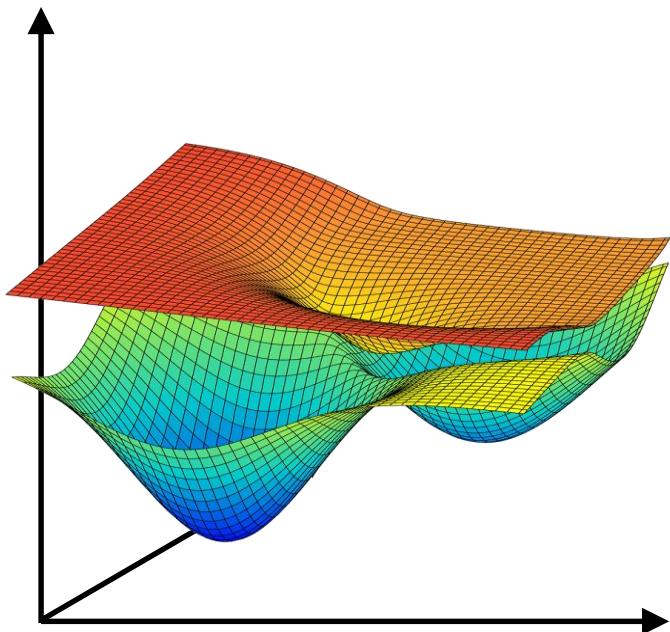


■ Adiabatic Dynamics:



BO approximation

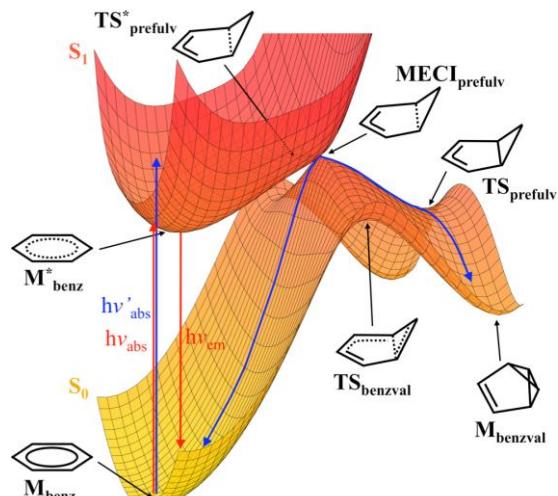
■ Nonadiabatic Dynamics:



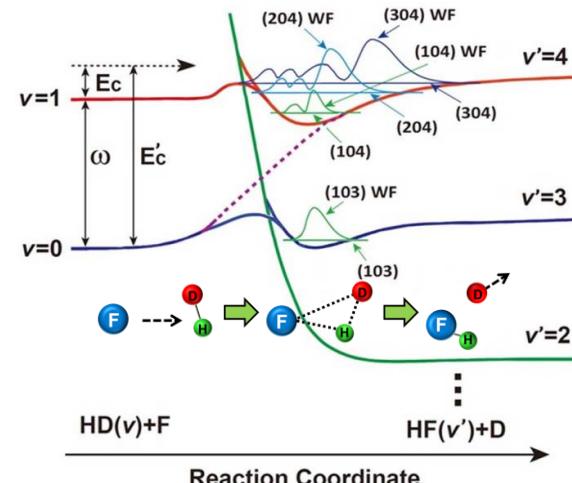
beyond BO approximation

In nonadiabatic dynamics, electron and nuclear dynamics are strongly coupled

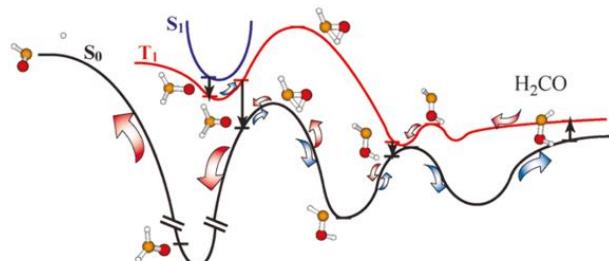
Nonadiabatic Dynamics in Photochemistry and Thermochemistry



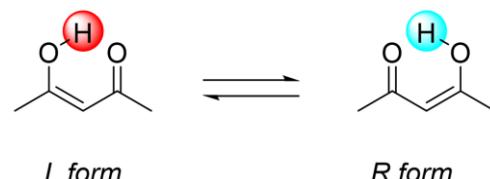
Photoisomerization



Thermal Reaction

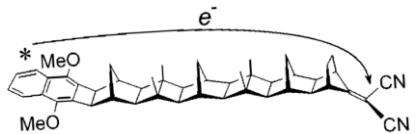


Photodissociation

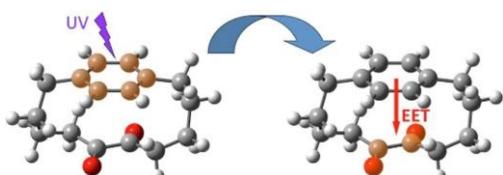


Proton Transfer

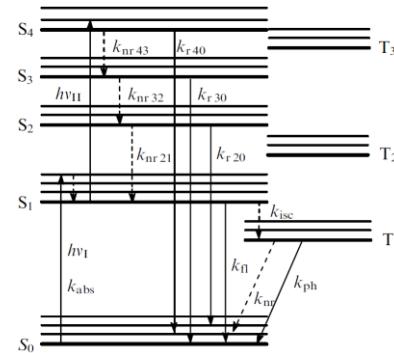
Nonadiabatic Dynamics in Electrochemistry, Materials, Physics, and Biology



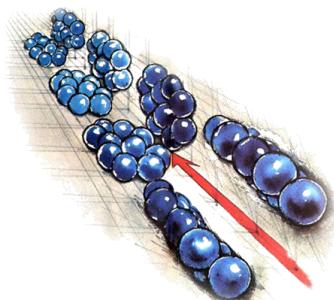
Charge Transfer



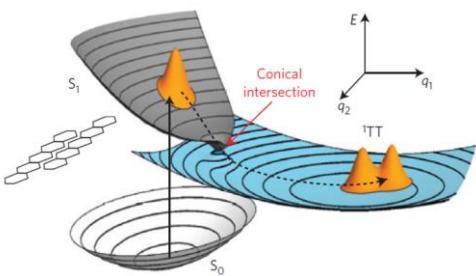
Energy Transfer



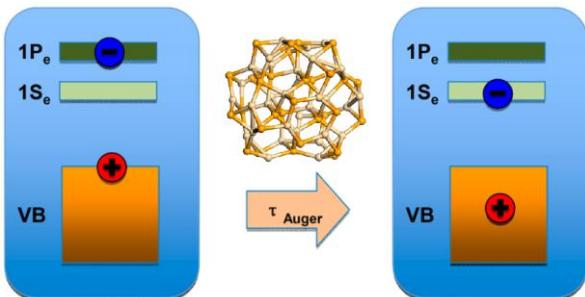
Nonradiative Decay



Charge Transport



Singlet Fission



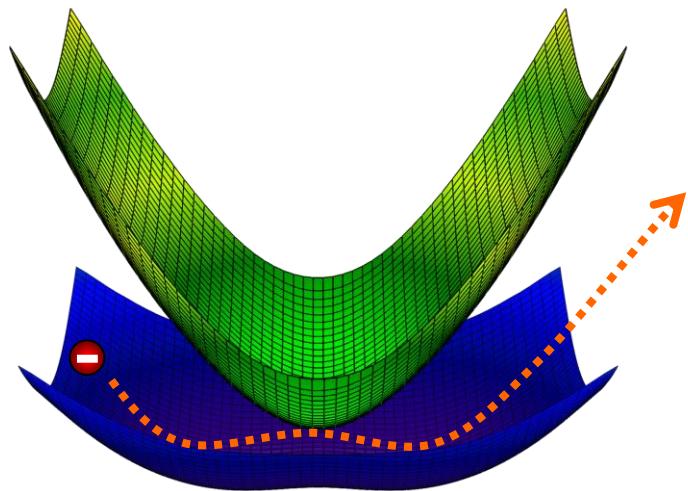
Auger Relaxation

Mixed Quantum-Classical Description of Nonadiabatic Dynamics



■ Mean field (MF):

$$\frac{\partial|\psi\rangle}{\partial t} = \frac{\mathbf{H}|\psi\rangle}{i\hbar} \quad m_i \ddot{x}_i = -\frac{\partial\langle\psi|\mathbf{H}|\psi\rangle}{\partial x_i}$$

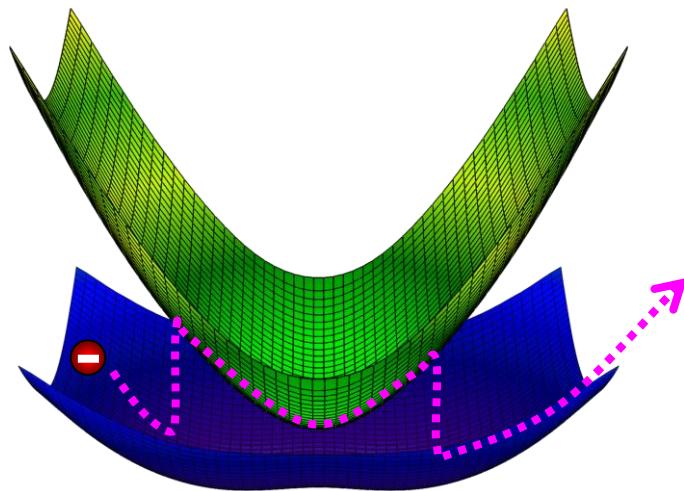


Ehrenfest Dynamics
Ehrenfest, Z. Phys. 45, 445 (1927)

more widely used in physics

■ Surface hopping (SH):

$$\frac{\partial|\psi\rangle}{\partial t} = \frac{\mathbf{H}|\psi\rangle}{i\hbar} \quad m_i \ddot{x}_i = -\frac{\partial\langle\psi_k|\mathbf{H}|\psi_k\rangle}{\partial x_i}$$



Fewest Switches Surface Hopping
Tully, J. Chem. Phys. 93, 1061 (1990)

more widely used in chemistry

The treatment of nuclear dynamics is different in MF and SH approaches,₉



Advantages of Ehrenfest Mean Field (EMF)

■ Clear physical picture:

The classical part experiences average forces from the quantum part

$$|\Psi(\mathbf{r}, \mathbf{R}, t)\rangle = |\psi(\mathbf{r}, t)\rangle |\chi(\mathbf{R}, t)\rangle \exp\left[\frac{i}{\hbar} \int_0^t E_0(t') dt'\right]$$

■ Representation independence:

$$\frac{\partial |\psi\rangle}{\partial t} = \frac{\mathbf{H}|\psi\rangle}{i\hbar} \quad m_i \ddot{x}_i = -\frac{\partial \langle \psi | \mathbf{H} | \psi \rangle}{\partial x_i}$$

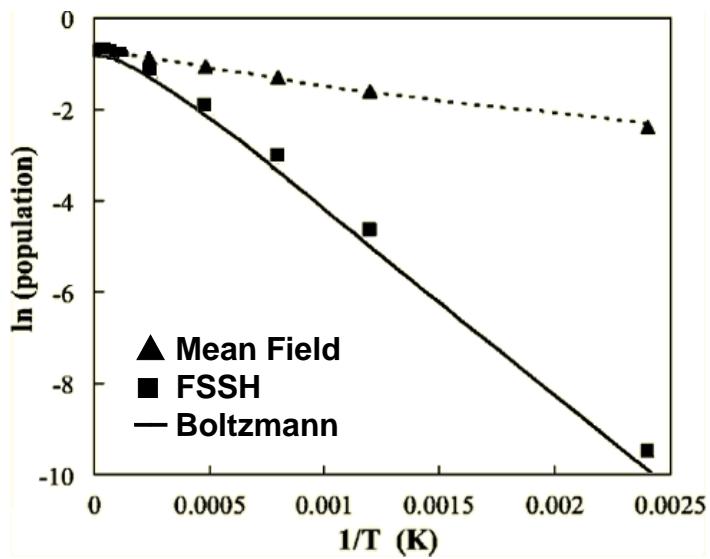
Diabatic and adiabatic representations give the same results

■ High efficiency:

Only one trajectory is used to describe the classical dynamics, and thus the statistical error is minimized

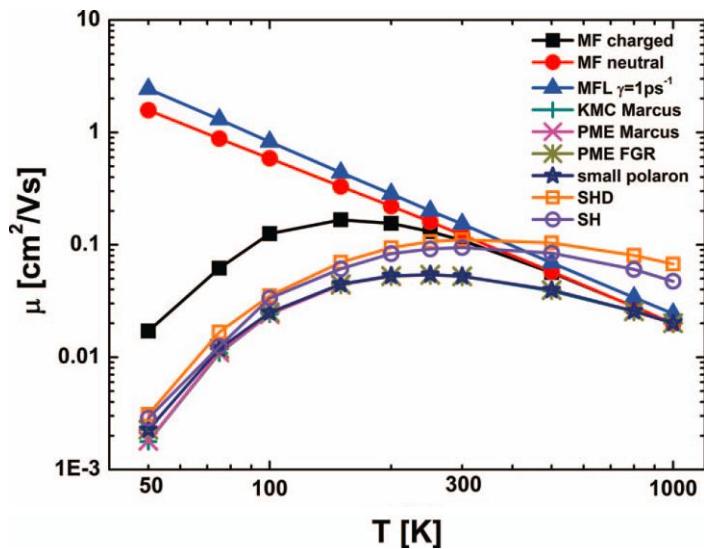
Limitations of Ehrenfest Mean Field

■ Detailed balance:



Parandekar and Tully
J. Chem. Phys. 122, 094102 (2005)

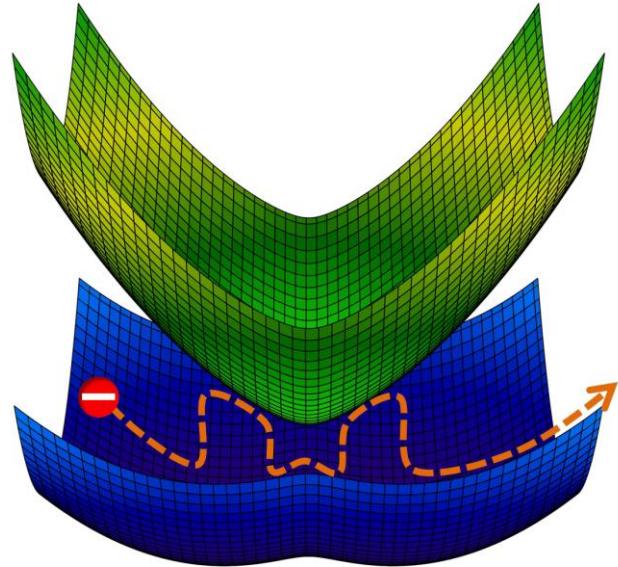
■ Polaronic effect:



Wang* and Beljonne
J. Chem. Phys. 139, 064316 (2013)

Feedback between the electron and nuclei is not properly described
and thus the simulation results are not always reliable

Working Equations of Fewest Switches Surface Hopping (FSSH)



wave function propagation

$$|\psi\rangle = \sum_i c_i |\phi_i\rangle$$

$$i\hbar \dot{c}_i = \sum_j c_j \left(V_{ij} - i\hbar \sum_k v_k \cdot d_{ij}^k \right)$$

nonadiabatic coupling

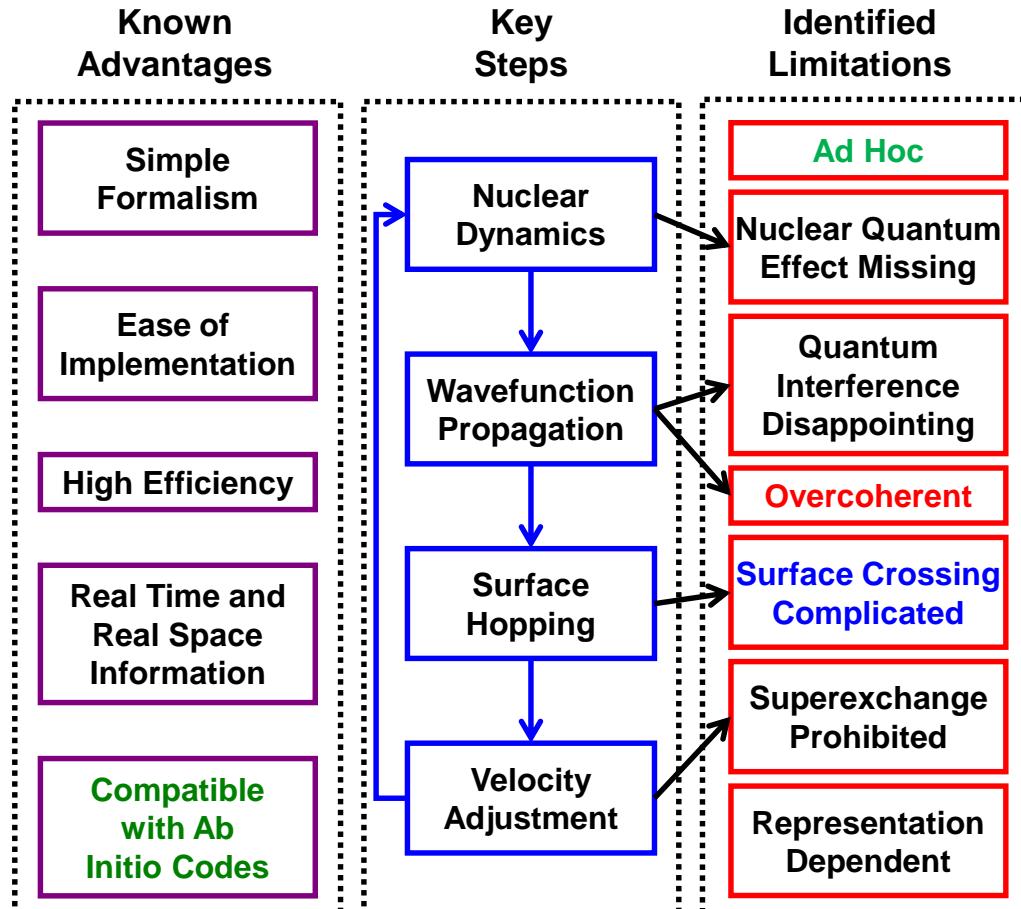
$$d_{ij}^k = \langle \phi_i | \frac{\partial}{\partial x_k} | \phi_j \rangle$$

$$\dot{a}_{ii} = \sum_{j \neq i} b_{ij} \quad b_{ij} = 2\hbar^{-1} \operatorname{Im} \left(a_{ij}^* V_{ij} \right) - 2 \operatorname{Re} \left(a_{ij}^* \sum_k v_k \cdot d_{ij}^k \right) \quad g_{ij} = -\frac{\Delta t b_{ij}}{a_{ii}}$$

hopping probability

Surface hopping characterize the different motion on different surfaces
 Adiabatic representation is a natural and preferred choice for surface hopping

Beyond Traditional EMF and FSSH



- J. Chem. Phys. 134, 244116 (2011)
 J. Phys. Chem. Lett. 3, 1888 (2013)
 J. Chem. Phys. 139, 064316 (2013)
 J. Chem. Phys. 139, 174109 (2013)
 J. Phys. Chem. Lett. 5, 713 (2014)
 J. Chem. Theory Comput. 10, 3598 (2014)
 J. Phys. Chem. Lett. 6, 3827 (2015)
 J. Chem. Phys. 143, 191102 (2015)
 J. Chem. Phys. 148, 104106 (2018)
 J. Phys. Chem. Lett. 9, 4319 (2018)
 J. Chem. Phys. 149, 244113 (2018)
 J. Phys. Chem. Lett. 10, 637 (2019)
 J. Chem. Phys. 150, 164101 (2019)
 DOI: [10.1063/1674-0068/cjcp2006098](https://doi.org/10.1063/1674-0068/cjcp2006098) (2020)
 DOI: [10.26434/chemrxiv.12820238](https://doi.org/10.26434/chemrxiv.12820238) (2020)
- J. Phys. Chem. Lett. 5, 3345 (2014)
 Phys. Chem. Chem. Phys. 17, 12395 (2015)
 Annu. Rev. Phys. Chem. 66, 549 (2015)
 J. Phys. Chem. Lett. 7, 2100 (2016)
 WIREs Comput. Mol. Sci. 10, e1435 (2020)

