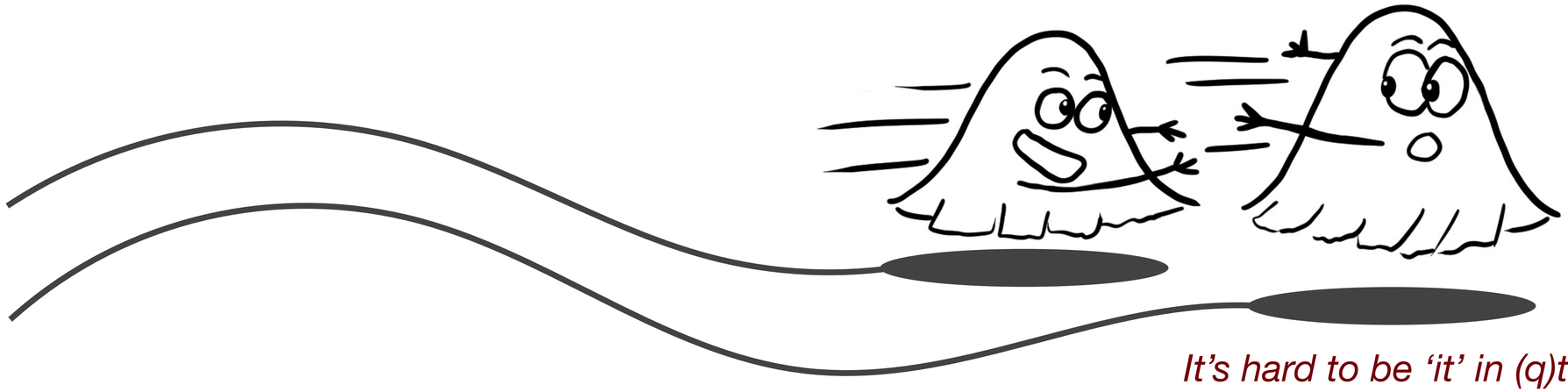
The QTAG Approach to Nonadiabatic Dynamics

VISTA Seminar #40



It's hard to be 'it' in (q)tag when you're following Bohmian paths.

Matthew Dutra

7/20/22

A Rich History of Trajectory-Based Dynamics…

AIMS

DISH

Surface Hopping

CTMQC

QTAG

FSSH

Ehrenfest Trajectories

aTG

FMS

AI-MCE

qtag

Prof. Sophya Garashchuk

Garashchuk/ Rassolov Research Groups **2021**

University of South Carolina

quantum tag

South Carolina

quantum trajectory-guided ag

South Carolina

q *uantum*
t *rajectory-guided*
a ***daptable***
g

South Carolina

q *uantum*
t *rajectory-guided*
a *daptable*
g ***aussians***

South Carolina

de Broglie - Bohm Mechanics

PHYSICAL REVIEW VOLUME 85, NUMBER 2 JANUARY 15, 1952

A Suggested Interpretation of the Quantum Theory in Terms of "Hidden" Variables. I

DAVID BOHM*
Palmer Physical Laboratory, Princeton University, Princeton, New Jersey
(Received July 5, 1951)

The usual interpretation of the quantum theory is self-consistent, but it involves an assumption that cannot be tested experimentally, *viz.*, that the most complete possible specification of an individual system is in terms of a wave function that determines only probable results of actual measurement processes. The only way of investigating the truth of this assumption is by trying to find some other interpretation of the quantum theory in terms of at present "hidden" variables, which in principle determine the precise behavior of an individual system, but which are in practice averaged over in measurements of the types that can now be carried out. In this paper and in a subsequent paper, an interpretation of the quantum theory in terms of just such "hidden" variables is suggested. It is shown that as long as the mathematical theory retains its present general form, this suggested interpretation leads to precisely the same results for all physical processes as does the usual interpretation. Nevertheless, the suggested interpretation provides a broader conceptual framework than the usual interpretation, because it makes possible a precise and continuous description of all processes, even at the quantum level. This broader conceptual framework allows more general mathematical formulations of the theory than those allowed by the usual interpretation. Now, the usual mathematical formulation seems to lead to insoluble difficulties when it is extrapolated into the domain of distances of the order of 10^{-13} cm or less. It is therefore entirely possible that the interpretation suggested here may be needed for the resolution of these difficulties. In any case, the mere possibility of such an interpretation proves that it is not necessary for us to give up a precise, rational, and objective description of individual systems at a quantum level of accuracy.

1. INTRODUCTION

THE usual interpretation of the quantum theory is based on an assumption having very far-reaching implications, *viz.*, that the physical state of an individual system is completely specified by a wave function that determines only the probabilities of actual results that can be obtained in a statistical ensemble of similar experiments. This assumption has been the object of severe criticisms, notably on the part of Einstein, who has always believed that, even at the quantum level, there must exist precisely definable elements or dynamical variables determining (as in classical physics) the actual behavior of each individual system, and not merely its probable behavior. Since these elements or variables are not now included in the quantum theory and have not yet been detected experimentally, Einstein has always regarded the present tions have as yet been suggested. The purpose of this paper (and of a subsequent paper hereafter denoted by II) is, however, to suggest just such an alternative interpretation. In contrast to the usual interpretation, this alternative interpretation permits us to conceive of each individual system as being in a precisely definable state, whose changes with time are determined by definite laws, analogous to (but not identical with) the classical equations of motion. Quantum-mechanical probabilities are regarded (like their counterparts in classical statistical mechanics) as only a practical necessity and not as a manifestation of an inherent lack of complete determination in the properties of matter at the quantum level. As long as the present general form of Schroedinger's equation is retained, the physical results obtained with our suggested alternative interpretation are precisely the same as those obtained

*Physical Review, (**1952**), 166-179, 85(2)*

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$$\Psi(x,t) = A(x,t)e^{iS(x,t)/\hbar} \qquad (1)$$

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(1) + (2) and separation into real and imaginary components

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Switching to Lagrangian frame; label trajectory momentum