EMF and FSSH share common advantages and limitations

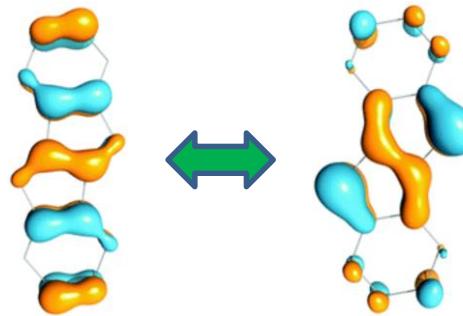


Outline

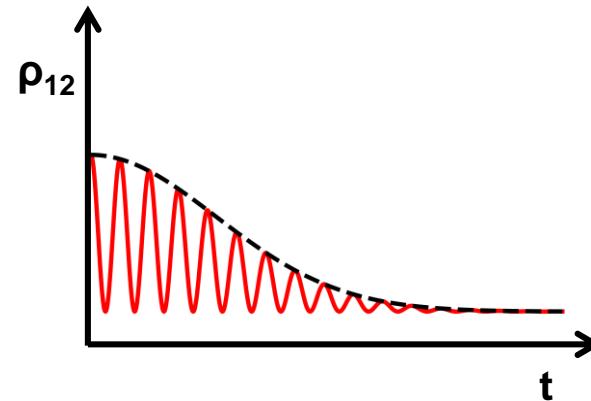
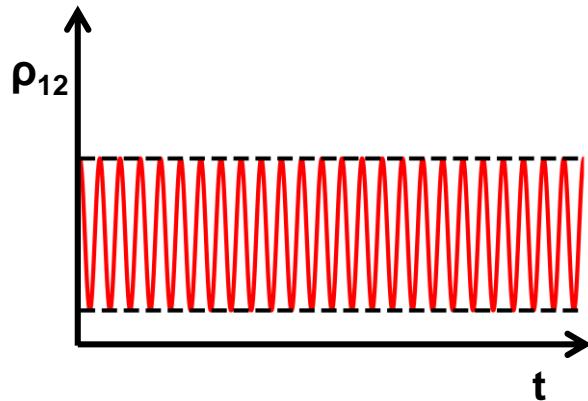
- Introduction to Mixed Quantum-Classical Dynamics
- **Interpretation of Decoherence Correction**
- Branching Corrected Surface Hopping
- New Energy-Based Decoherence Time Formulas
- Branching Corrected Mean Field

Quantum Coherence and Decoherence

■ Schrödinger's cat (thought experiment, 1935):



■ Coherence and Decoherence:



Coherence decays with time for a quantum system in contact with a classical bath

Decoherence Correction Approaches in Mixed Quantum-Classical Dynamics



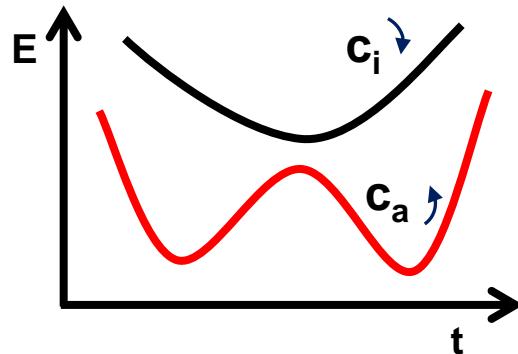
■ Existed approaches:

- 1994, Webster, Rossky, Friesner, **SPSH**
- 1995, Schwartz, Bittner, Prezhdo, Rossky, **FBD**
- 1997, Prezhdo, Rossky, **MF/SH**
- 1999, Fang, Hammes-Schiffer, **MDQT***
- 2004, Zhu, Jasper, Truhlar, **SCDM**
- 2004, Zhu, Nangia, Jasper, Truhlar, **CSDM**
- 2005, Zhu, Jasper, Truhlar, **LDM, PDDM**
- 2005, Bedard-Hearn, Larsen, Schwartz, **MF-SD**
- 2007, Granucci, Persico, **EBD**
- 2008, Cheng, Zhu, Truhlar, **CSDM-D**
- 2010, Granucci, Persico, Zoccant, **ODC**
- 2011, Shenvi, Subotnik, Yang, **STSH**
- 2011, Subotnik, Shenvi, **A-FSSH**
- 2012, Jaeger, Fischer, Prezhdo, **DISH**
- 2013, Gorshkov, Tretiak, Mozyrsky, **SCMC**
- 2013, Nelson, Tretiak, **ID**
- 2014, Akimov, Prezhdo, **CPF**
- 2014, Zheng, Truhlar, **AAT-CDSM**
- 2016, Martens, **CSH**
- 2017, Gao, Thiel, **nH-EOM**
- 2018, Ha, Lee, Min, **DISH-XF**
- 2019, Martens, **QTSH**

■ Decoherence time:

$$c'_i = c_i e^{-dt/\tau_i}$$

$$c'_a = c_a \left[\frac{1 - \sum_{j \neq a} |c'_j|^2}{|c_a|^2} \right]^{\frac{1}{2}}$$

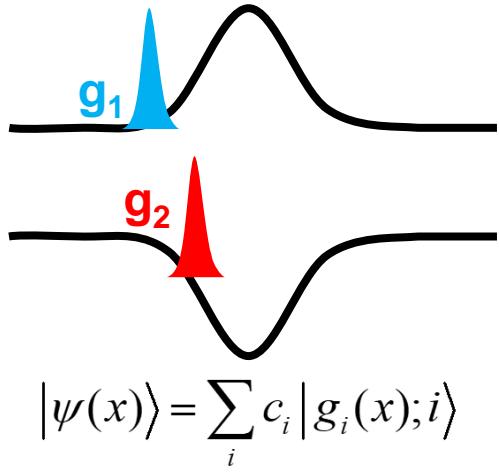


$$\text{FBD: } \tau_i^{-2} = \sum_j \frac{(F_a^j - F_i^j)^2}{4\hbar\sqrt{Km}}$$

$$\text{EBD: } \tau_i = \frac{\hbar}{|E_i - E_a|} \left(1 + \frac{C}{E_{kin}} \right)$$

$$\text{AFSSH: } \tau_i^{-1} = \sum_j Z_{ai}^j \Theta(Z_{ai}^j) \Theta \left[(\delta R_{aa}^j - \delta R_{ii}^j) (\delta P_{aa}^j - \delta P_{ii}^j) \right]$$

Traditional Interpretation of Decoherence Decay of Mixing



■ Frozen Gaussian approximation:

$$g_i(x) = (\sqrt{2\pi}\sigma)^{-1/2} \exp\left[-\frac{(x-x_i)^2}{4\sigma^2} + \frac{ip_i(x-x_i)}{\hbar}\right]$$

$$g_j(x) = (\sqrt{2\pi}\sigma)^{-1/2} \exp\left[-\frac{(x-x_j)^2}{4\sigma^2} + \frac{ip_j(x-x_j)}{\hbar}\right]$$

$$| \langle g_i | g_j \rangle | = \exp\left[-\frac{(x_i-x_j)^2}{8\sigma^2} - \frac{\sigma^2(p_i-p_j)^2}{2\hbar^2}\right]$$

■ First-order approximation:

$$x_i = x_i(0) + \frac{p_i(0)}{m}t \quad p_i = p_i(0) + F_i(0)t$$

decoherence rate

$$| \langle g_i | g_j \rangle | \approx c \exp\left\{ - \left[\frac{(x_i(0)-x_j(0))(p_i(0)-p_j(0))}{4\sigma^2 m} + \frac{\sigma^2(p_i(0)-p_j(0))(F_i(0)-F_j(0))}{\hbar^2} \right] t \right\}$$

Heller, J. Chem. Phys. 75, 2923 (1981)

Neria and Nitzan, J. Chem. Phys. 99, 1109 (1993)

Zhu, Nangia, Jasper, and Truhlar, J. Chem. Phys. 121, 7658 (2004)

Bedard-Hearn, Larsen, and Schwartz, J. Chem. Phys. 123, 234106 (2005)

Subotnik and Shenvi, J. Chem. Phys. 134, 024105 (2011)

Time-Dependent Schrödinger Equation

■ Mixed quantum-classical description:

$$i\hbar \frac{\partial |\psi(\mathbf{r}, t)\rangle}{\partial t} = [\hat{H}_e] |\psi(\mathbf{r}, t)\rangle$$

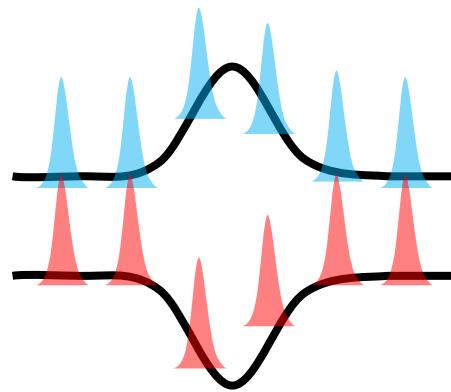
adiabatic bases

$$|\psi(\mathbf{r}, t)\rangle = \sum_i c_i(t) |\phi_i(\mathbf{r}; \mathbf{R}(t))\rangle$$

■ Fully quantum Description:

$$i\hbar \frac{\partial |\psi(\mathbf{r}, \mathbf{R}, t)\rangle}{\partial t} = \hat{H} |\psi(\mathbf{r}, \mathbf{R}, t)\rangle$$

$$|\psi(\mathbf{r}, \mathbf{R}, t)\rangle = \sum_i c_i(t) |\phi_i(\mathbf{r}; \mathbf{R})\rangle \otimes |\chi_i(\mathbf{R})\rangle$$

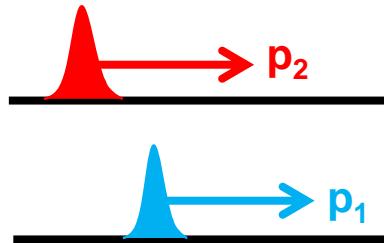


■ Hidden requirements:

1. There is only one wave packet (WP) on each potential energy surface
2. WPs on different surfaces move with similar trajectories

Phase Correction

- Two Gaussian WPs propagate with different momenta:



$$|\psi(\mathbf{r}, \mathbf{R}, t)\rangle = \sum c_i(t) |\phi_i(\mathbf{r}; \mathbf{R}_i(t))\rangle \otimes |g_i(\mathbf{R}, t)\rangle$$

$$|g_i(\mathbf{R}, t)\rangle = \frac{1}{(\sqrt{2\pi}\sigma)^{1/2}} \exp\left[-\frac{(\mathbf{x} - \mathbf{x}_i(t))^2}{4\sigma^2} + \frac{i}{\hbar} \mathbf{p}_i(t) \cdot (\mathbf{x} - \mathbf{x}_i(t)) + i\gamma_i(t) \right]$$

- First-order Approximation:

$$\mathbf{x}_i(t) = \mathbf{x}_i(0) + \frac{\mathbf{p}_i(0)}{m} t \quad \mathbf{p}_i(t) = \mathbf{p}_i(0) + \frac{\mathbf{F}_i(0)}{m} t \quad \gamma_i(t) = \gamma_i(0) + \frac{\mathbf{p}_i \cdot \mathbf{p}_i - E}{\hbar} t$$

- Effective Hamiltonian:

$$\frac{g_2(\mathbf{R}_1, t)}{g_1(\mathbf{R}_1, t)} = \exp\left[\frac{i}{m\hbar} \mathbf{p}_1 \cdot (\mathbf{p}_1 - \mathbf{p}_2) \right] \quad H_{eff} = \begin{pmatrix} \frac{-\mathbf{p}_1(t) \cdot \mathbf{p}_a(t)}{m} & -\frac{i}{m\hbar} \mathbf{p}_a(t) \cdot \mathbf{d}_{12}(t) \\ -\frac{i}{m\hbar} \mathbf{p}_a(t) \cdot \mathbf{d}_{21}(t) & \frac{-\mathbf{p}_2(t) \cdot \mathbf{p}_a(t)}{m} \end{pmatrix}$$

Heller, J. Chem. Phys. 75, 2923 (1981)

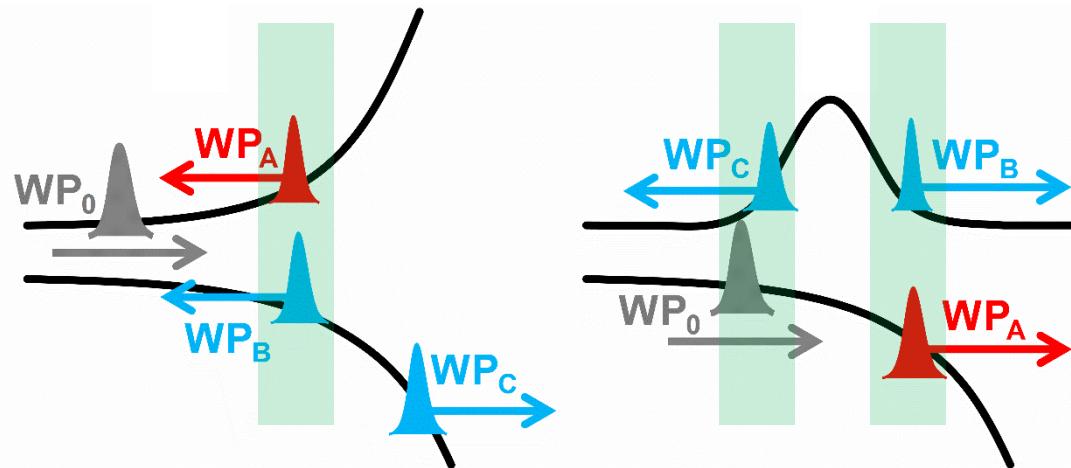
Shenvi and Subotnik, J. Chem. Phys. 134, 024105 (2011)

Shenvi, Subotnik, and Yang, J. Chem. Phys. 135, 024101 (2011)

Zhu, Sci. Rep. 6, 24198 (2016)

Branching due to Wave Packet Reflection

- Multiple Gaussian WPs on a PES generated due to reflection:



$$|\psi\rangle = c_A |g_A(x); 1\rangle + c_B |g_B(x); 2\rangle + c_C |\cancel{g_C}(x); 2\rangle$$

$$|\psi\rangle = c_A |g_A(x); 2\rangle + c_B |g_B(x); 1\rangle + c_C |\cancel{g_C}(x); 1\rangle$$

Multiple Gaussian WPs are necessary in certain cases

The WP away from the active trajectory needs to be eliminated,
which gives “decoherence correction”

Branching due to wave packet reflection cannot be treated as perturbation



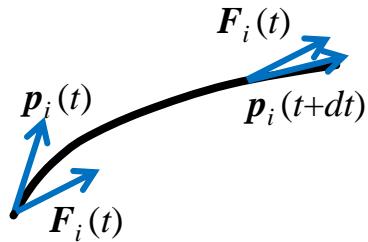
Outline

- Introduction to Mixed Quantum-Classical Dynamics
- Interpretation of Decoherence Correction
- **Branching Corrected Surface Hopping**
- New Energy-Based Decoherence Time Formulas
- Branching Corrected Mean Field

Branching Corrected Surface Hopping (BCSH)

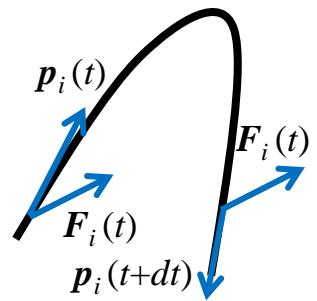


- Resetting wavefunction by judgment of trajectory reflection:



no reflection

$$\text{sign}\{\mathbf{F}_i(t) \cdot \mathbf{p}_i(t)\} = \text{sign}\{\mathbf{F}_i(t) \cdot \mathbf{p}_i(t + dt)\}$$



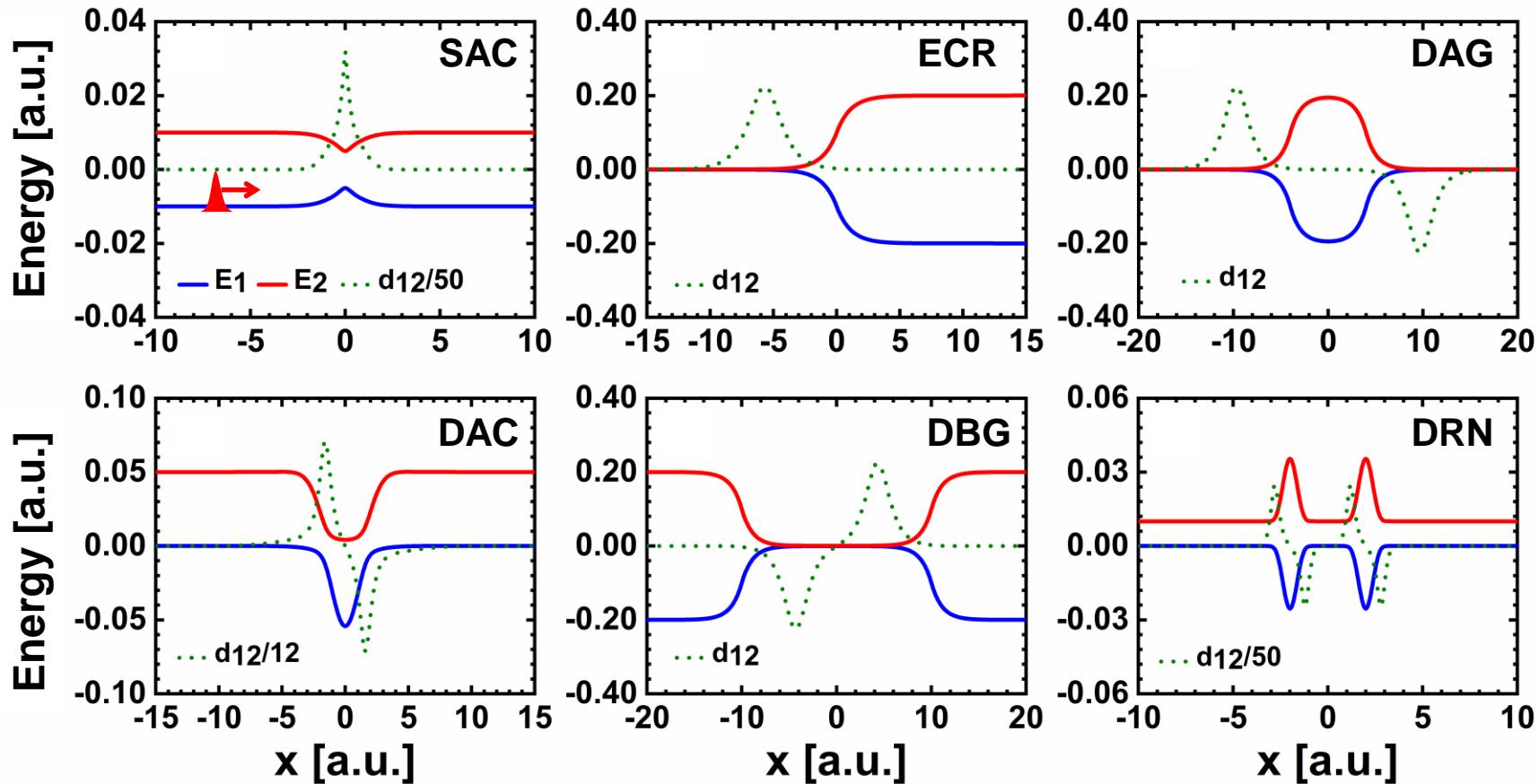
reflection

$$\text{sign}\{\mathbf{F}_i(t) \cdot \mathbf{p}_i(t)\} = -\text{sign}\{\mathbf{F}_i(t) \cdot \mathbf{p}_i(t + dt)\}$$

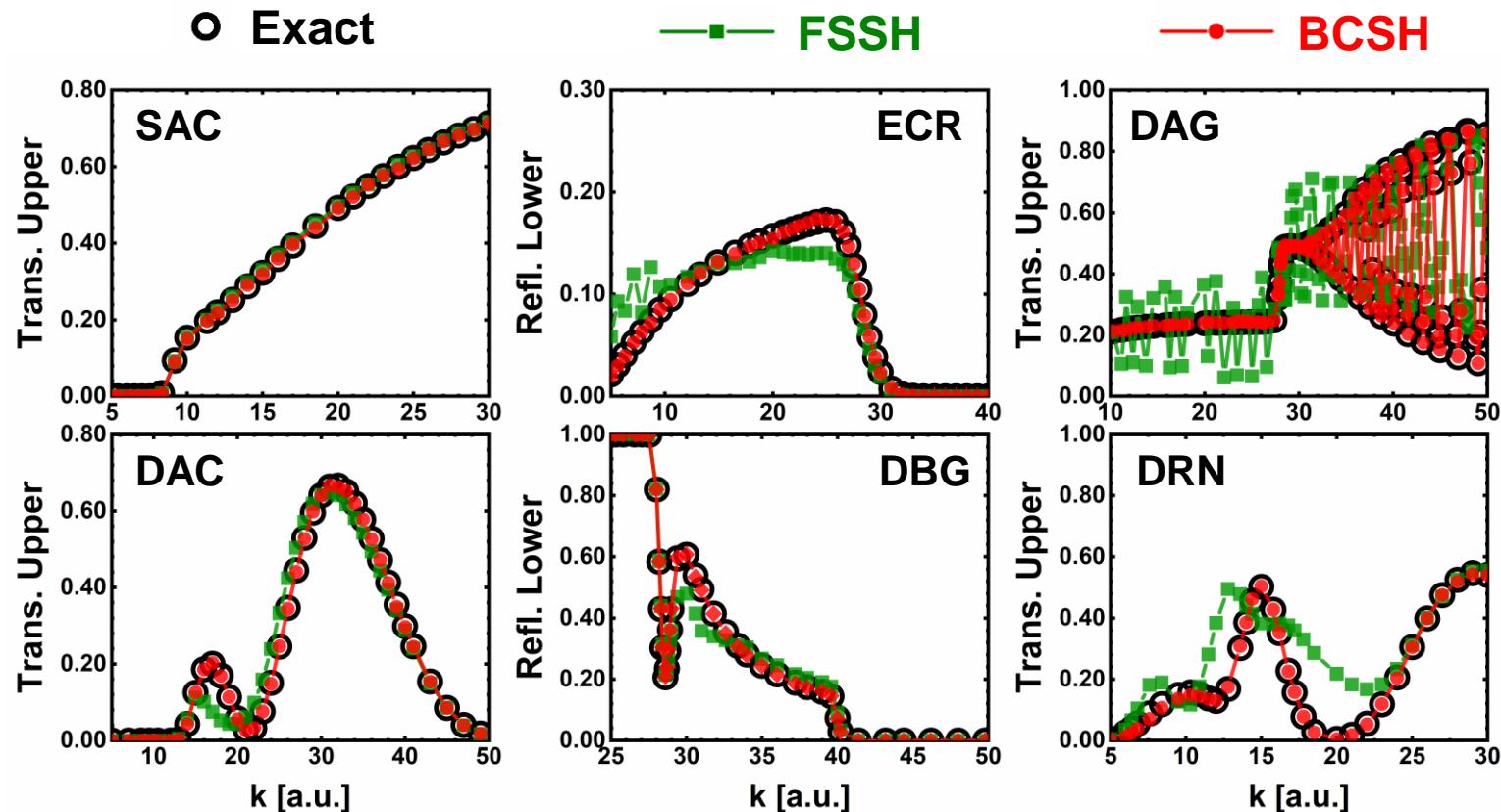
In two-level systems, when the active or the non-active surface is reflected, the wave function is collapsed to the active state ($c_a = 1$ and $c_{na} = 0$)

In multilevel systems, we classify states into two groups

Standard Scattering Models

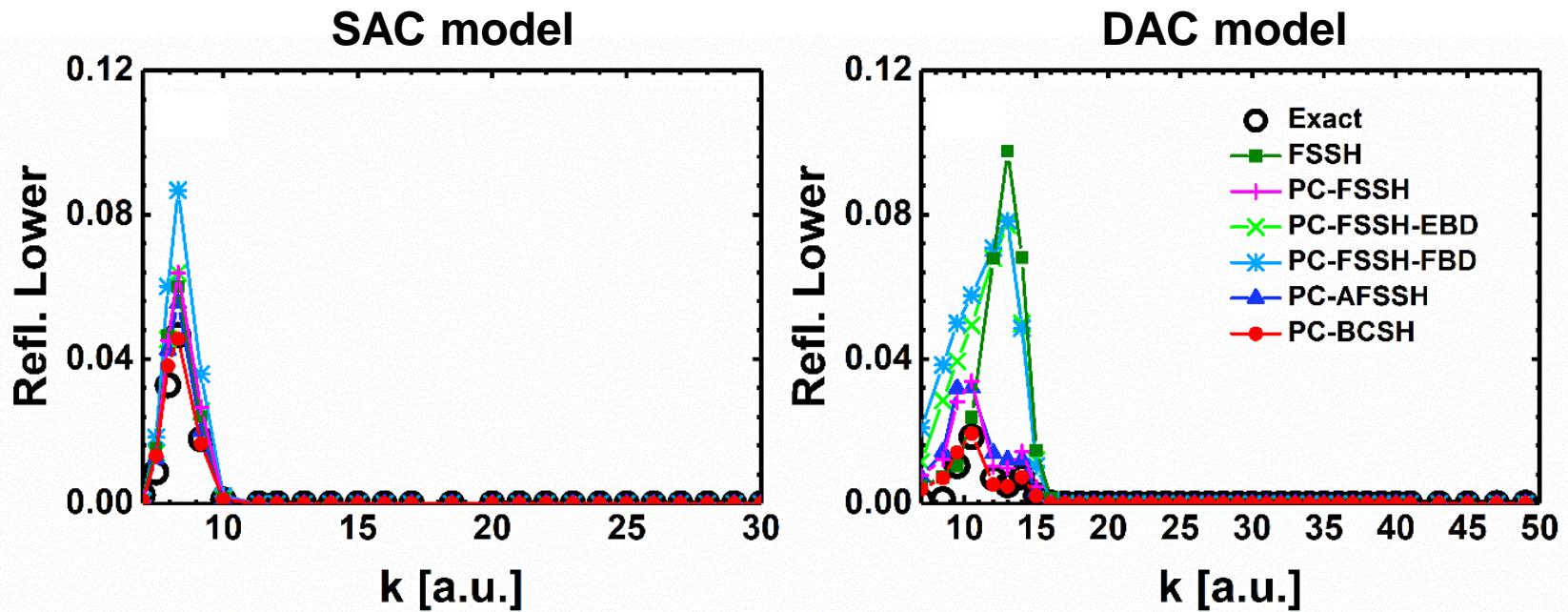


Major Channel Performance of BCSH



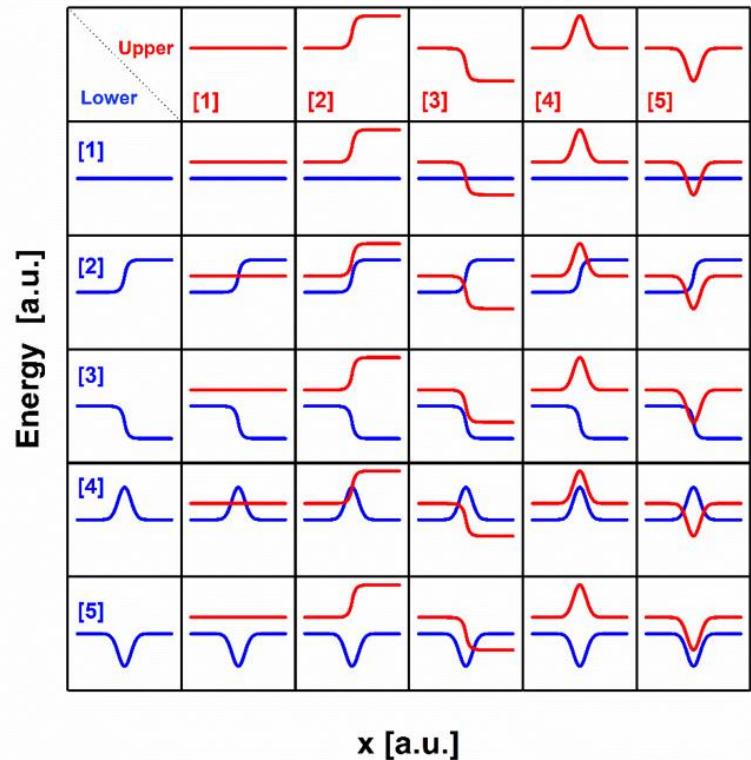
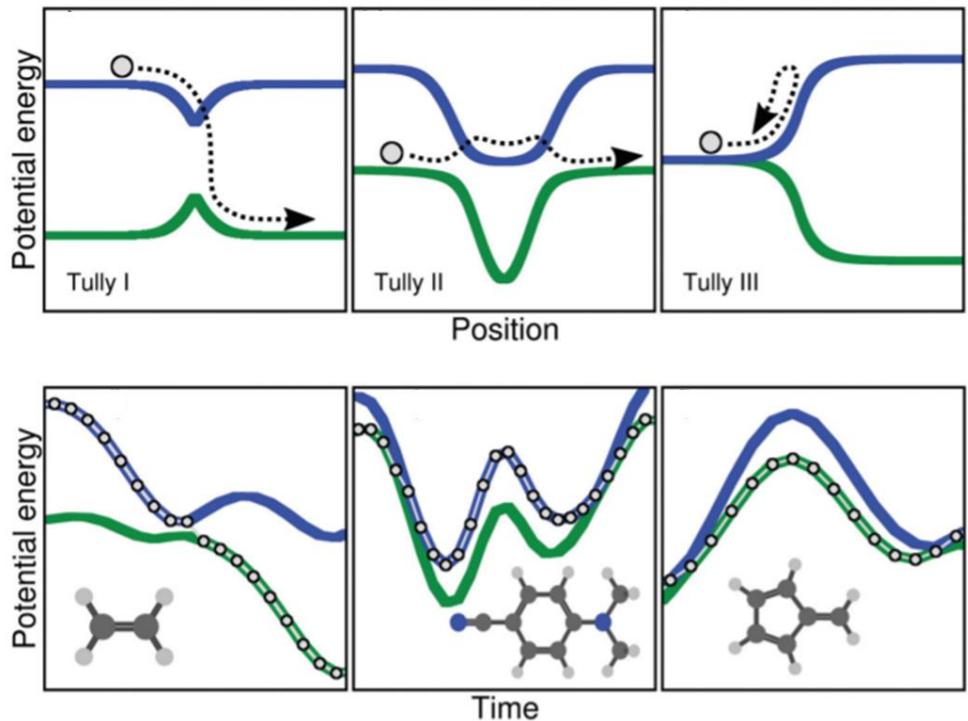
BCSH reproduces the quantum results almost exactly

Minor Channel Performance of BCSH



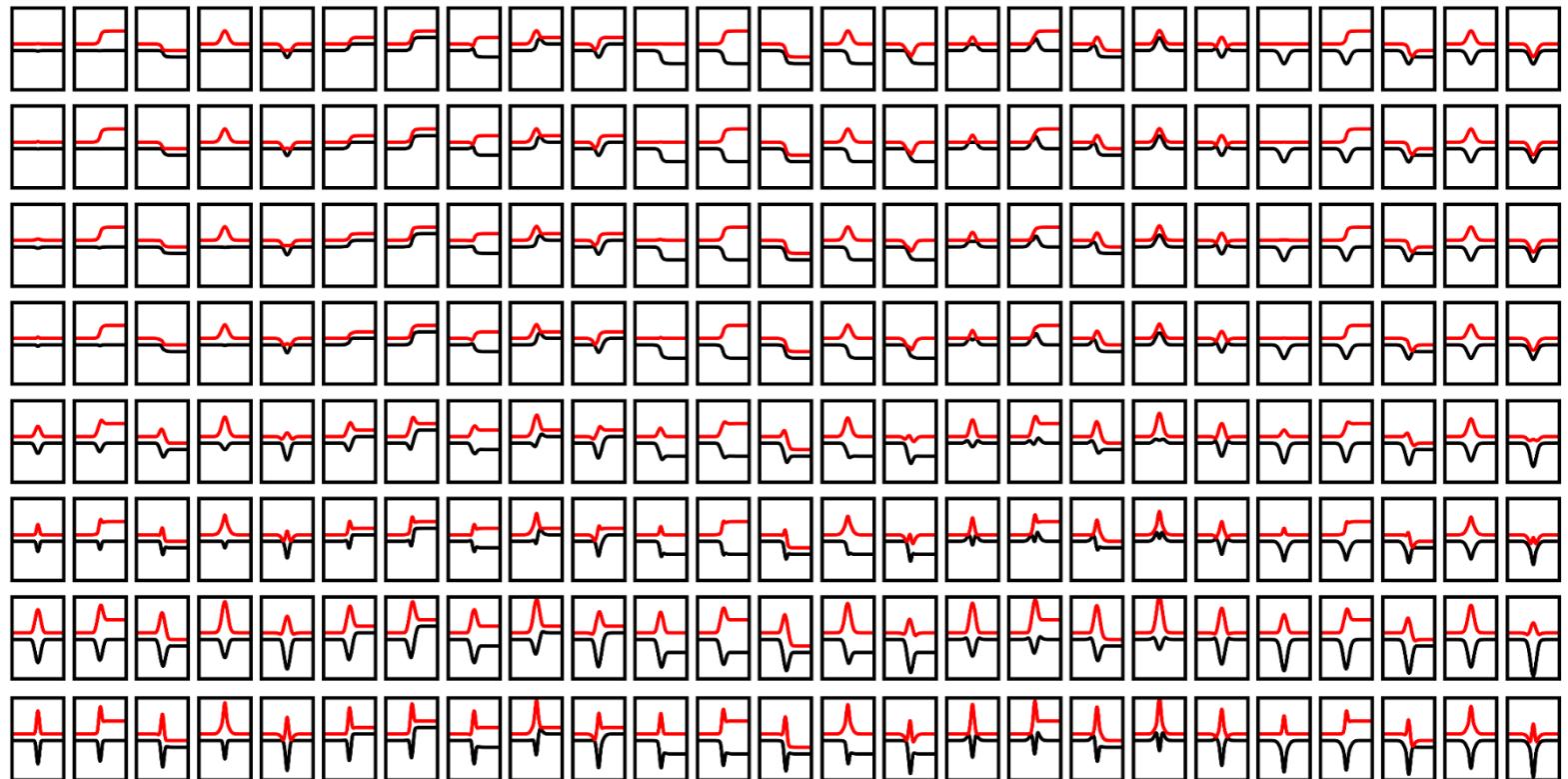
Decoherence correction is not very important in these models
BCSH reproduces the quantum results even for minor channels

Two-Level Model Base



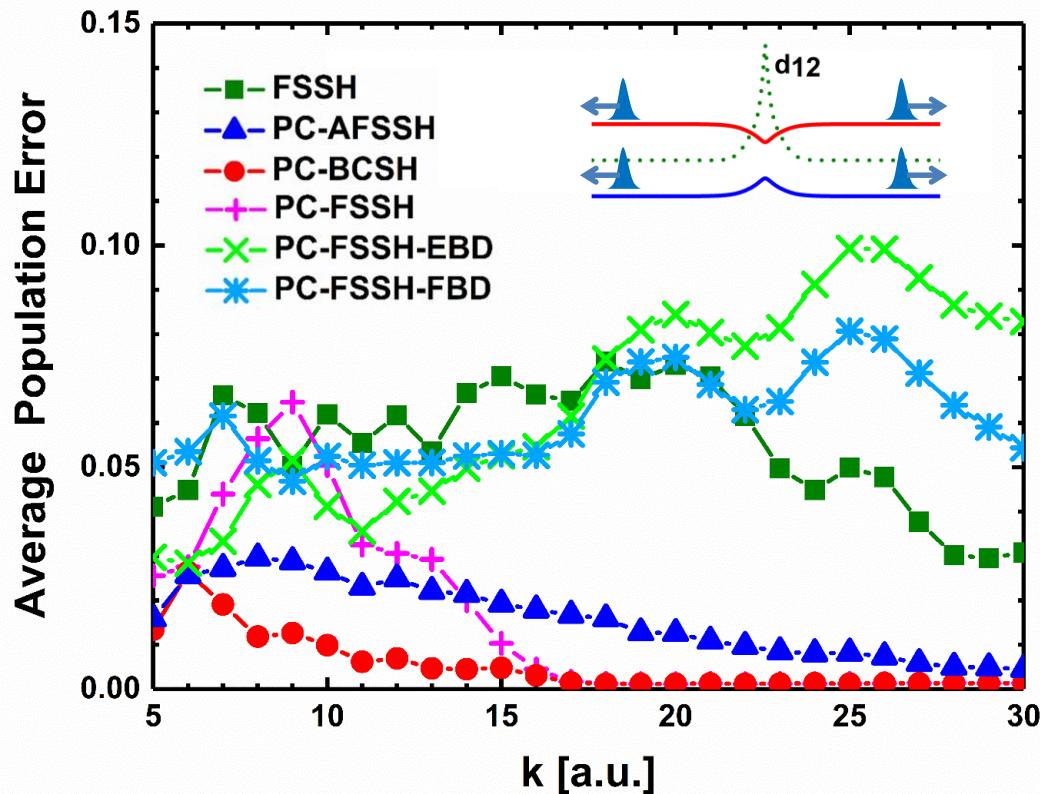
25 combinations of diabatic potential energy surfaces are constructed

Two-Level Model Base



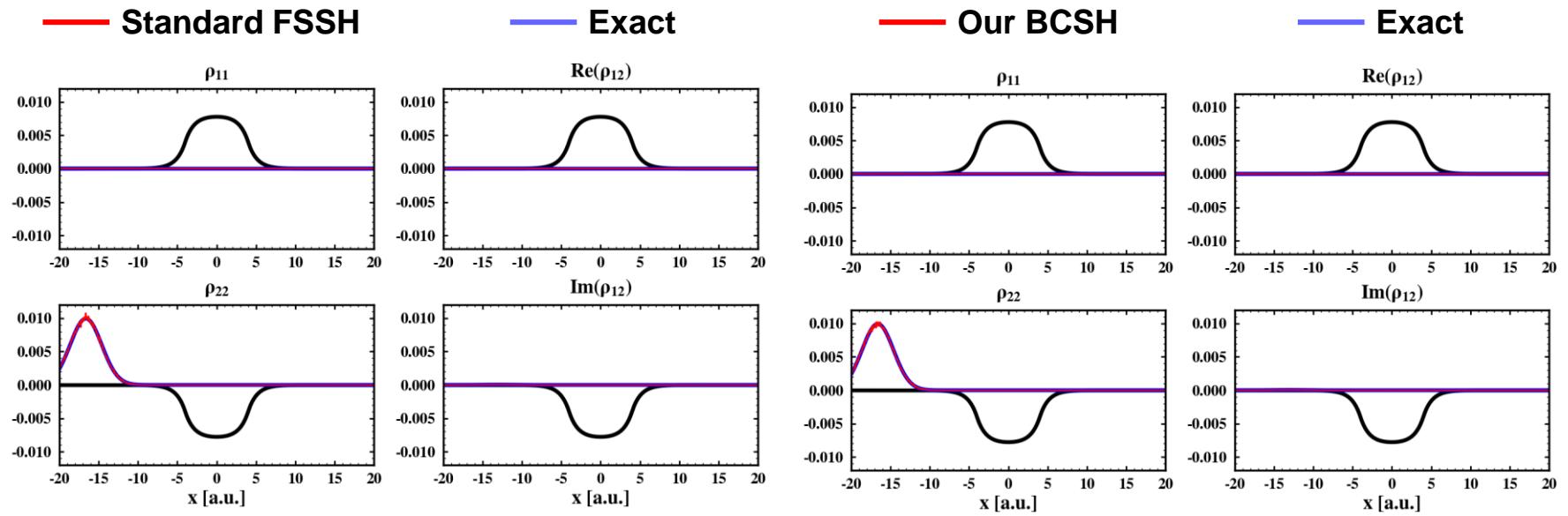
**200 two-level models are constructed to build the model base
with 4 strengths and 2 widths for the diabatic coupling**