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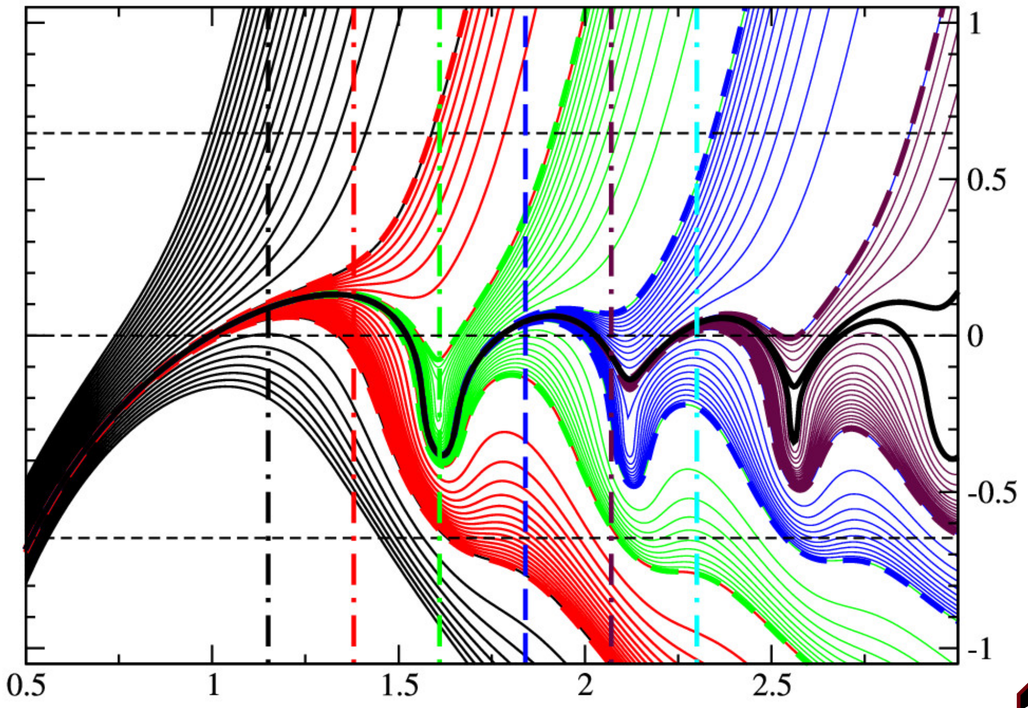

Gaussian parameters are consistent with Bohmian trajectories

$$G(x,t) = \left(\frac{a_t}{\pi}\right)^{1/4} \exp\Big[-\frac{a_t}{2}(x-q_t)^2 + \underbrace{i\mathcal{S}(q_t) + i\mathcal{S}'(q_t)(x-q_t) + \frac{i\mathcal{S}''(q_t)}{2}(x-q_t)^2}_{\approx iS(x,t)} \Big]$$

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Substitute into TDSE and divide by G(x,t), separate real and imaginary parts, switch to Lagrangian frame

$$Q_G + V + \frac{d\mathcal{S}}{dt} - \frac{(\nabla\mathcal{S})^2}{2m} = 0 \longrightarrow \frac{d\mathcal{S}}{dt} = \frac{(\nabla\mathcal{S})^2}{2m} - V - Q_G$$

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Real component…

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$$\dot{q}_t = \frac{\mathcal{S}'(q_t)}{m} \qquad \dot{a}_t = -\frac{2\mathcal{S}''(q_t)}{m} a_t$$

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From QHJE, with p = ∇S

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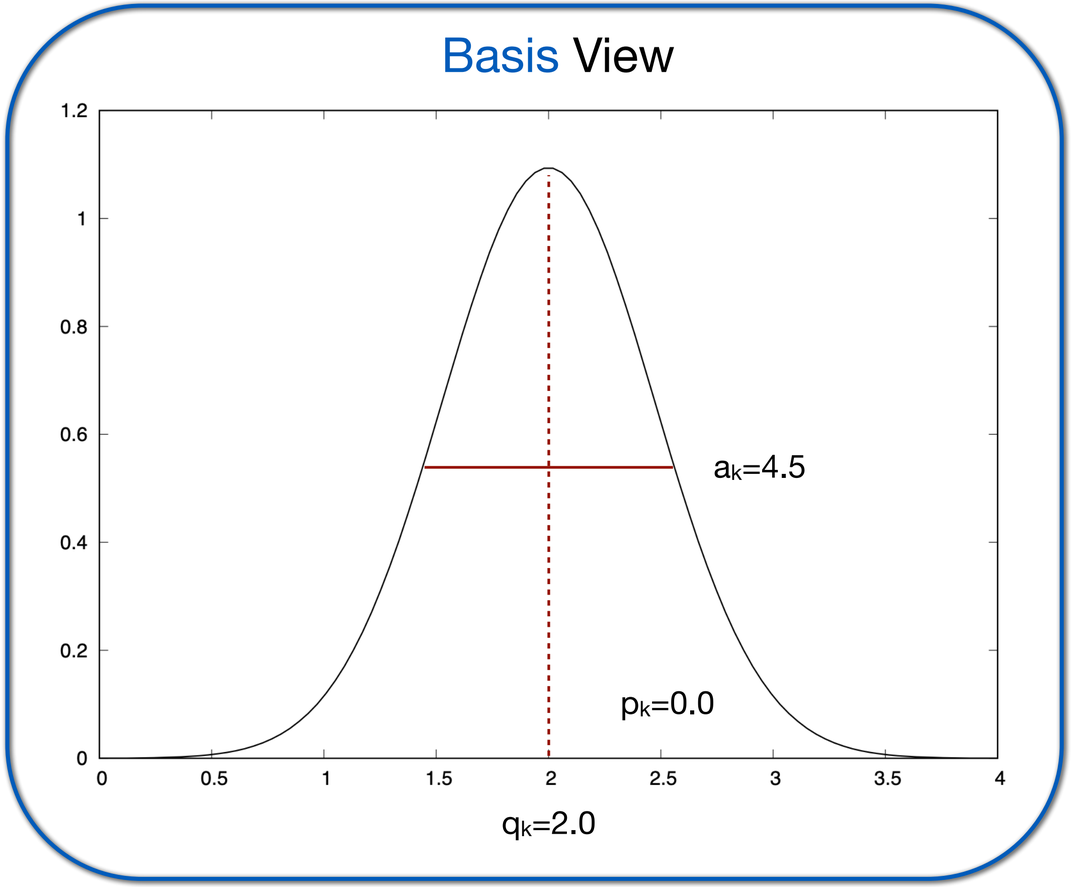
Can think about Bohmian trajectories defining a path for a Gaussian wavepacket, or for a set of Gaussian basis functions.