Performance of BCSH in the Model Base



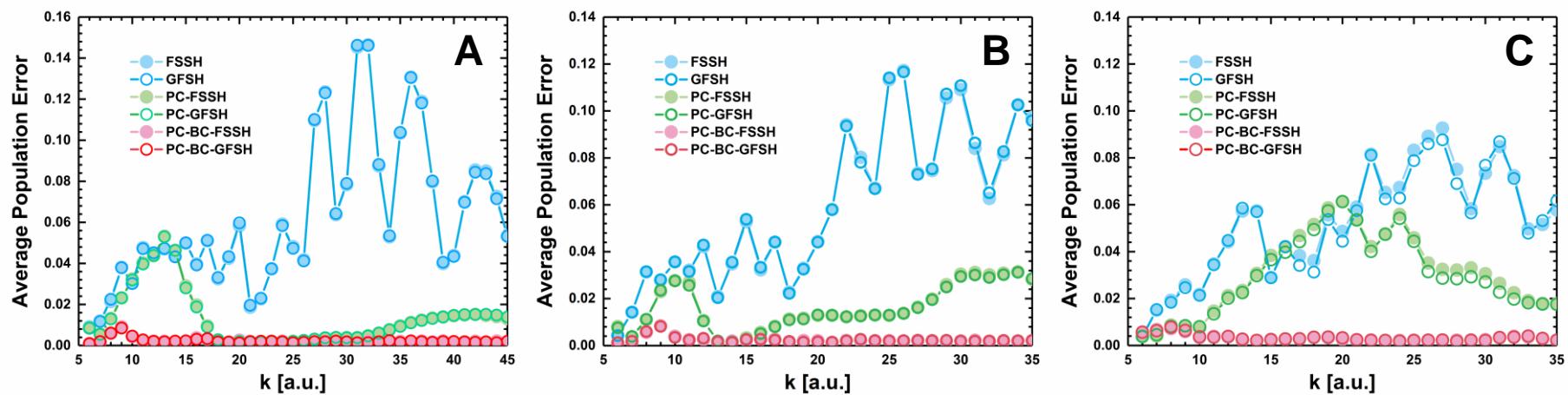
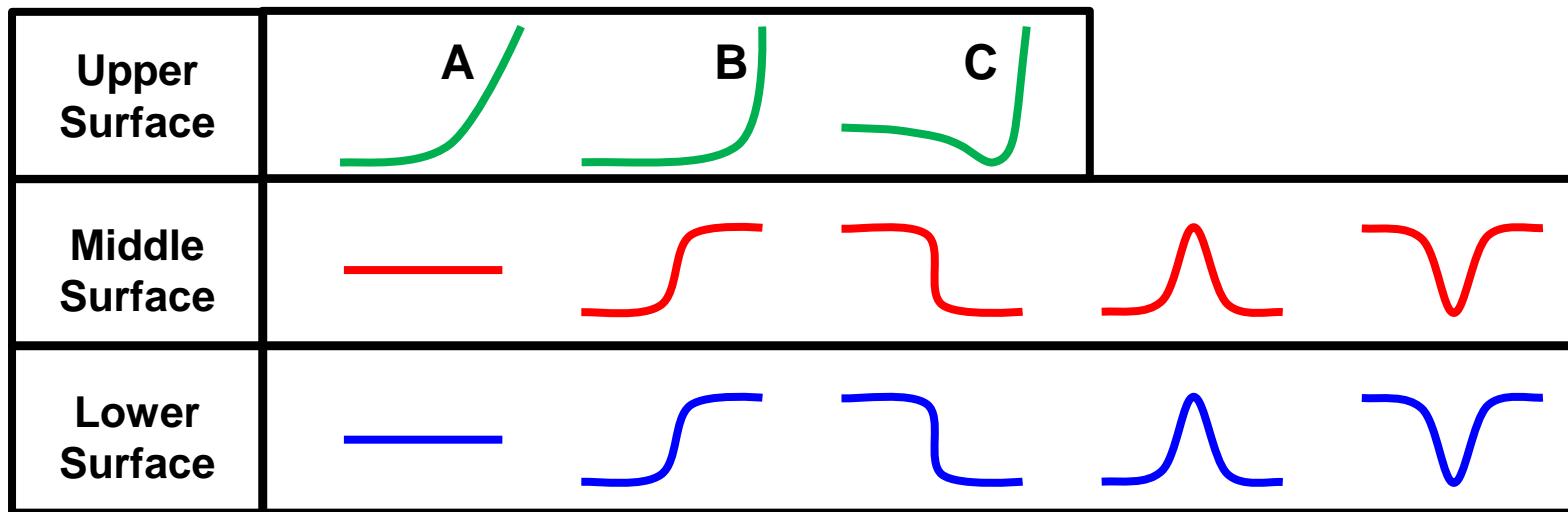
BCSH shows the highest performance in the 200 diverse models

Time-Dependent Population and Coherence

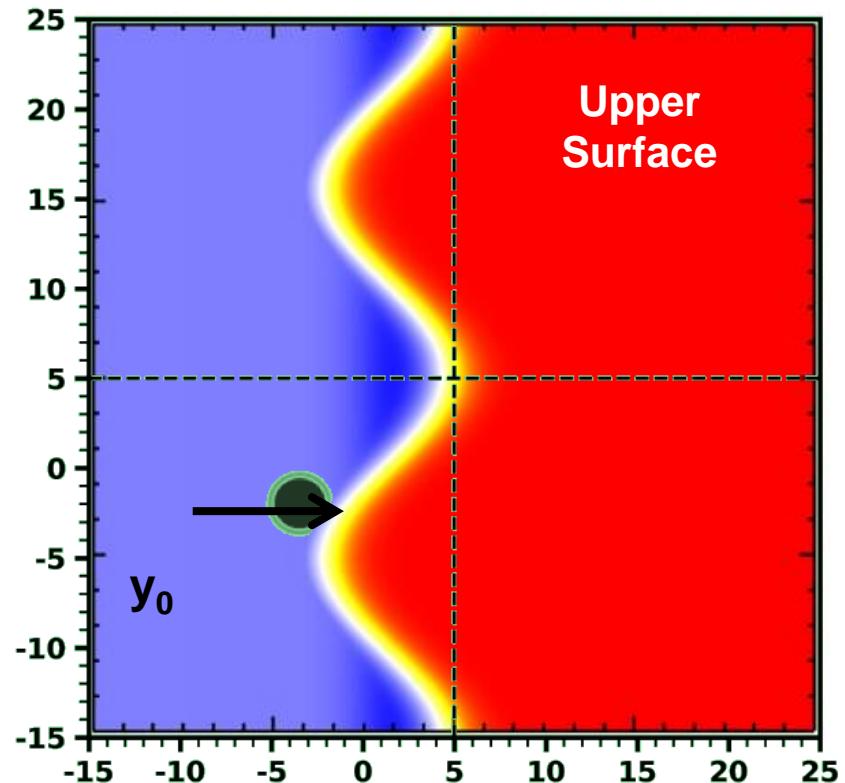
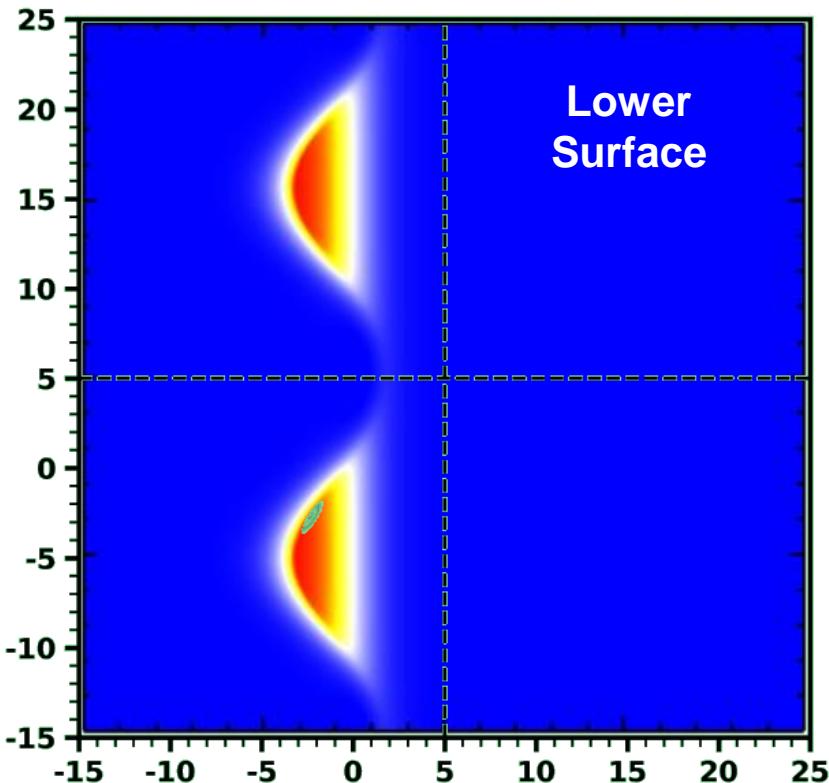


BCSH reproduces both the population and coherence of the quantum dynamics
as demonstrated in the DAG model with $k = 25$

Three-Level Model Base

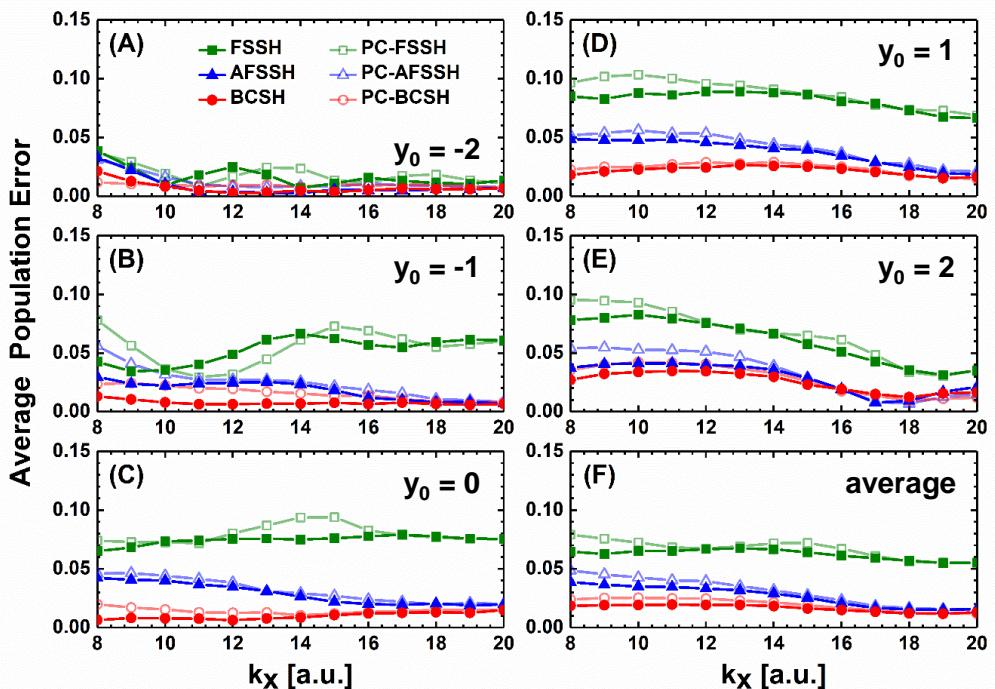
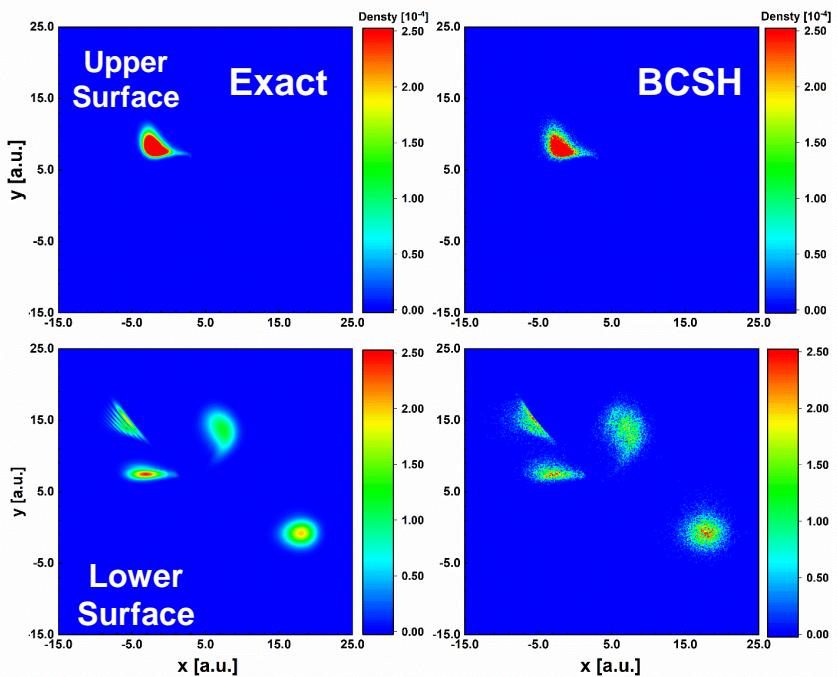


Subotnik's Two-Dimensional Model



2D models are still not extensively investigated in the literature

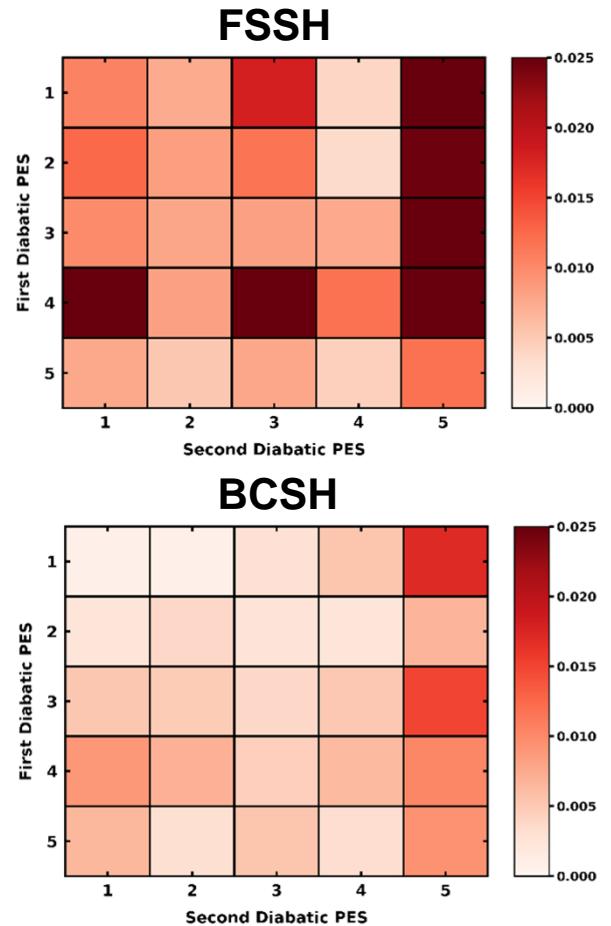
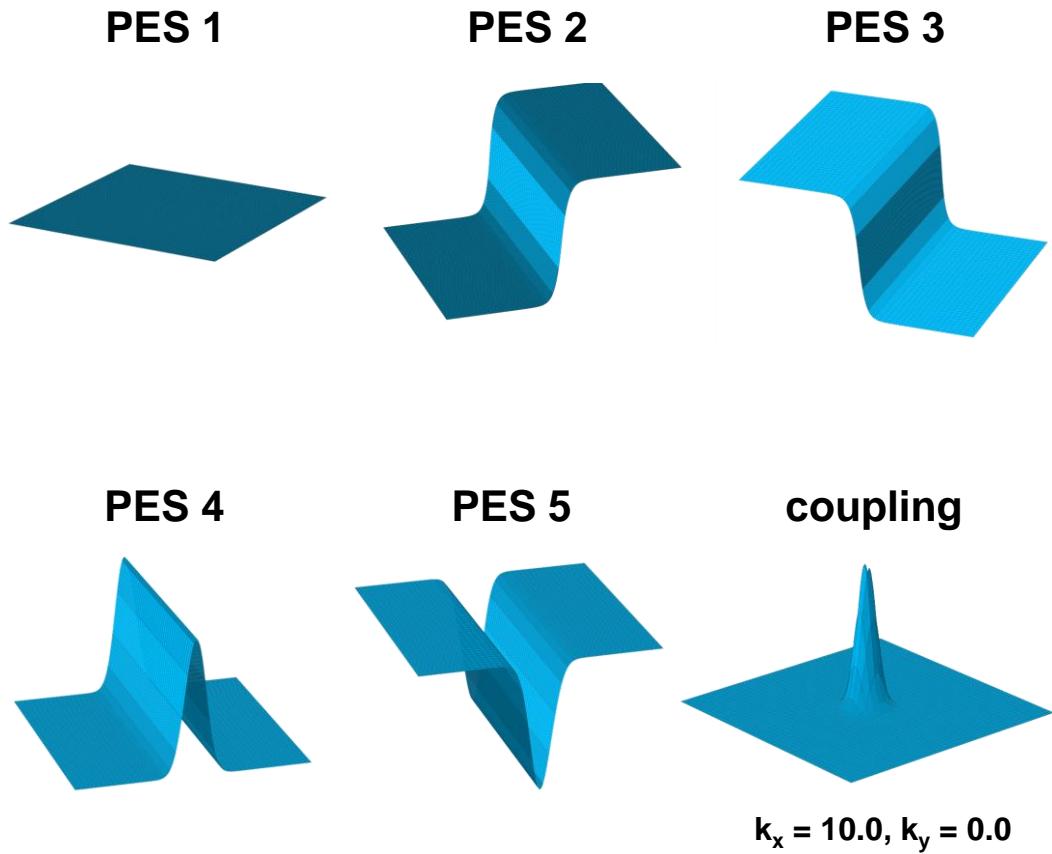
Performance of BCSH



BCSH obtains almost the exact population distribution of different channels



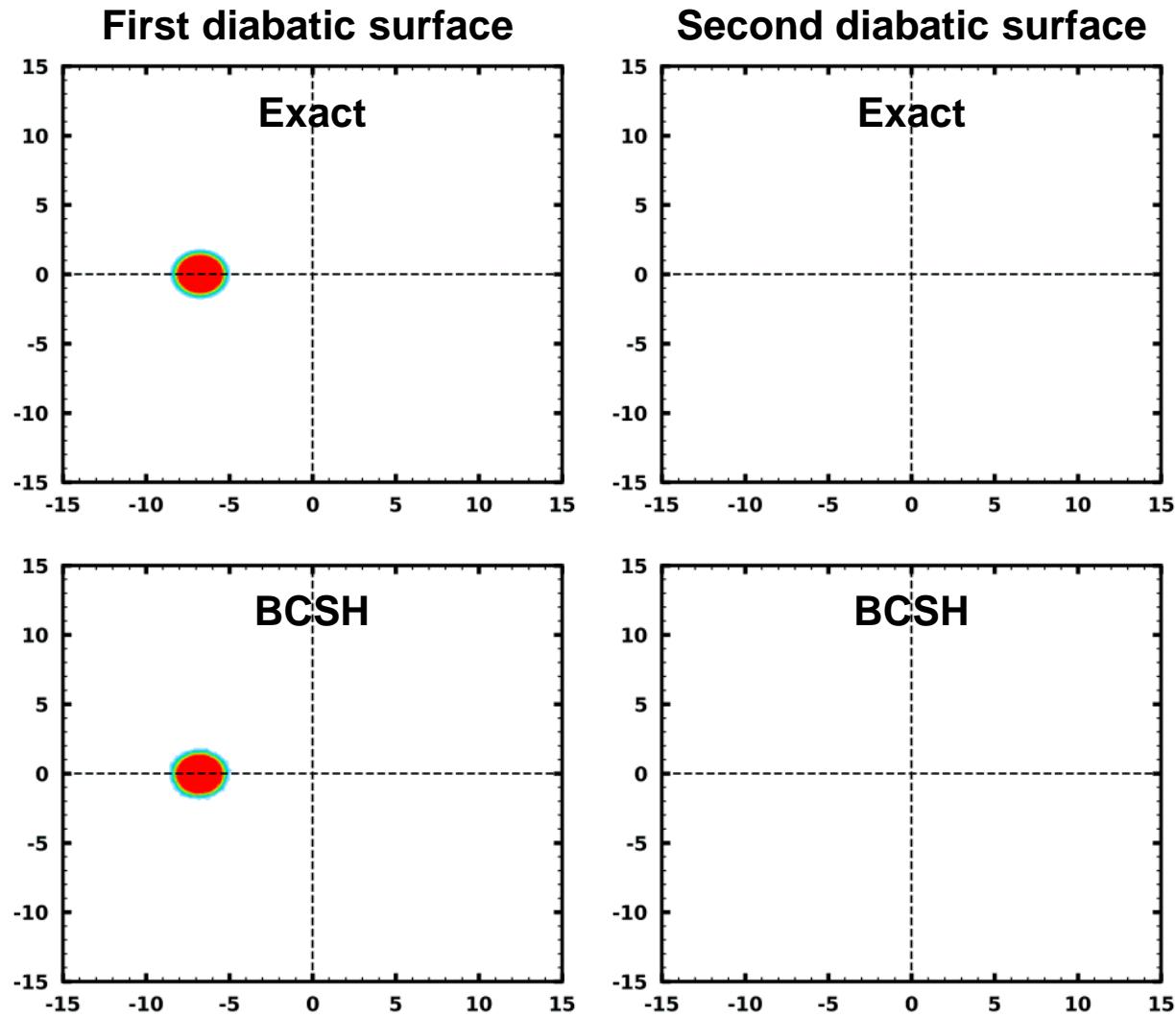
Two-Dimensional Two-Level Model Base



BCSH significantly increases the accuracy in 2D systems



Time Evolution of Quantum Population





Outline

- Introduction to Mixed Quantum-Classical Dynamics
- Interpretation of Decoherence Correction
- Branching Corrected Surface Hopping
- **New Energy-Based Decoherence Time Formulas**
- Branching Corrected Mean Field



New Decoherence Time Formula

■ Traditional Energy-Based Formula

$$\tau_{ai} = \frac{\hbar}{|E_a - E_i|} \left(1 + \frac{A}{E_{kin}} \right)$$

Decoherence is stronger for larger kinetic energy, which is against the branching picture



■ Modified Linear Formula

$$\tau_{ai} = \frac{\hbar}{|E_a - E_i|} (A + B \cdot E_{kin})$$

Hold the basic formalism and uncertainty principle

■ Modified Exponential Formula

$$\tau_{ai} = A \exp\left(\frac{B \cdot E_{kin}}{|E_a - E_i|}\right)$$

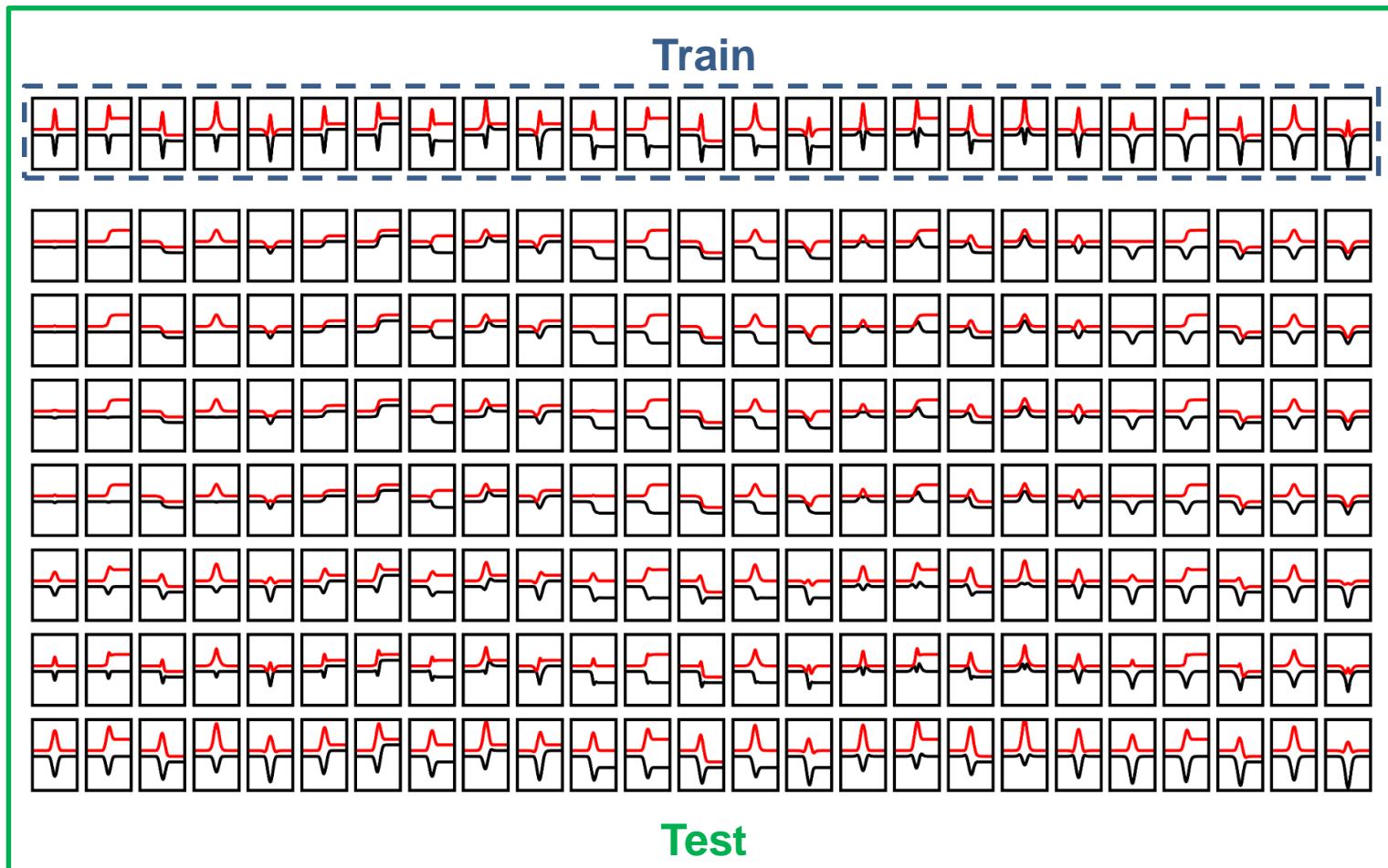
Tune the dependence on nuclear kinetic energy

Zhu, Nangia, Jasper, and Truhlar, J. Chem. Phys. 121, 7658 (2004)

Granucci and Persico, J. Chem. Phys. 126, 134114 (2007)

Xiao, Xu, and Wang*, DOI:10.1063/1674-0068/cjcp2006098 (2020)

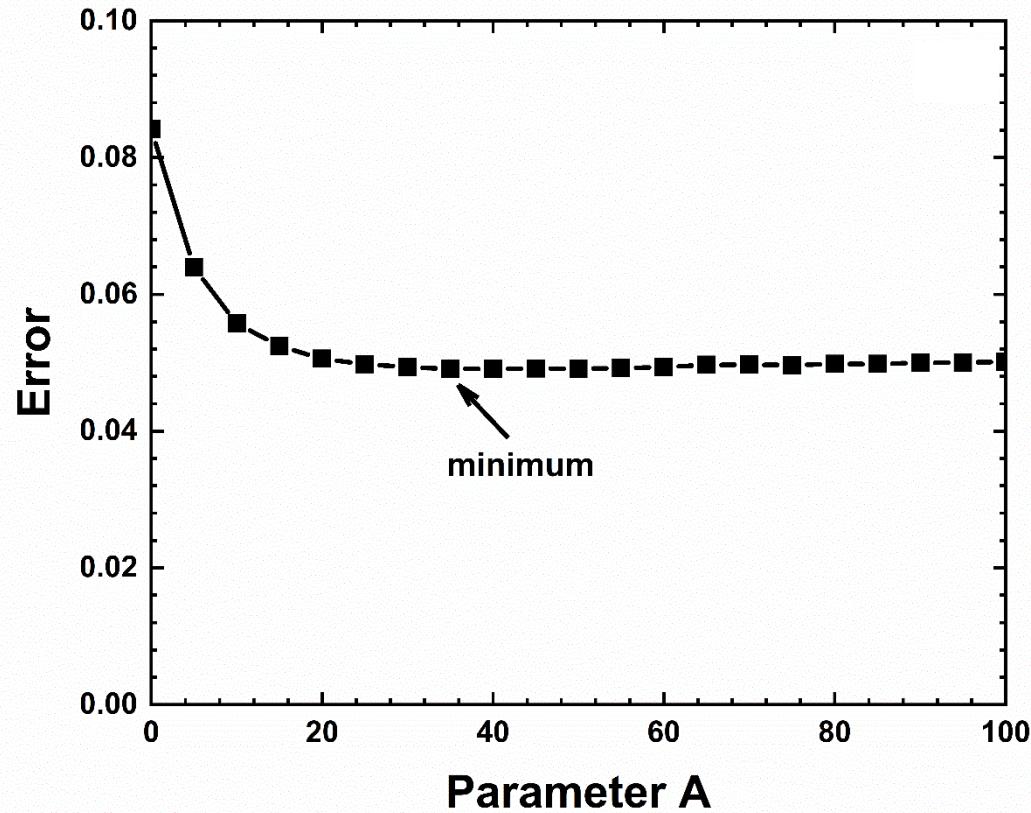
Parameter Scan



The parameters are obtained in a machine-learning fashion

Traditional Decoherence Time Formula

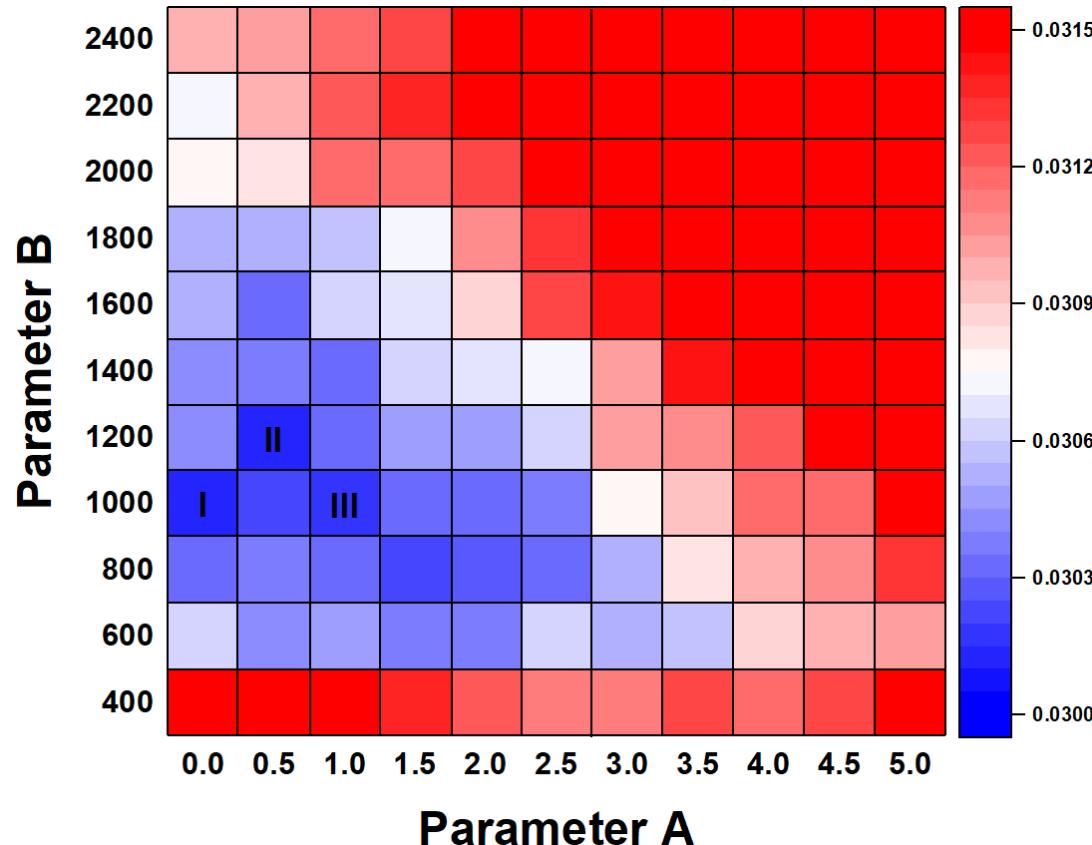
$$\tau_{ai} = \frac{\hbar}{|E_a - E_i|} \left(1 + \frac{A}{E_{kin}} \right)$$



The optimal parameter gives no decoherence correction

Linear Decoherence Time Formula

$$\tau_{ai} = \frac{\hbar}{|E_a - E_i|} (A + B \cdot E_{kin})$$

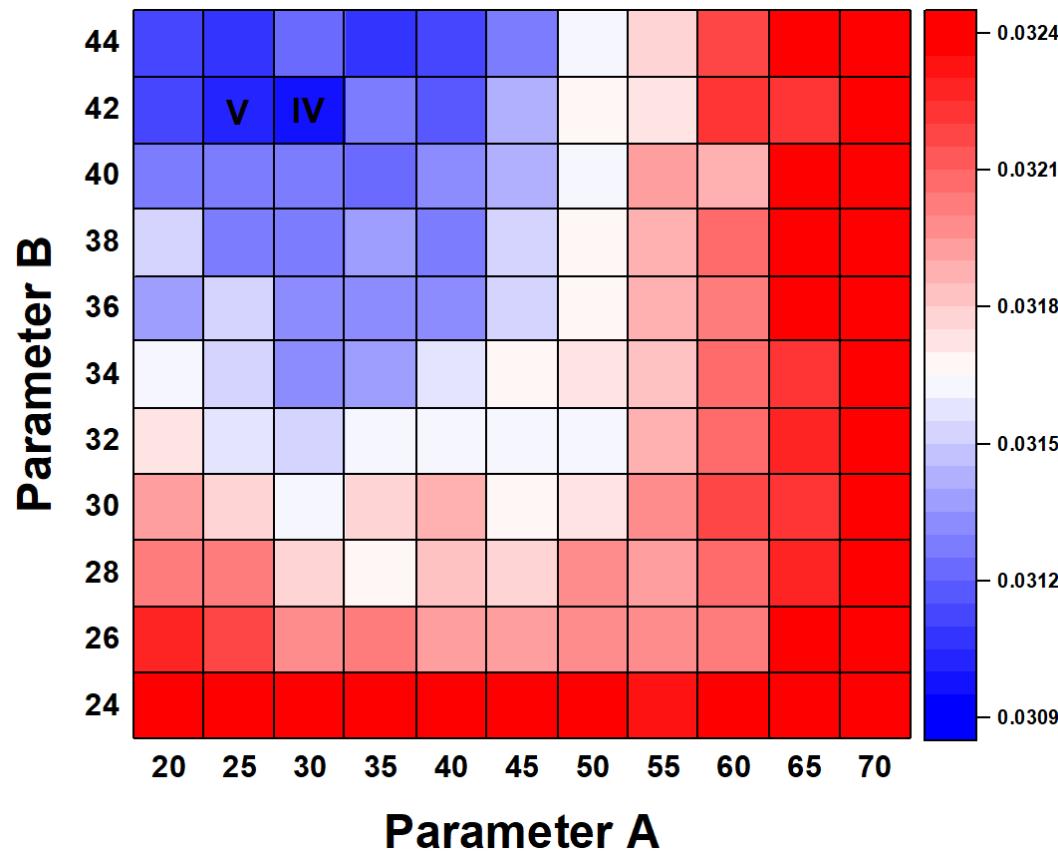


Optimal parameter set corresponds to small A and medium B



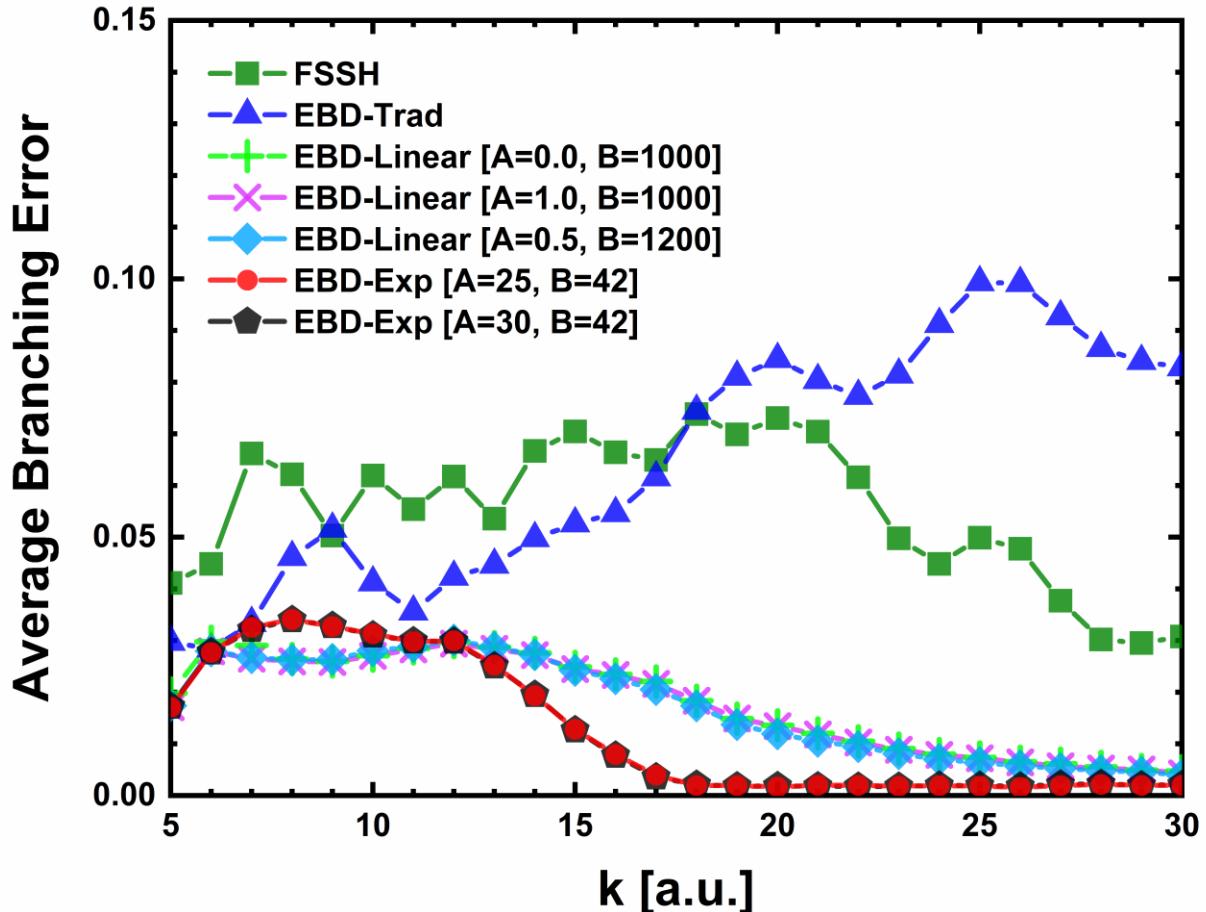
Exponential Decoherence Time Formula

$$\tau_{ai} = A \exp\left(\frac{B \cdot E_{kin}}{|E_a - E_i|}\right)$$



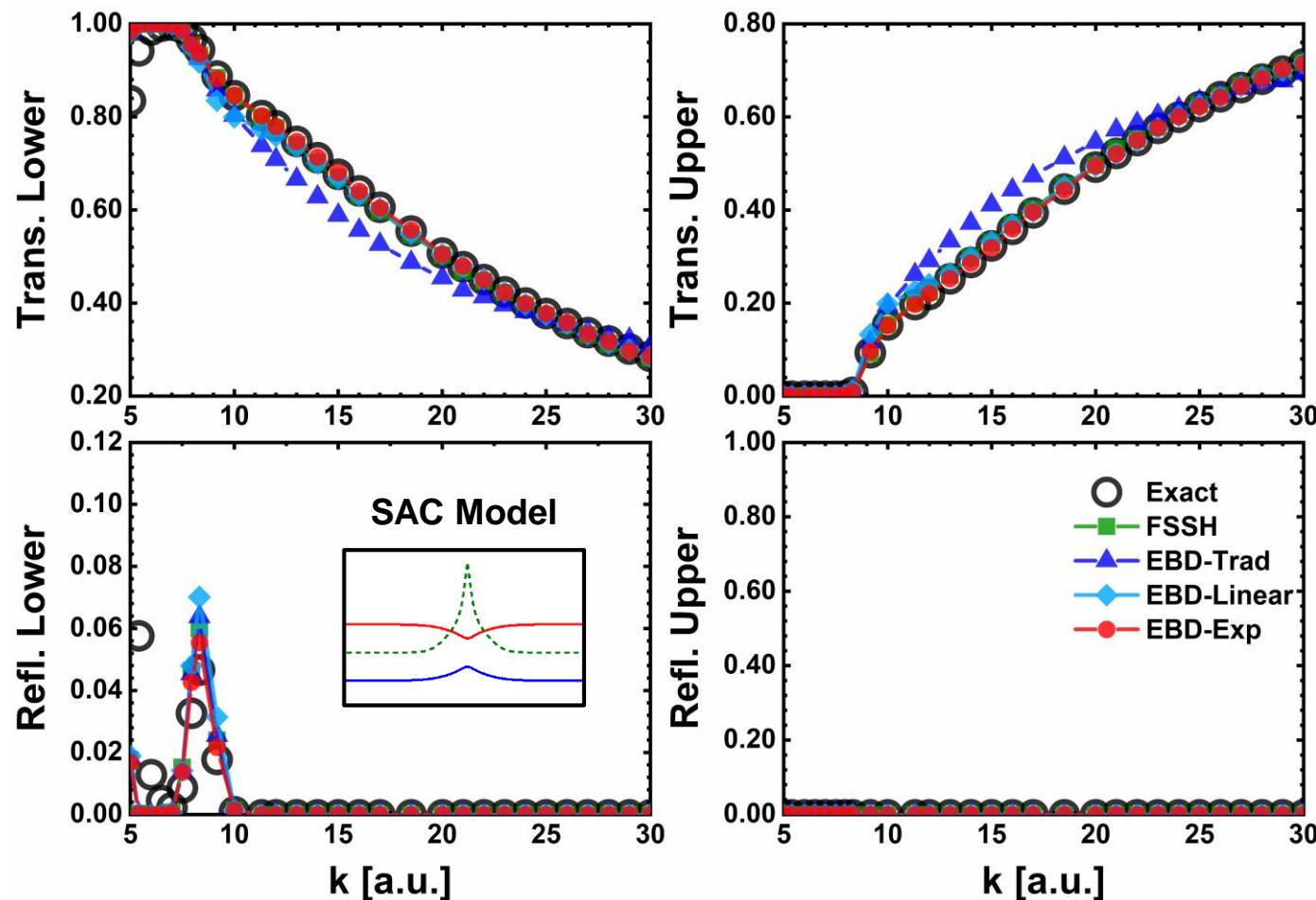
Optimal parameter set corresponds to small A and large B