The time-dependent wavefunction is constructed from adaptable Gaussians

$$g_k = \prod_{\nu=1}^{N_d} \left(\frac{a_{\nu,k}}{\pi}\right)^{1/4} \exp\left(-\frac{a_{\nu,k}}{2}(x_\nu - q_{\nu,k})^2 + \imath p_{\nu,k}(x_\nu - q_{\nu,k})\right)$$

N_d-dimensional Gaussian basis function with position (***q***), phase (***p***), and width (***a***) parameters



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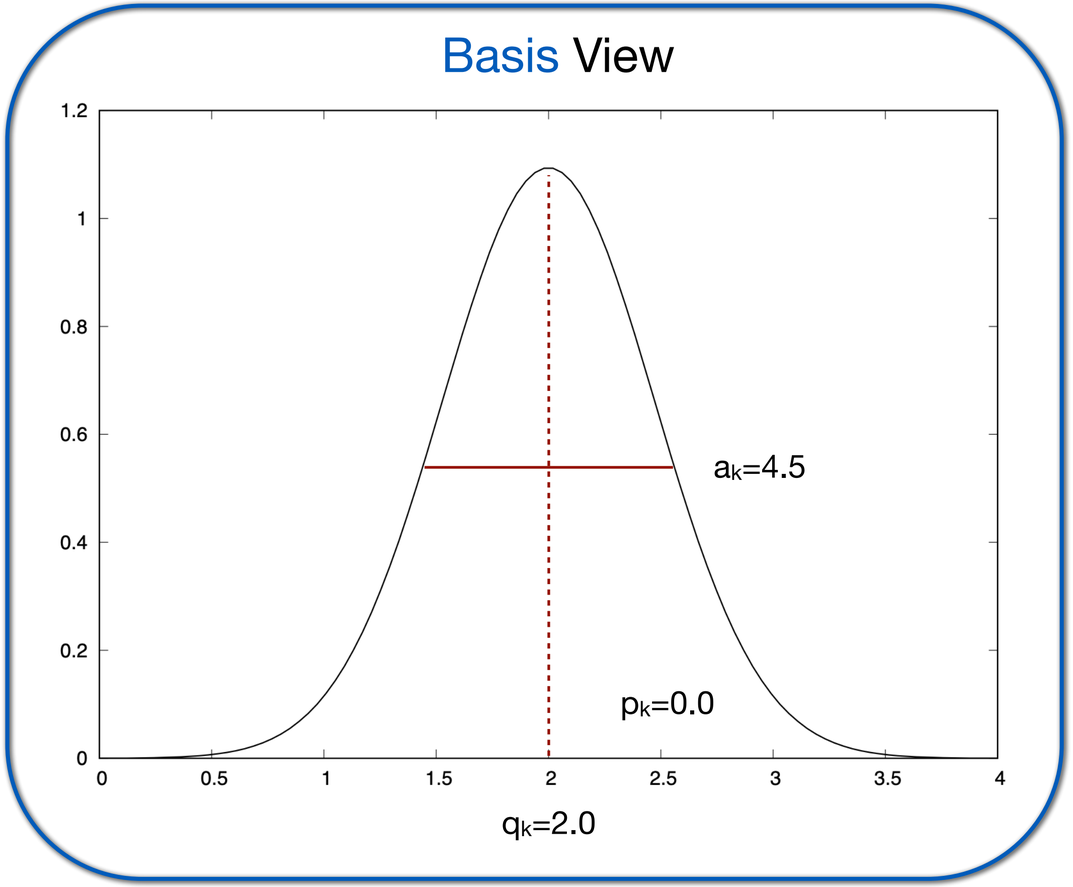
N_d-dimensional Gaussian basis function with position (***q***), phase (***p***), and width (***a***) parameters

$$\psi(\mathbf{x}, t) = \sum_{k=1}^{N_b} c_k(t) g_k(\mathbf{x}, t)$$

Generic wavefunction constructed from Gaussian basis functions, each multiplied by a complex amplitude ***c(t)***



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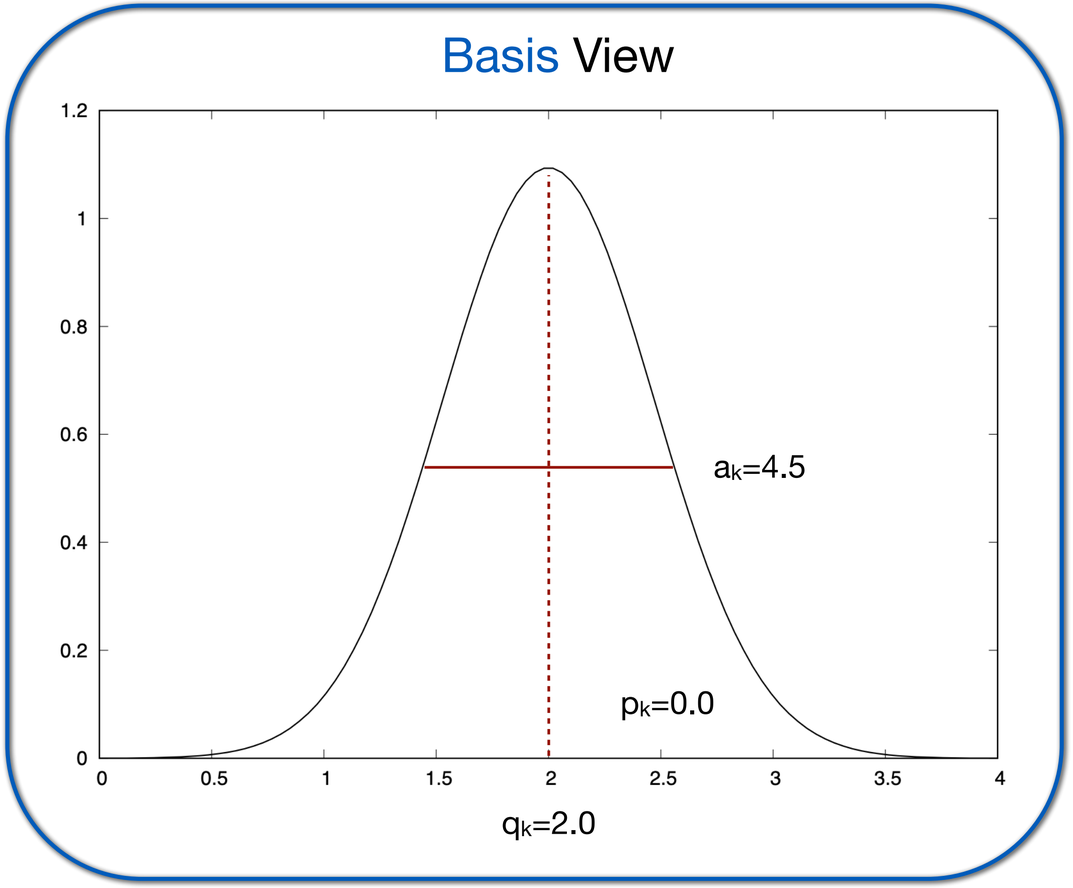

Time-Evolution of Gaussian Parameters

$$\frac{dq_t}{dt} = \frac{p_t}{m} \qquad \frac{dp_t}{dt} = -\nabla(V+Q)\Big|_{x=q_t} \qquad \frac{da_t}{dt} = -\frac{2\nabla p_t}{m} a_t$$

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A quick aside…

$$i\hbar\frac{d\vec{c}}{dt} = \mathbf{S^{-1}}(\mathbf{H} - i\hbar\mathbf{D})\vec{c}$$

*bold-face indicates a matrix, arrows indicate a vector

$$S_{ij} = \langle g_i | g_j \rangle \qquad H_{ij} = \langle g_i | K + V | g_j \rangle$$

$$D_{ij} = \left\langle g_i \middle| \sum_{d=1}^{f} \dot{\lambda}_{jd} \middle| \left(\frac{\partial g_j}{\partial \lambda_{jd}}\right) \right\rangle$$

$$\lambda_j = \{q_j, p_j, a_j, s_j\}$$

Set of basis parameters defining the j-th GBF

B. Gu and S. Garashchuk, Quantum Dynamics with Gaussian Bases Defined by the Quantum Trajectories, *Journal of Physical Chemistry A, (**2016**),* 3023-3031, 120(19)

The time-dependent wavefunction is constructed from adaptable Gaussians

$$g_k = \prod_{\nu=1}^{N_d} \left(\frac{a_{\nu,k}}{\pi}\right)^{1/4} \exp\left(-\frac{a_{\nu,k}}{2}(x_\nu - q_{\nu,k})^2 + \imath p_{\nu,k}(x_\nu - q_{\nu,k})\right)$$

N_d-dimensional Gaussian basis function (GBF) with position (***q***), phase (***p***), and width (***a***) parameters

$$\psi(\mathbf{x},t) = \sum_{k=1}^{N_b} c_k(t) g_k(\mathbf{x},t)$$

Generic wavefunction constructed from Gaussian basis functions, each multiplied by a complex amplitude ***c(t)***

$$i\hbar\frac{\partial\Psi}{\partial t} = -\left(\frac{\hbar^2}{2m}\right)\nabla^2\Psi + V(x)\Psi$$

Time-dependent Schrodinger Equation (TDSE)

A quick aside…

$$i\hbar\frac{d\vec{c}}{dt} = \mathbf{S^{-1}}(\mathbf{H} - i\hbar\mathbf{D})\vec{c}$$

*bold-face indicates a matrix, arrows indicate a vector

$$S_{ij} = \langle g_i | g_j \rangle \qquad H_{ij} = \langle g_i | \hat{\mathbf{K}} + V | g_j \rangle$$

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…and can be calculated at an arbitrary time via matrices K and T

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Time-dependent Schrodinger Equation (TDSE)

The time-dependent wavefunction in the QTAG algorithm is constructed from solutions to the time-independent eigenproblem w/ eigenvectors **Z** and eigenvalues ε :

$$\mathbf{HZ} = \mathbf{SZ}\mathcal{E}$$

H and **S** denote the Hamiltonian and overlap matrices, respectively, whose elements are integrals over the appropriate GBFs:

$$H_{ij} = \langle g_i | K + V | g_j \rangle \qquad S_{ij} = \langle g_i | g_j \rangle$$

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$$H_{ij} = \langle g_i|K + V|g_j\rangle \qquad S_{ij} = \langle g_i|g_j\rangle$$

Propagation over time is done via the propagator matrix **K** and time-overlap matrix **T**:

$$\mathbf{K}^{(m)} = \mathbf{Z}^{(m)}\exp(-i\mathcal{E}^{(m)}\tau)(\mathbf{Z}^{(m)})^\dagger$$

$$T_{ij}^{(m,m-1)} = \langle g_i^{(m)}|g_j^{(m-1)}\rangle$$

For M time steps:

$$\psi(x, M\tau) = (\vec{g}^{(M-1)})^T\left(\prod_{m=2}^{M}\mathbf{K}^{(m-1)}\mathbf{T}^{(m-1,m-2)}\right)\mathbf{K}^{(0)}\vec{b}^{(0)}(0)$$

$$b^{(0)} = \langle\vec{g}^{(0)}(x)|\psi(x,0)\rangle$$

The QTAG algorithm evolves basis coefficients and trajectories

1. Computing Basis Coefficients

Compute Overlap Matrix Elements

↓

Compute Hamiltonian Matrix Elements

↓

Solve Eigenvalue Problem $HZ=SZ\varepsilon$

↓

Update Basis Coefficients from Eigenvalues/ vectors

2. Updating Trajectory Parameters

Calculate Momentum from Wavefunction

↓

Update Basis Parameters {p,a,s}

↓

Update Positions (q)