Average Errors of the Model Base



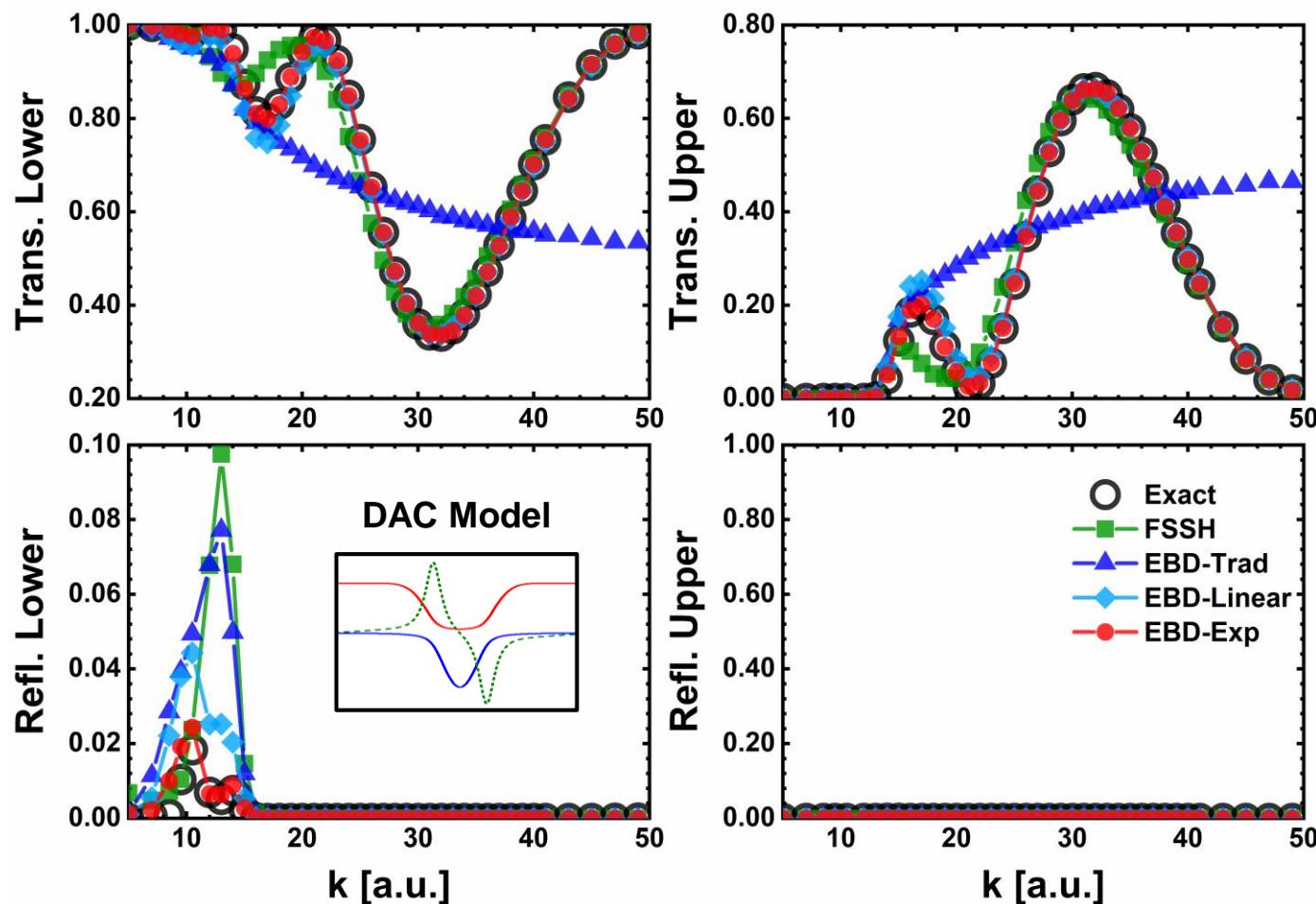
Average errors of the two modified formulas are systematically reduced

SAC Model



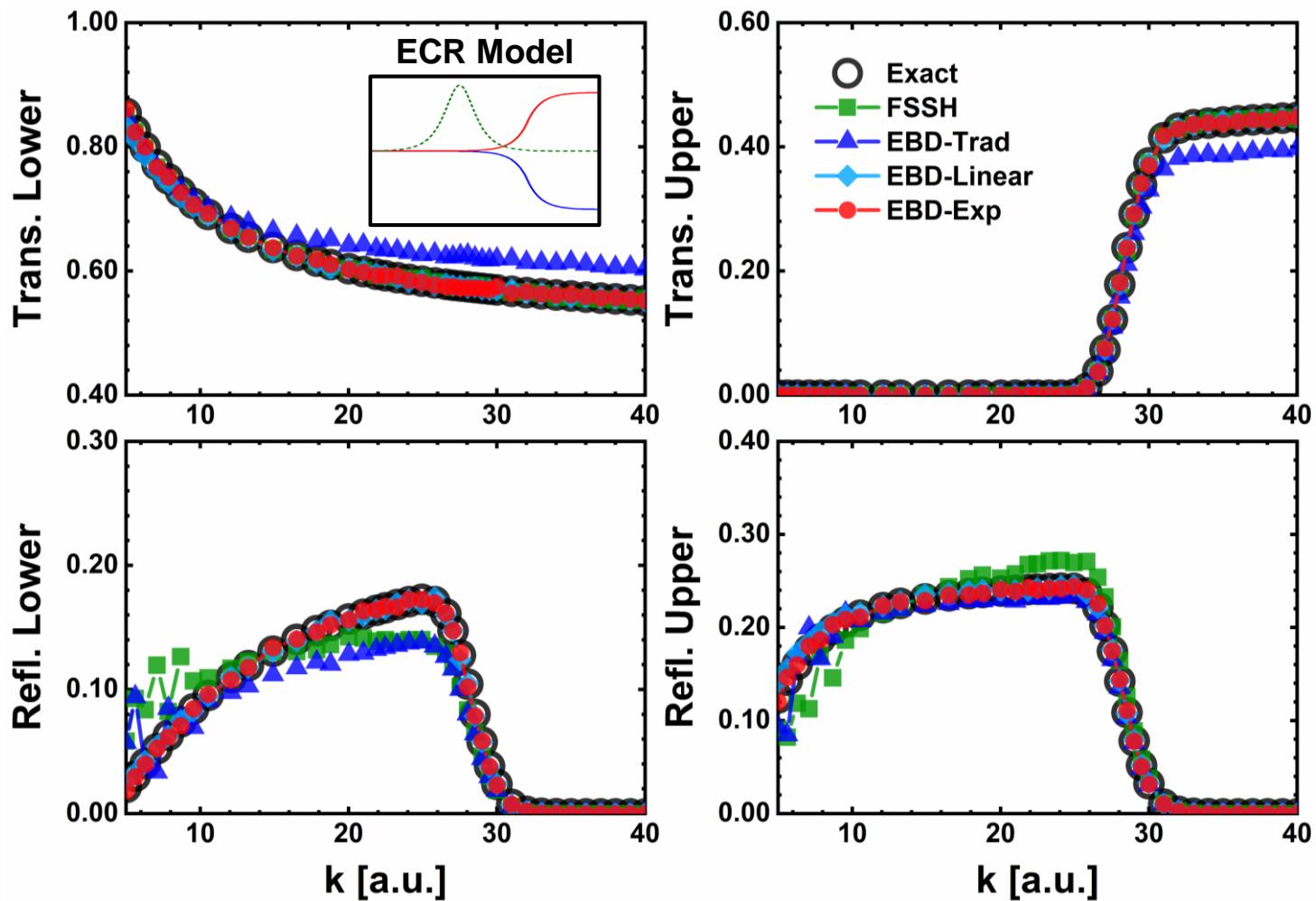
Our modified decoherence time formulas work well the SAC model

DAC Model



Our formulas correctly describe the quantum interference effects

ECR Model



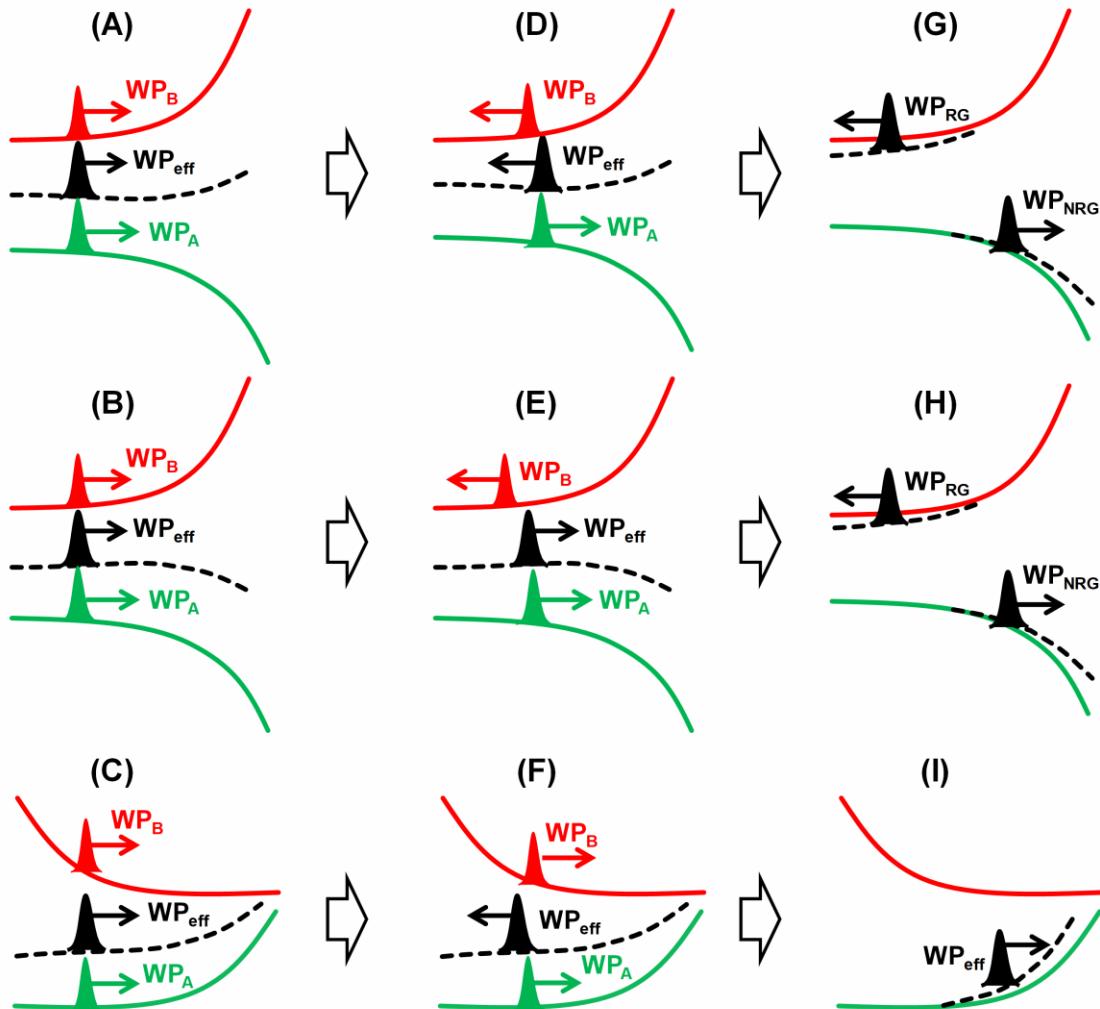
Both our formulas capture the correct strength of decoherence



Outline

- Introduction to Mixed Quantum-Classical Dynamics
- Interpretation of Decoherence Correction
- Branching Corrected Surface Hopping
- New Energy-Based Decoherence Time Formulas
- **Branching Corrected Mean Field**

Branching in the Mean Field Picture



■ Reference Trajectory:

In surface hopping, the reference trajectory is characterized by the active state. In mean field dynamics, it is the mean field trajectory

■ Branching:

Besides the WPs on adiabatic PESs, the mean field WP can be also reflected. When the mean field trajectory cannot describe all WPs, corrections are needed

Branching Corrected Mean Field BCMF-s and BCMF-w

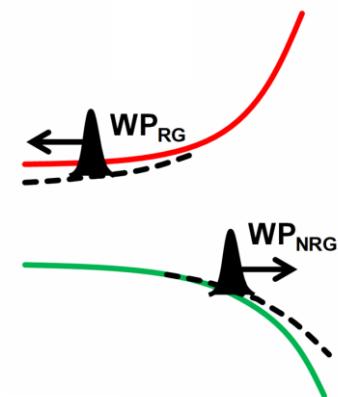


- Propagate the wave function and nuclei with the average forces
- Check whether the adiabatic WPs and the mean field WP are reflected and classify the adiabatic WPs into RG and NRG groups

$$P_{RG} = \sum_{i \in RG} |c_i|^2 \quad P_{NRG} = \sum_{i \in NRG} |c_i|^2$$

- In BCMF-s, choose either RG or NRG, and reset the corresponding wavefunction coefficients

$$c'_{i \in NRG} = 0 \quad c'_{i \in RG} = c_i / P_{RG}^{1/2} \quad c'_{i \in RG} = 0 \quad c'_{i \in NRG} = c_i / P_{NRG}^{1/2}$$

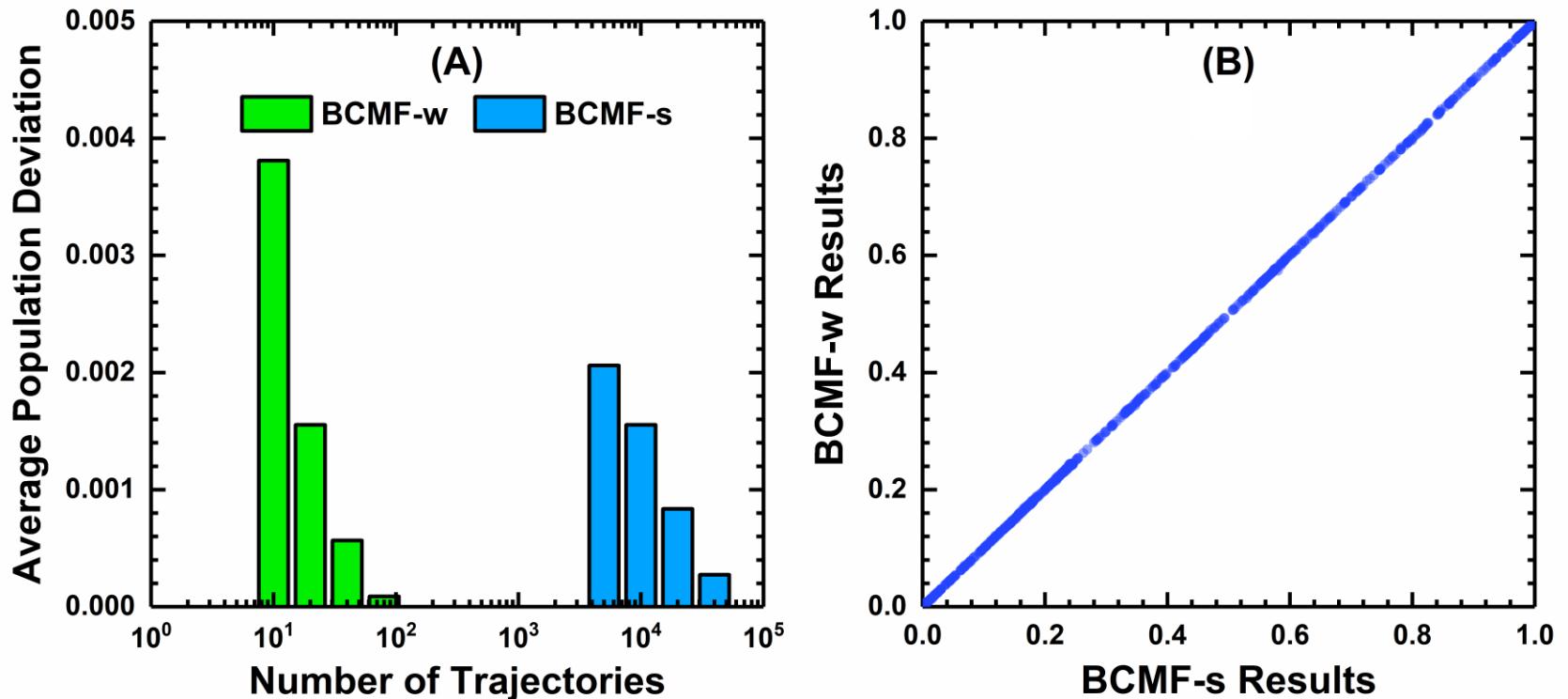


- In BCMF-w, run new mean field trajectories for both RG and NRG with modified weights

$$w_{RG} = w_p P_{RG} \quad w_{NRG} = w_p P_{NRG}$$

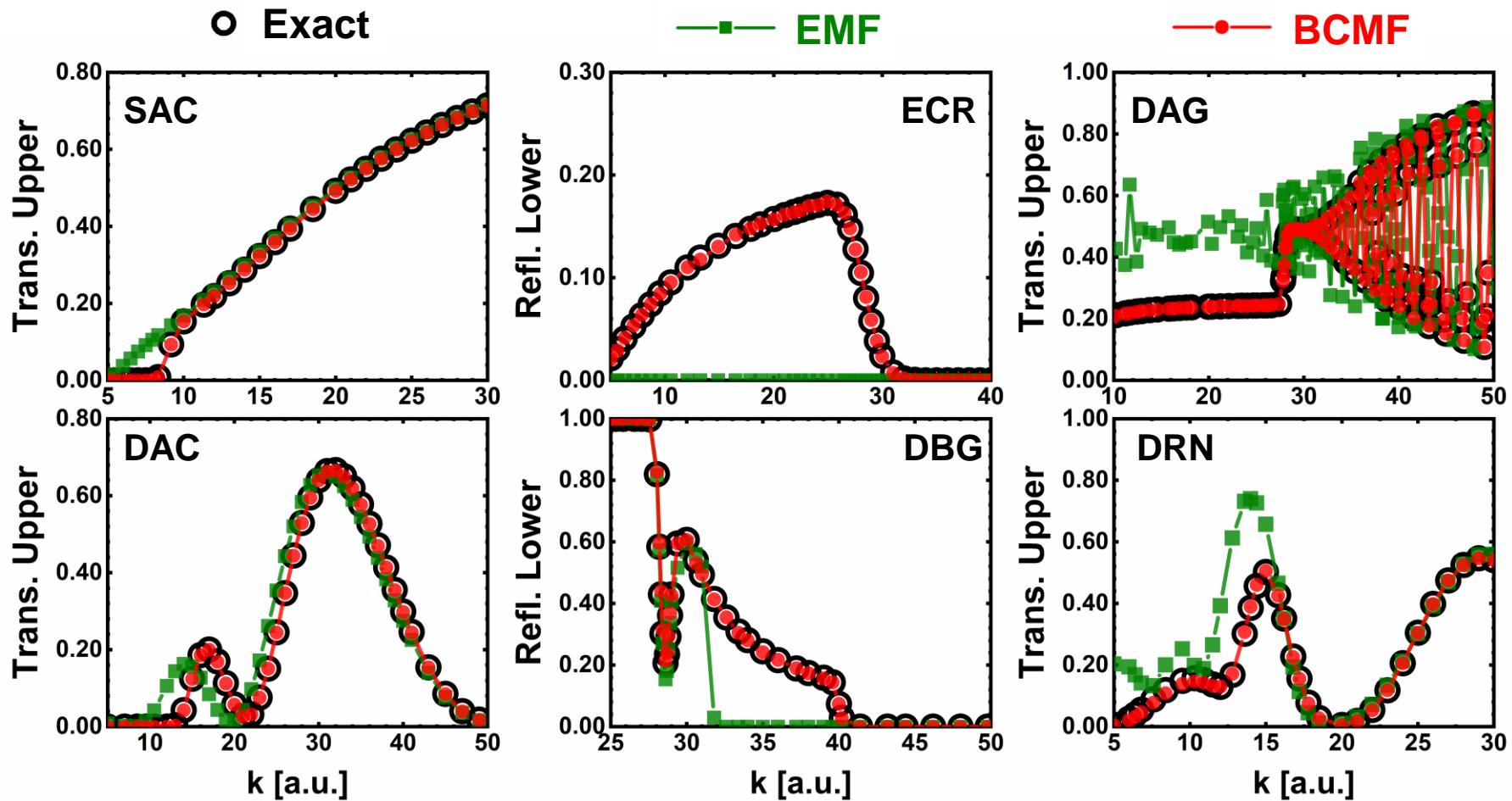
- Obtain the population of each state considering energy conservation