↓

Compute Time Overlap Matrix Elements

The QTAG algorithm evolves basis coefficients and trajectories

1. Computing Basis Coefficients

Compute Overlap Matrix Elements

↓

Compute Hamiltonian Matrix Elements

↓

Solve Eigenvalue Problem HZ=SZ$\mathcal{E}$

↓

Update Basis Coefficients from Eigenvalues/ vectors

(1a) $$S_{ij} = \langle g_i | g_j \rangle$$

(1b) $$H_{ij} = \langle g_i | K + V | g_j \rangle$$

(1c) $$\mathbf{HZ} = \mathbf{SZ}\mathcal{E}$$

(1d) $$\vec{c}^{(0)} = \mathbf{Z}^{(0)} \exp(-i\mathcal{E}^{(0)}\Delta t)(\mathbf{Z}^{(0)})^{\dagger}\vec{b}^{(0)}$$

Analytical integral if available, approximated using LHA or BAT if not

LHA = Local Harmonic Approximation

BAT — Bra-ket Averaged Taylor Expansion

The QTAG algorithm evolves basis coefficients and trajectories

Unaltered Bohmian trajectories are notoriously numerically challenging, can modify momenta for added stability:

- *Linear fitting (implemented here)*
- Momentum convolution
- Wavefunction convolution

$$p_t = Im\left(\frac{\nabla\psi}{\psi}\right) \quad (2a)$$

$$\frac{da_t}{dt} = -\frac{2\nabla p_t}{m} a_t \quad (2b)$$

$$\frac{dq_t}{dt} = \frac{p_t}{m} \quad (2c)$$

$$T_{ij}^{(m,m-1)} = \langle g_i^{(m)} | g_j^{(m-1)} \rangle \quad (2d)$$

$$\vec{b}^{(1)} = \mathbf{T}^{(1,0)} \vec{c}^{(0)}$$

2. Updating Trajectory Parameters

Calculate Momentum from Wavefunction

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Compute Time Overlap Matrix Elements

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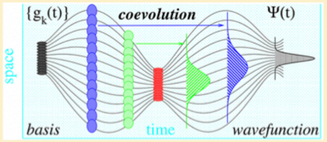
Quantum Dynamics with the Quantum Trajectory-Guided Adaptable Gaussian Bases

Matthew Dutra, Sachith Wickramasinghe, and Sophya Garashchuk*

Department of Chemistry and Biochemistry, University of South Carolina, Columbia, South Carolina 29208, United States

ABSTRACT: The computational cost of describing a general quantum system fully coupled by anharmonic interactions scales exponentially with the system size. Thus, an efficient basis representation of wave functions is essential, and when it comes to the large-amplitude motion of high-dimensional systems, the dynamic bases of Gaussian functions are often employed. The time dependence of such bases is determined from the variational principle or from classical dynamics; the former is challenging in implementation due to singular matrices, while the latter may not cover the configuration space relevant to quantum dynamics. Here we describe a method using Quantum Trajectory-guided Adaptable Gaussian (QTAG) bases "tuned"—including the basis position, phase, and width—to the wave function evolution, thanks to the continuity of the probability density in the course of the quantum trajectory dynamics. Thus, an efficient basis in configuration space is generated, bypassing the variational equations on the parameters of the Gaussians. We also propose a time propagator with basis transformation by projections which lends efficiency and stability to the QTAG dynamics, as demonstrated on standard tests and the ammonia inversion model.



Applications to single-surface systems w/ quantum features, molecular tunneling, coupled system-bath models, etc.

THE JOURNAL OF PHYSICAL CHEMISTRY A
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Article

Multidimensional Tunneling Dynamics Employing Quantum-Trajectory Guided Adaptable Gaussian Bases

Matthew Dutra, Sachith Wickramasinghe, and Sophya Garashchuk*

Cite This: J. Phys. Chem. A 2020, 124, 9314−9325
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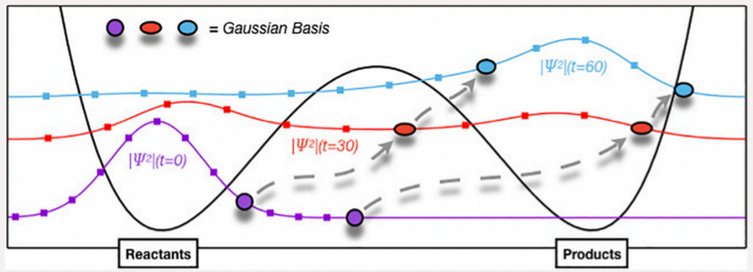

ABSTRACT: An efficient basis representation of time-dependent wavefunctions is essential for theoretical studies of high-dimensional molecular systems exhibiting large-amplitude motion. For fully coupled anharmonic systems, the complexity of a general wavefunction scales exponentially with the system size; therefore, for practical reasons, it is desirable to adapt the basis to the time-dependent wavefunction at hand. Often times on this quest for a minimal basis representation, time-dependent Gaussians are employed, in part because of their localization in both configuration and momentum spaces and also because of their direct connection to classical and semiclassical dynamics, guiding the evolution of the basis function parameters. In this work, the quantum-trajectory guided adaptable Gaussian (QTAG) bases method [*J. Chem. Theory Comput.* **2020**, *16*, 18−34] is generalized to include correlated, i.e., non-factorizable, basis functions, and the performance of the QTAG dynamics is assessed on benchmark system/bath tunneling models of up to 20 dimensions. For the popular choice of initial conditions describing tunneling between the reactant/product wells, the minimal "semiclassical" description of the bath modes using essentially a single multidimensional basis function combined with the multi-Gaussian representation of the tunneling mode is shown to capture the dominant features of dynamics in a highly efficient manner.

Libra

University at Buffalo

Prof. Alexey Akimov

Libra Winter School on Excited States and Nonadiabatic Dynamics in Materials 2022

Computational Chemistry Cyber Training

Nonadiabatic dynamics requires minor matrix modifications

1. Computing Basis Coefficients

Compute Overlap Matrix Elements

↓

Compute Hamiltonian Matrix Elements

↓

Solve Eigenvalue Problem HZ=SZ$\mathcal{E}$

↓

Update Basis Coefficients from Eigenvalues/ vectors

	Single-surface	*Multi-surface*
(1a)	$S_{ij}^{aa} = \langle g_i^a \vert g_j^a \rangle$	$S_{ij}^{ab} = 0$
(1b)	$H_{ij}^{aa} = \langle g_i^a \vert K + V^a \vert g_j^a \rangle$	$H_{ij}^{ab} = \langle g_i^a \vert V^{ab} \vert g_j^b \rangle$
(1c)	$\mathbf{HZ} = \mathbf{SZ}\mathcal{E}$	
(1d)	$\vec{c}^{(0)} = \mathbf{Z}^{(0)} \exp(-i\mathcal{E}^{(0)}\Delta t)(\mathbf{Z}^{(0)})^\dagger \vec{b}^{(0)}$	

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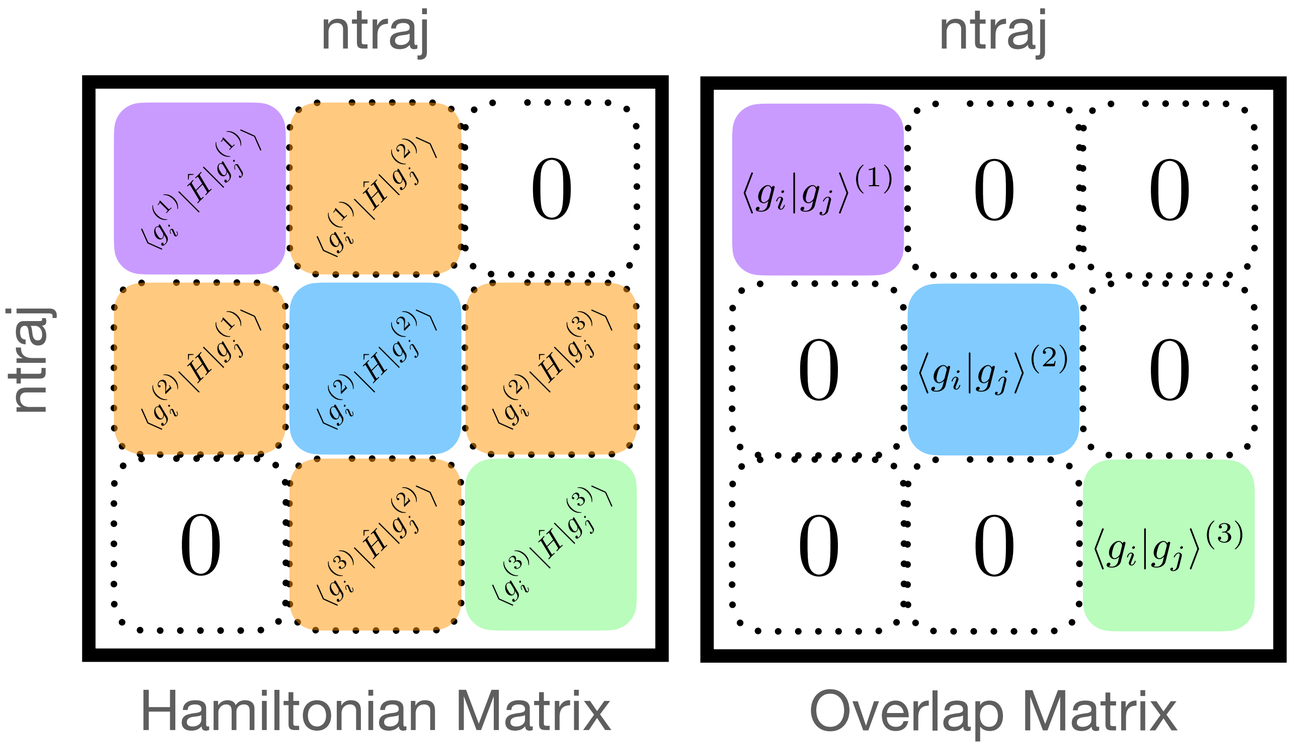


Hamiltonian Matrix

Overlap Matrix

Trajectories in the nonadiabatic picture still evolve on single surfaces*

*Momenta poorly defined for basis functions on surfaces w/ no density, may have to consider how to move them initially:

- *Synchronize to populated state (implemented here)*
- Move them classically
- Place them in coupling region

Single-surface

$$p_t = Im\left(\frac{\nabla\psi}{\psi}\right) \quad (2a)$$

$$\frac{da_t}{dt} = -\frac{2\nabla p_t}{m} a_t \quad (2b)$$

$$\frac{dq_t}{dt} = \frac{p_t}{m} \quad (2c)$$

$$T_{ij}^{(m,m-1)} = \langle g_i^{(m)} | g_j^{(m-1)} \rangle \quad (2d)$$

$$\vec{b}^{(1)} = \mathbf{T}^{(1,0)} \vec{c}^{(0)}$$

2. Updating Trajectory Parameters

Calculate Momentum from Wavefunction

↓

Update Basis Parameters {p,a,s}

↓

Update Positions (q)