BCMF-s vs. BCMF-w Algorithms



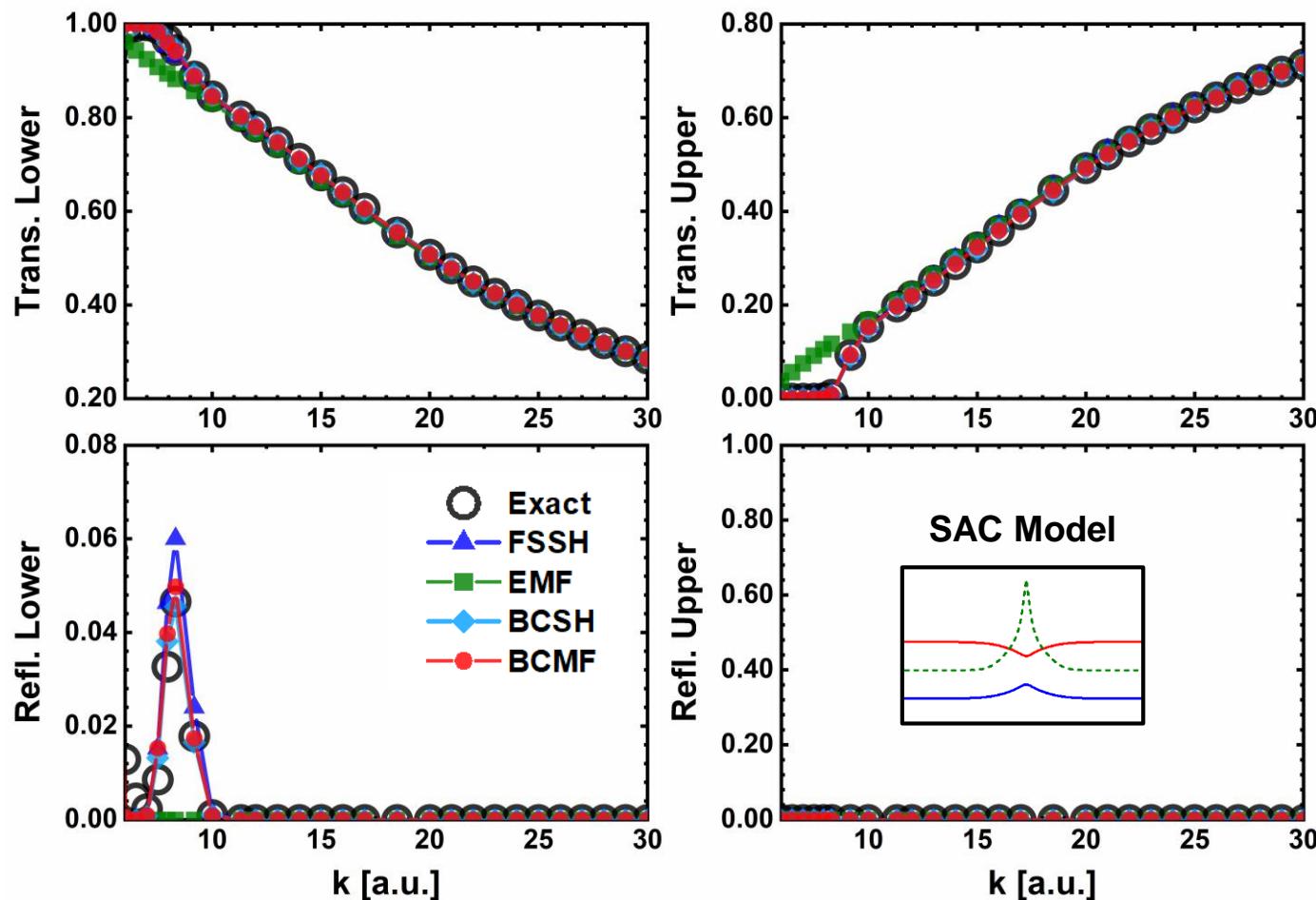
Converged results of BCMF-s and BCMF-w are intrinsically identical
 BCMF-s is more efficient in complex systems for long time simulations
 BCMF-w is more efficient for simpler cases

BCMF vs. EMF in Standard Models



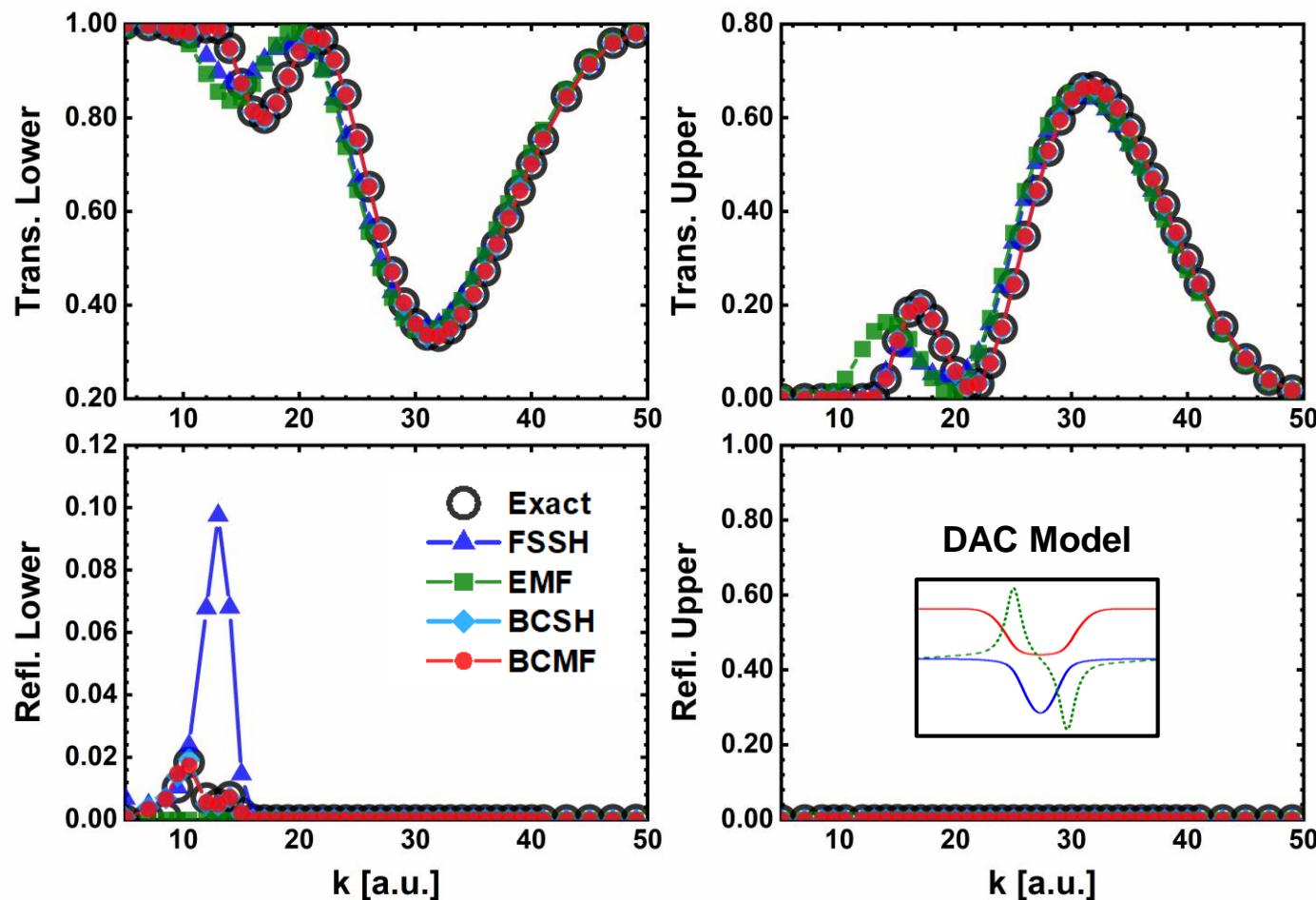
BCMF outperforms EMF in the six standard models

SAC Model



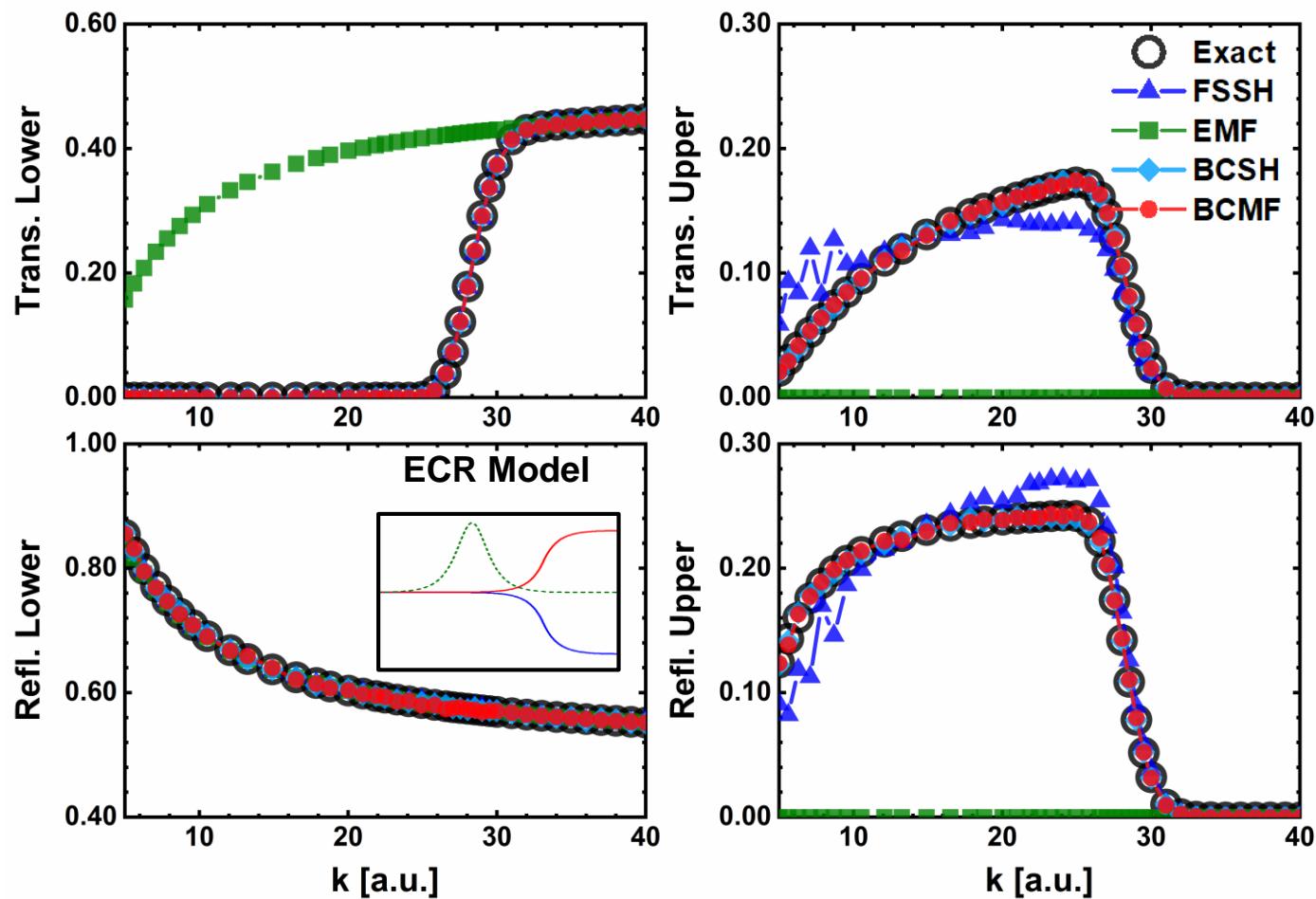
BCMF and BCSH work equally well for the SAC model

DAC Model



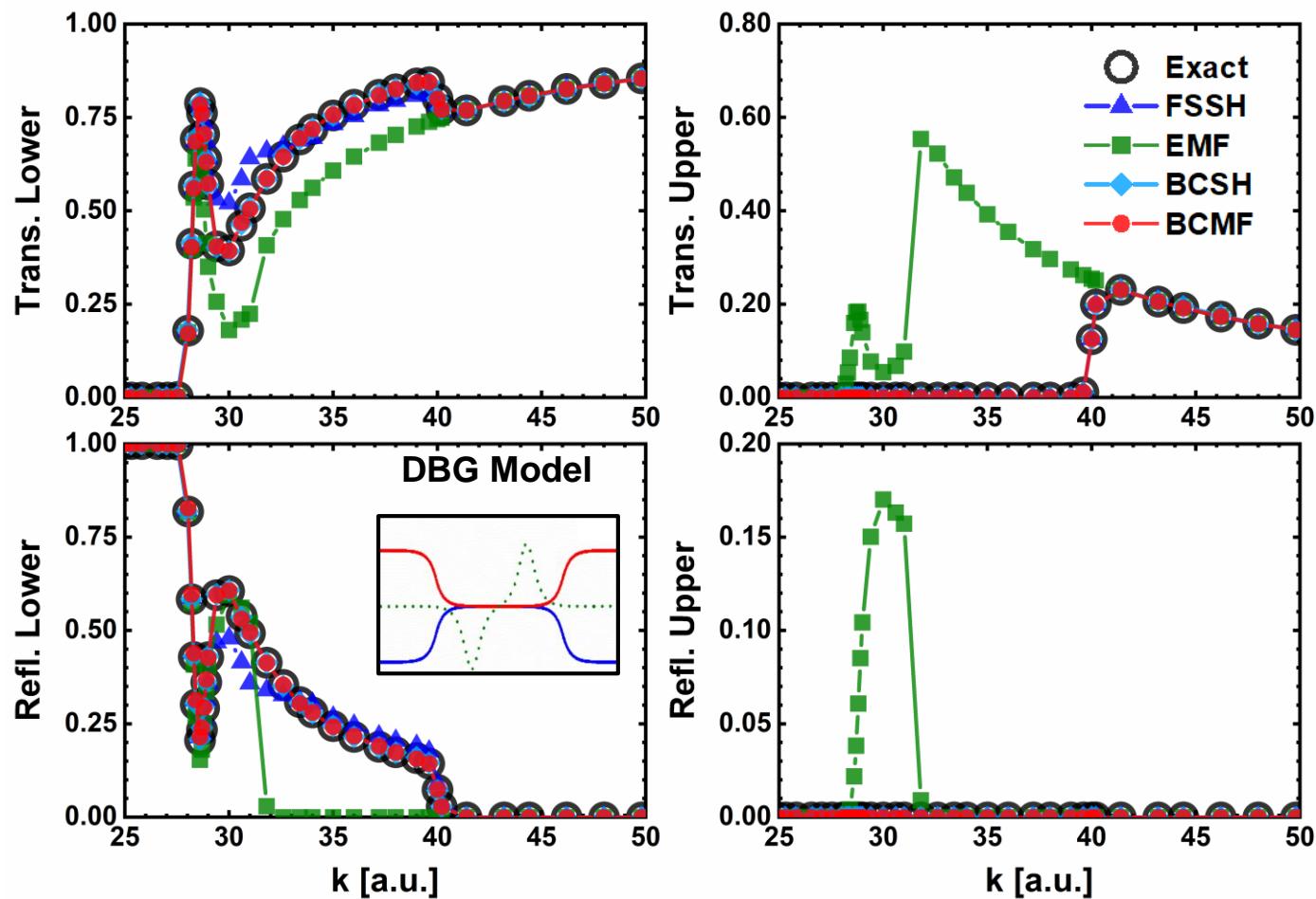
BCMF and BCSH work equally well for the DAC model

ECR Model



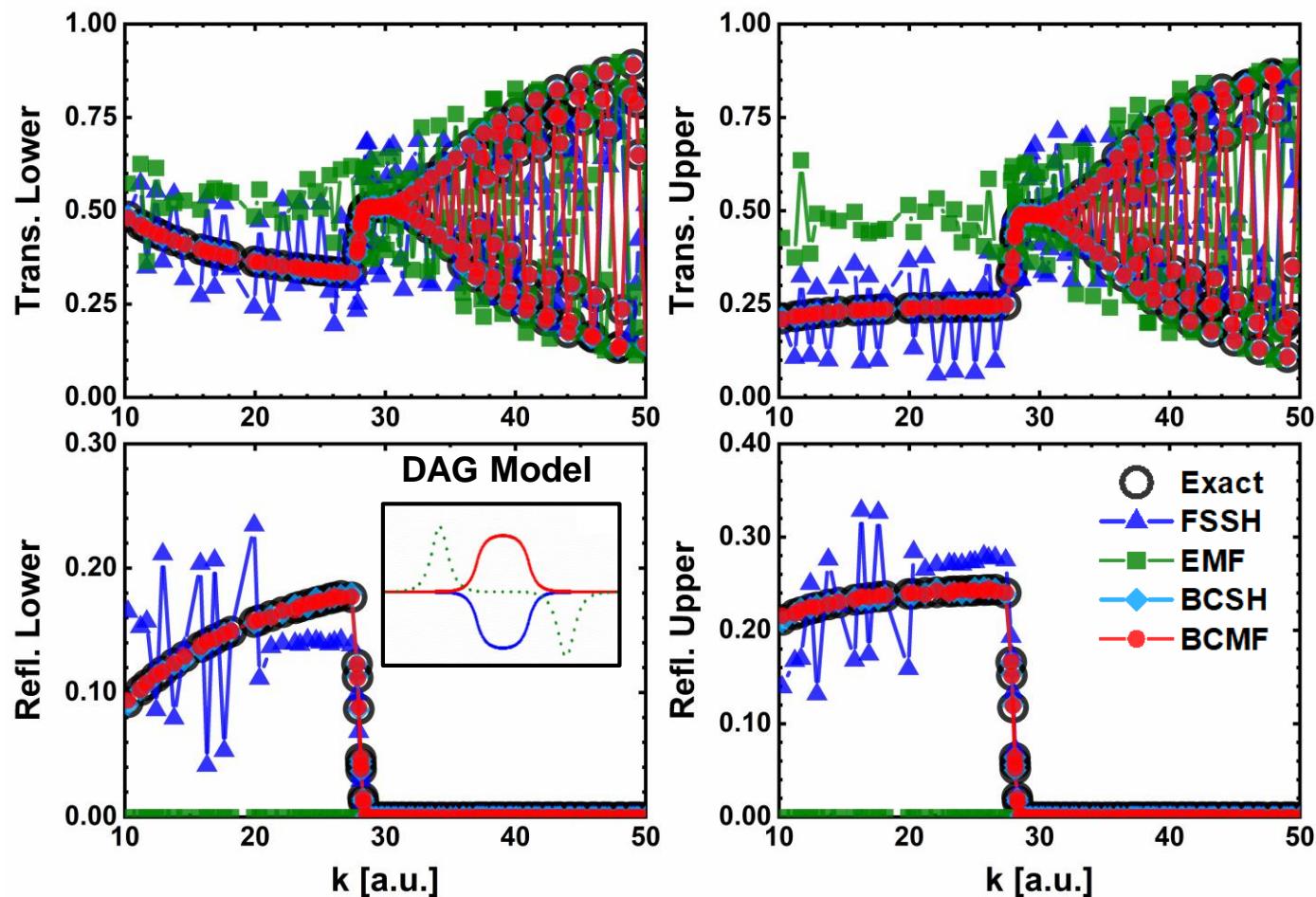
BCMF and BCSH work equally well for the ECR model