↓

Compute Time Overlap Matrix Elements

Holstein Model — Coupled Harmonic Oscillators

ψ_0

Q_0 = -2.0
P_0 = 0.0
A_0 = 1.0
S_0 = 0.0

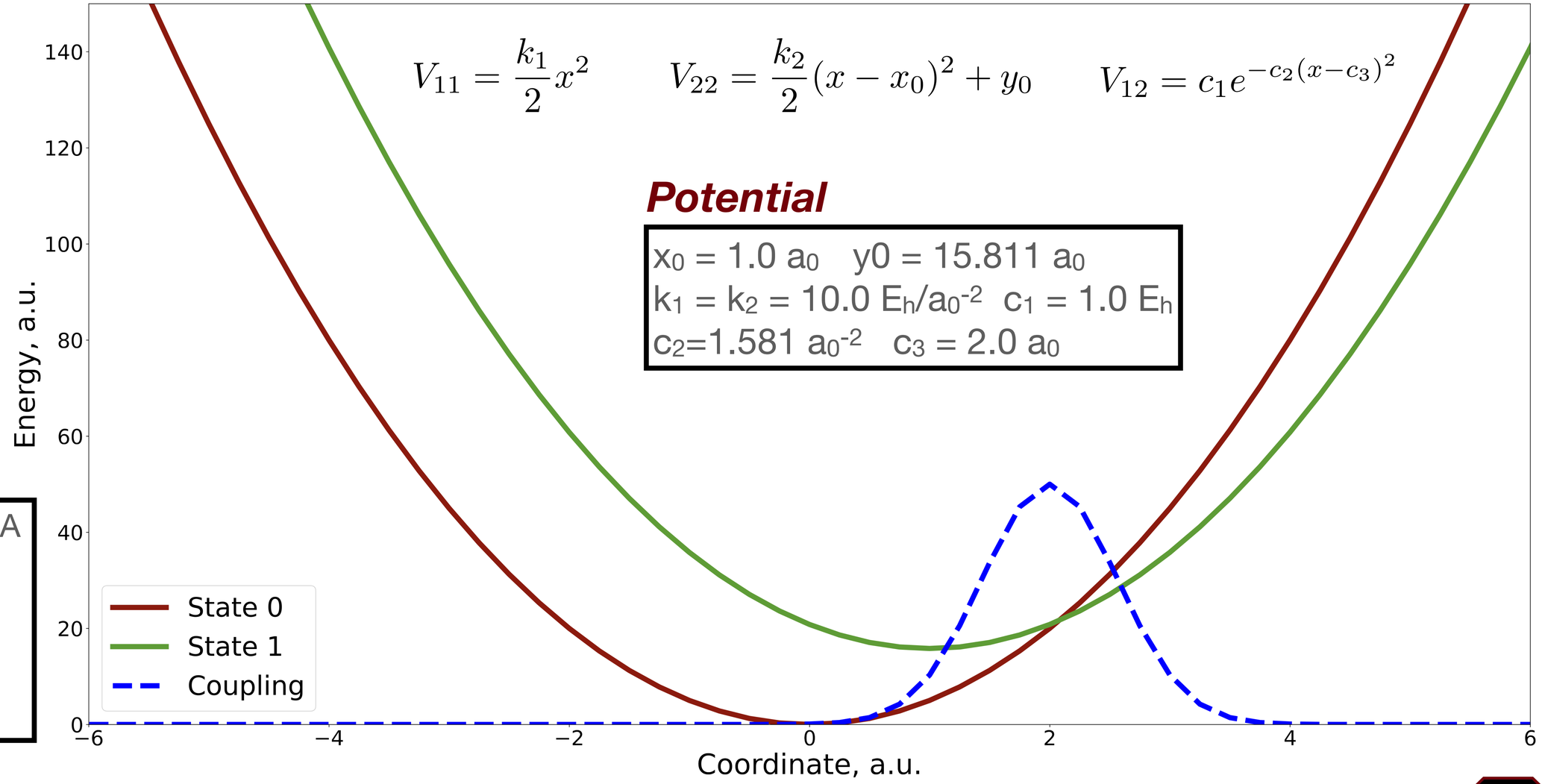
Parameters

Potential Approx. — LHA
Trajectories — 25
Width Scale — 6.0
Mass — 1.0 a.u.
Decpl. Pop. — 0.3
dt — 0.01

$$V_{11} = \frac{k_1}{2}x^2 \qquad V_{22} = \frac{k_2}{2}(x - x_0)^2 + y_0 \qquad V_{12} = c_1 e^{-c_2(x-c_3)^2}$$

Potential

x_0 = 1.0 a_0 y0 = 15.811 a_0
$k_1 = k_2$ = 10.0 E_h/a_0^{-2} c_1 = 1.0 E_h
c_2=1.581 a_0^{-2} c_3 = 2.0 a_0