DBG Model



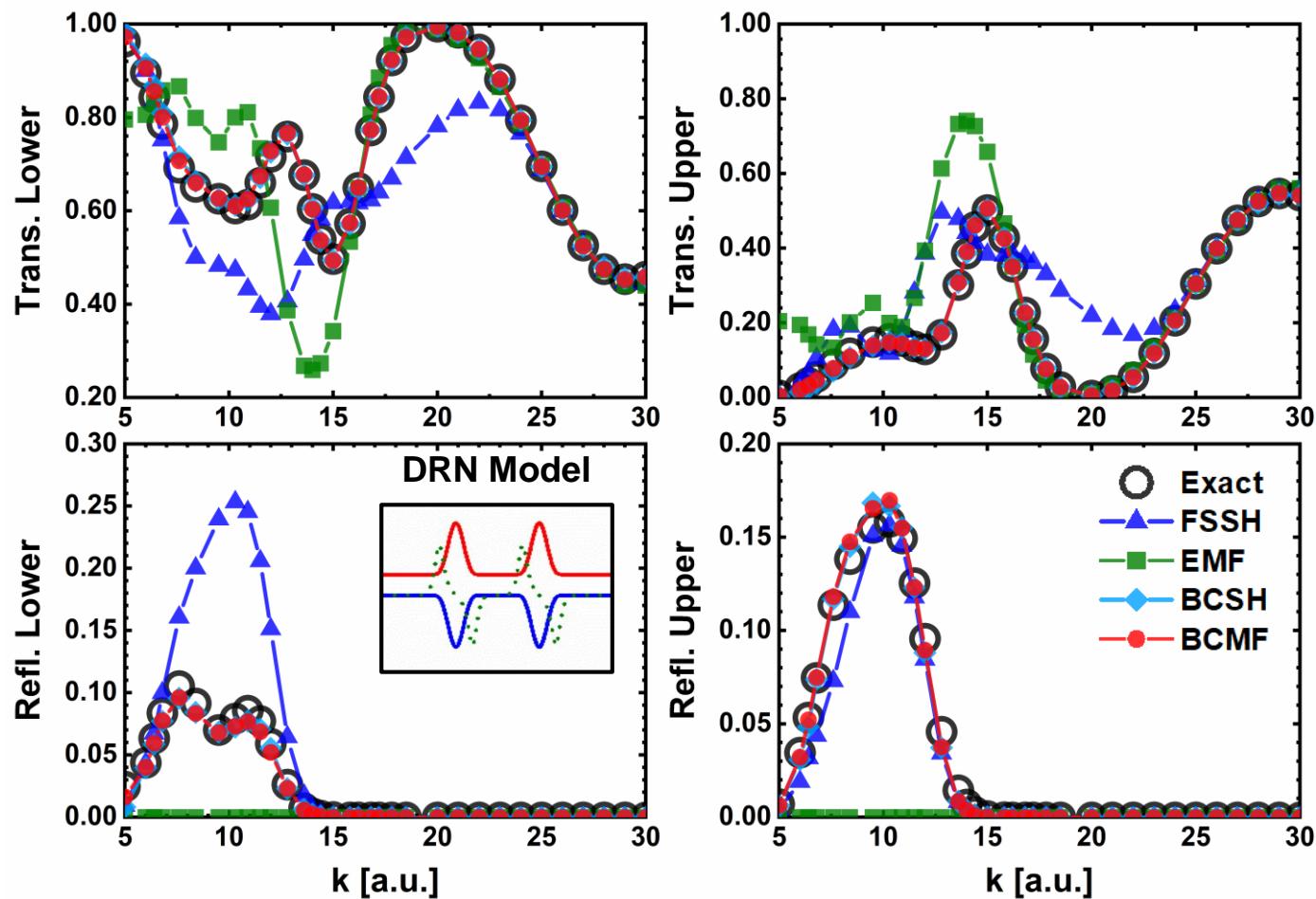
BCMF and BCSH work equally well for the DBG model

DAG Model



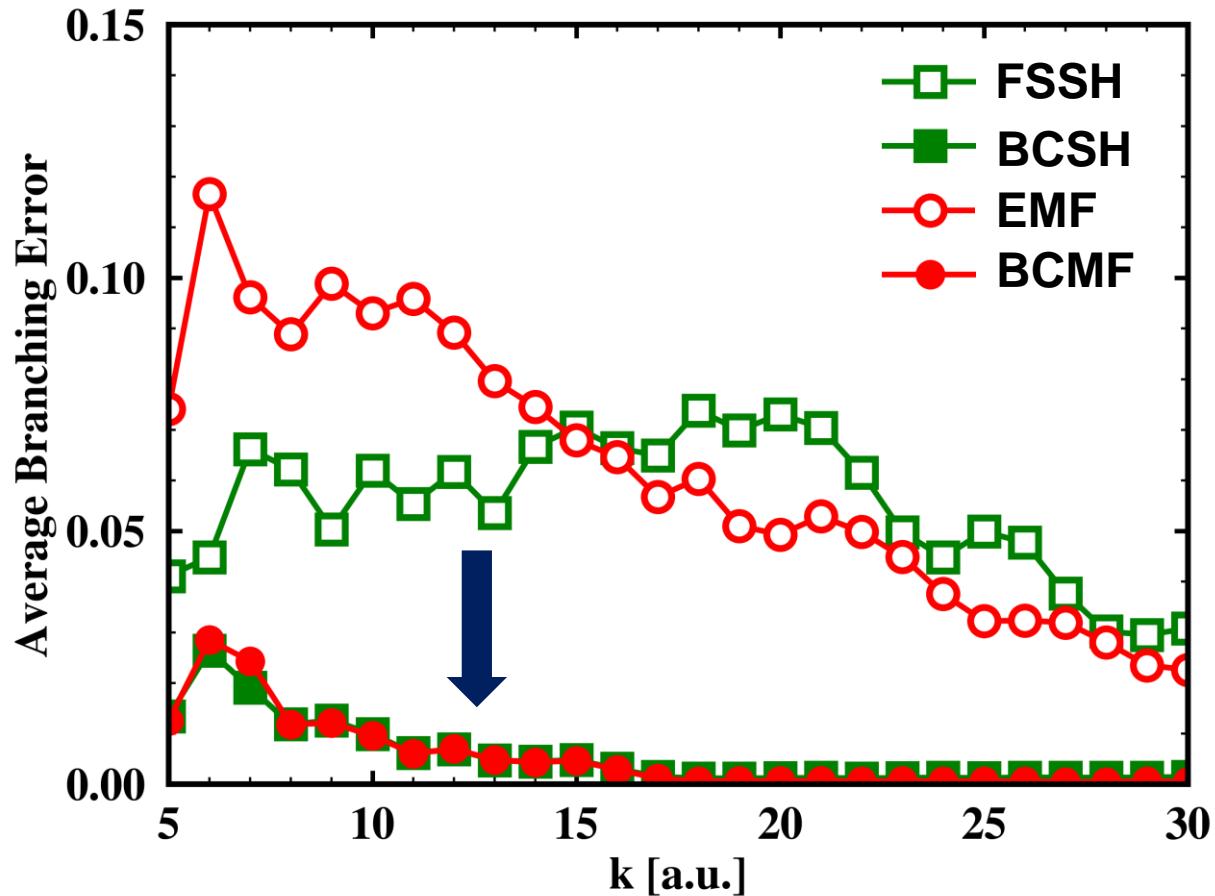
BCMF and BCSH work equally well for the DAG model

DRN Model



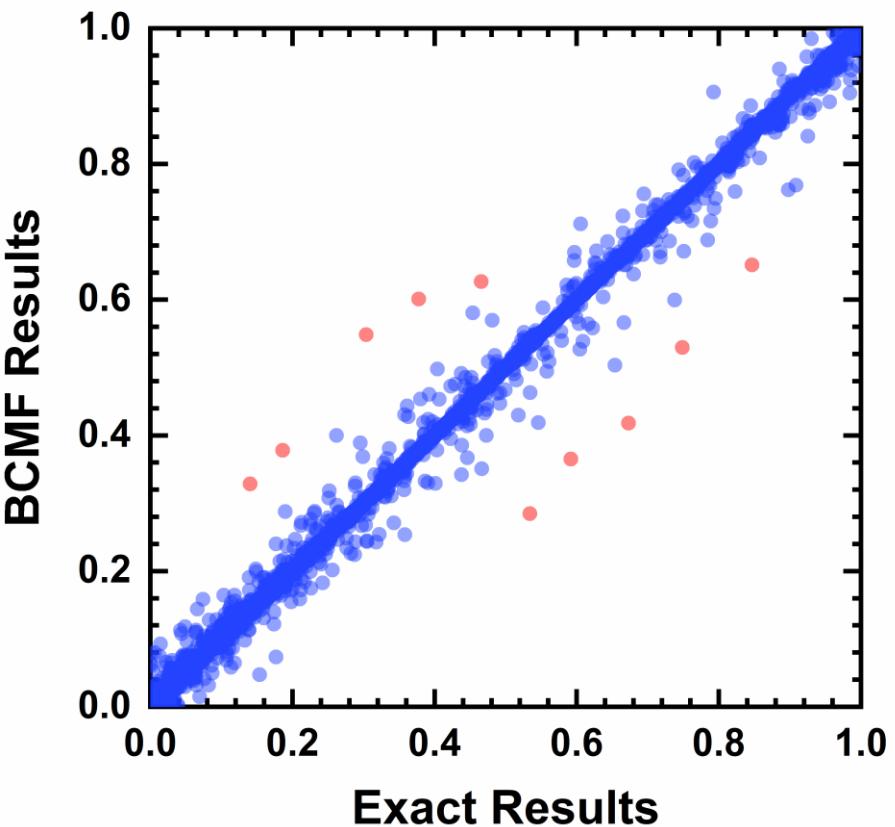
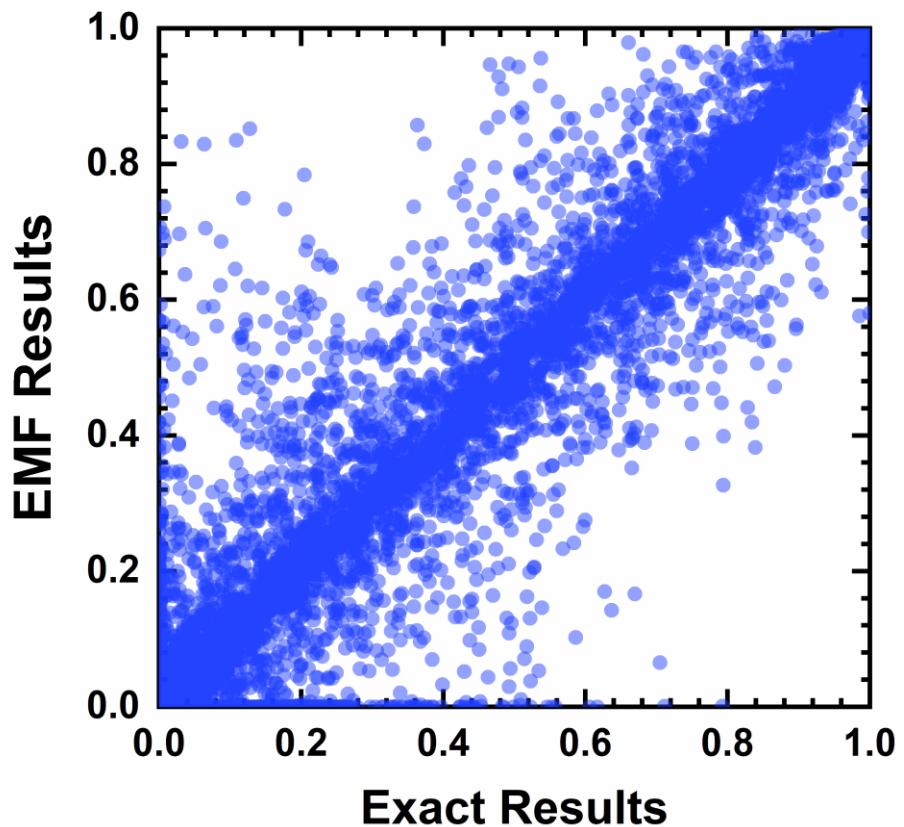
BCMF and BCSH work equally well for the DRN model

Average Error in the Two-Level Model Base



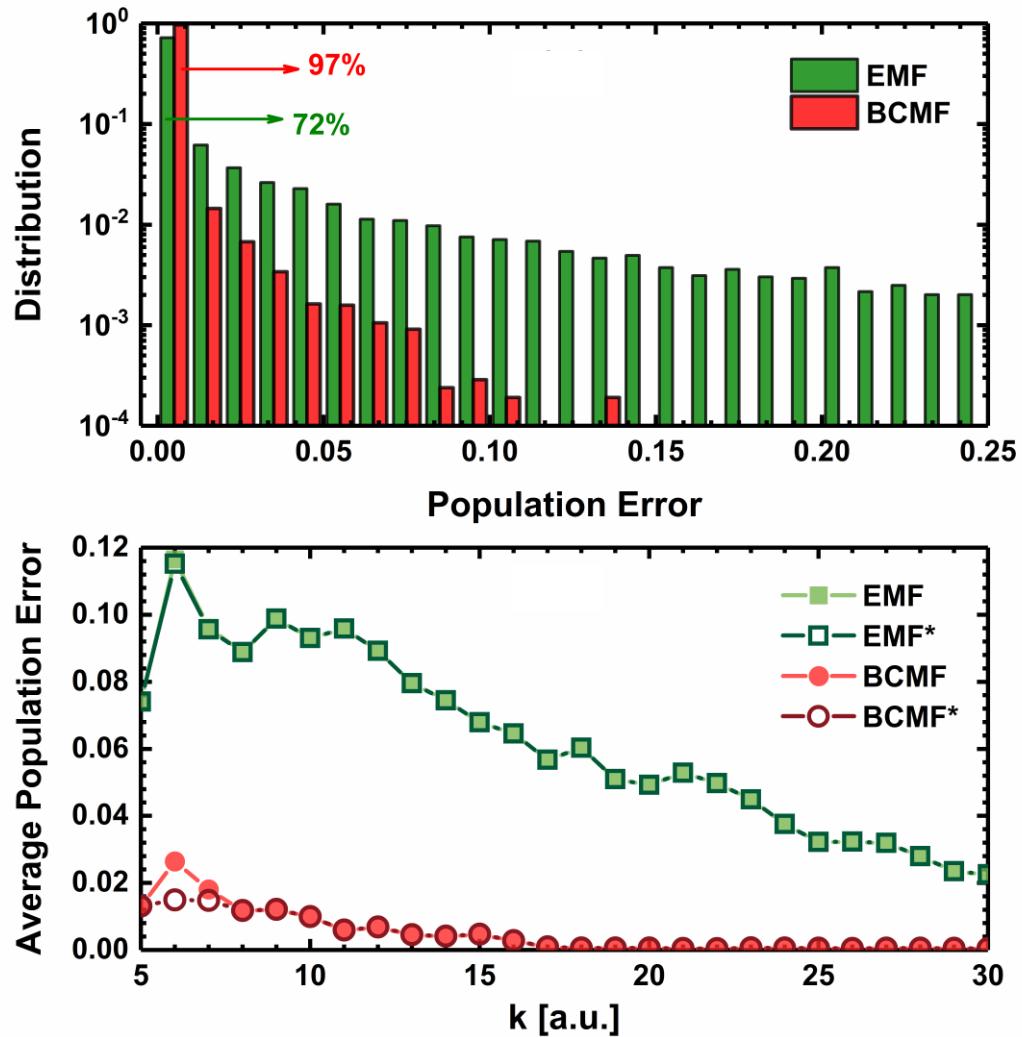
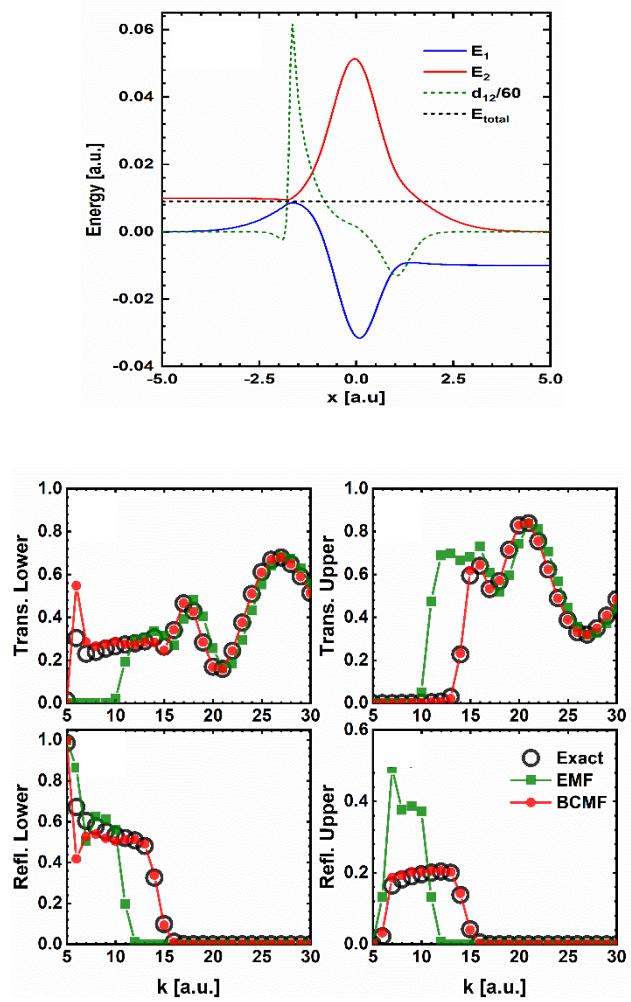
BCMF and BCSH work equally well in the 200 scattering problems

All Errors in the Two-Level Model Base



The population errors are significantly reduced in the 20800 channels

Error Distribution in the Two-Level Model Base



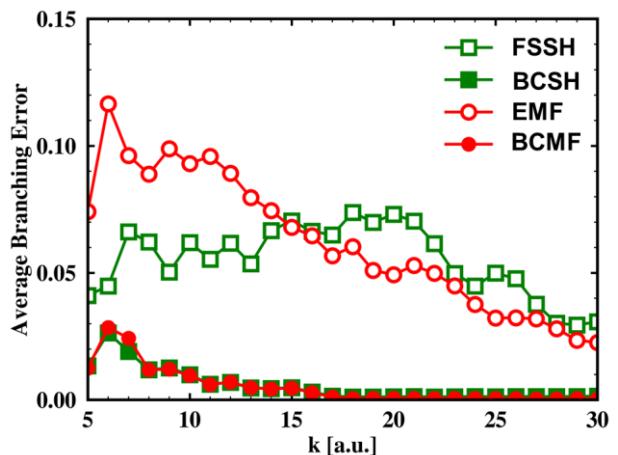
BCMF achieves 10-fold of accuracy compared with the traditional EMF 58

Summary



A novel branching correction has been proposed for mixed quantum-classical dynamics, promising to be applied to nonadiabatic dynamics simulations in chemistry, physics, biology, and material sciences.

- Reliability significantly improved
- Good for multilevel and high dimensions
- Reproduces time and spacial evolution
- Unifies mean field and surface hopping
- Leads to better decoherence time formulas





Acknowledgements



Prof. Oleg Prezhdo (USC)
Prof. Alexey Akimov (UB)
Prof. Qiang Shi (ICCAS)
Prof. Yijing Yan (USTC)
Prof. Jiushu Shao (BNU)
Prof. David Beljonne (UMons)
Prof. Zhigang Shuai (THU)



Thank you for your attention!