Holstein Model

Coupled Harmonic Oscillators

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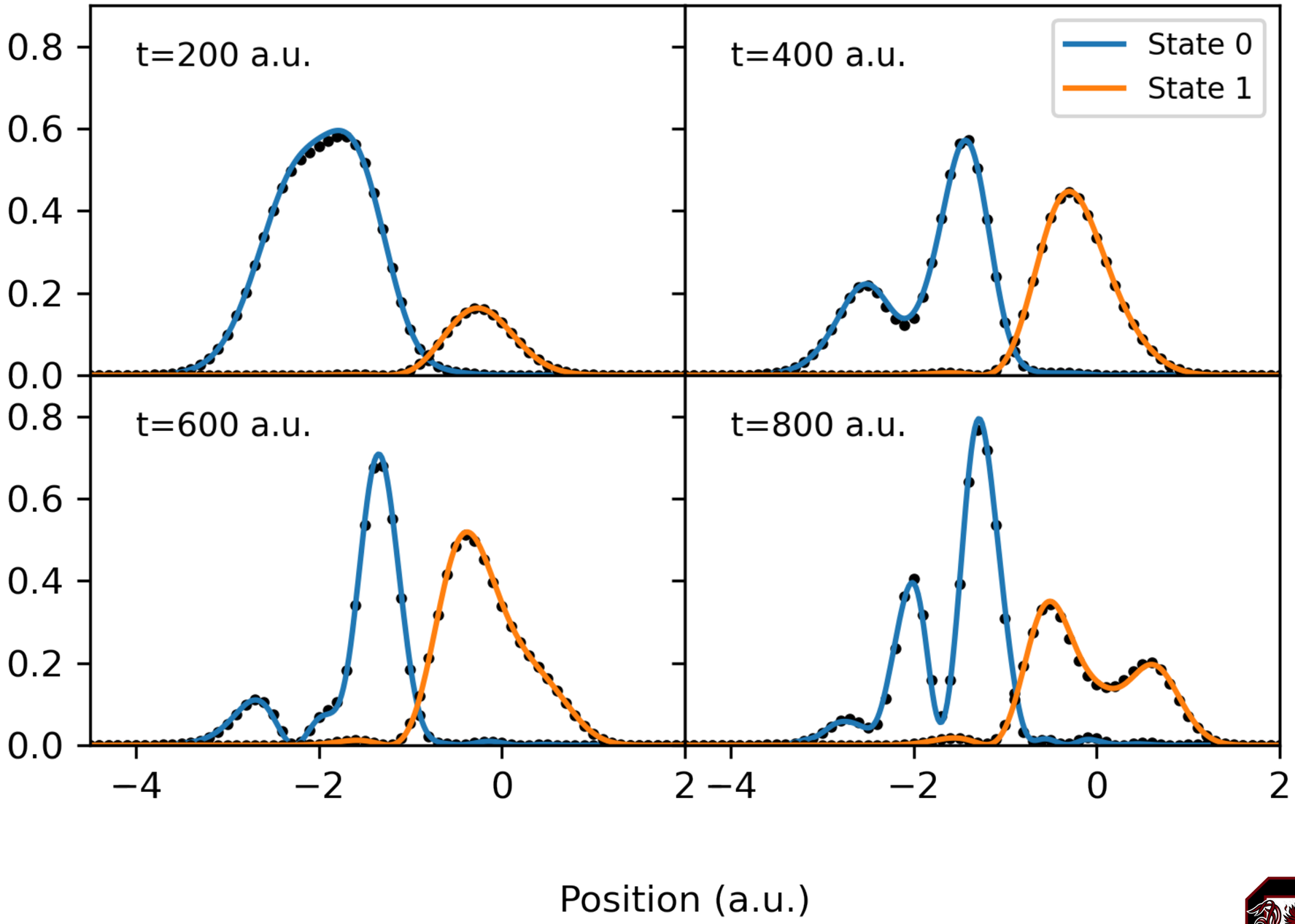

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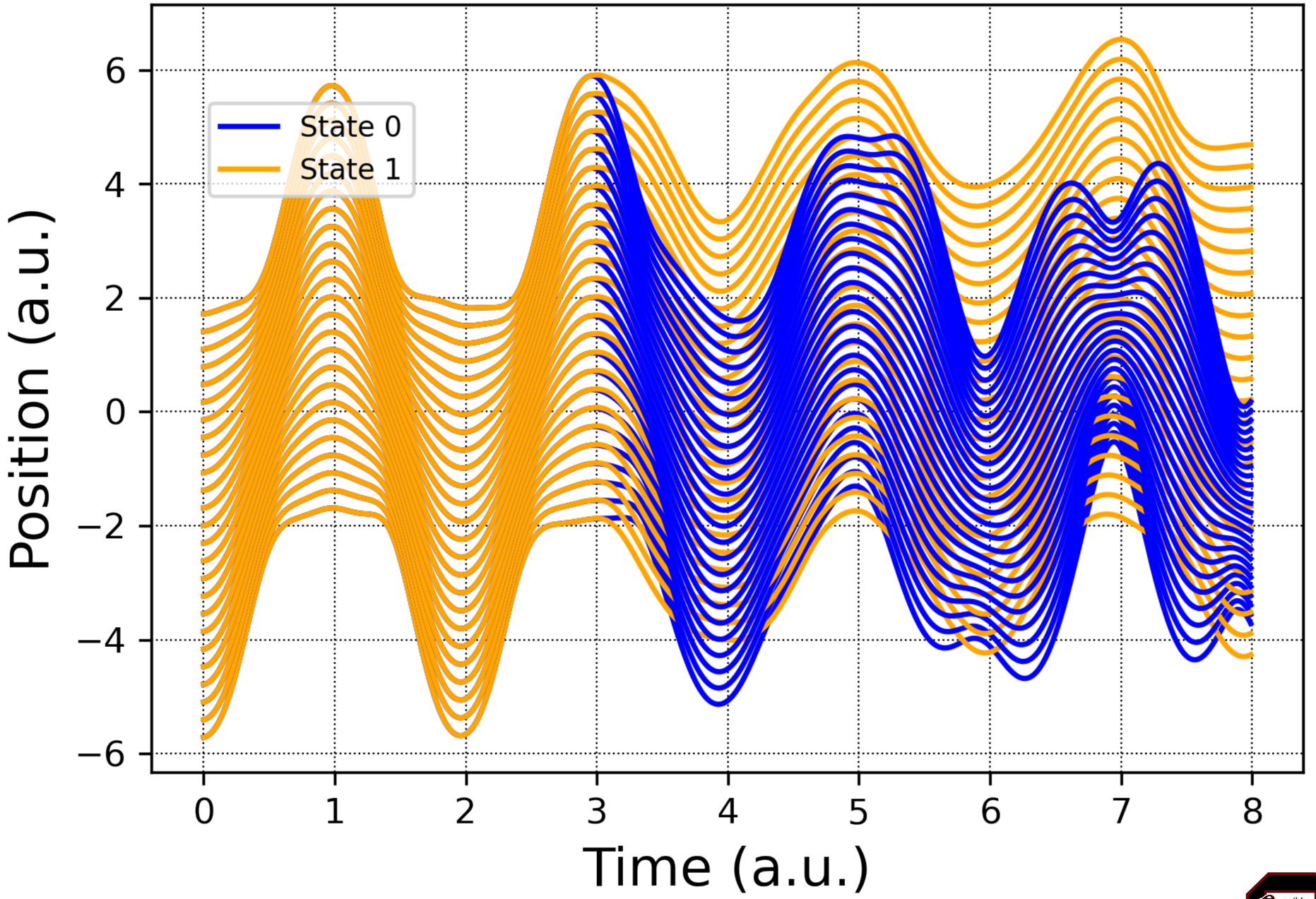

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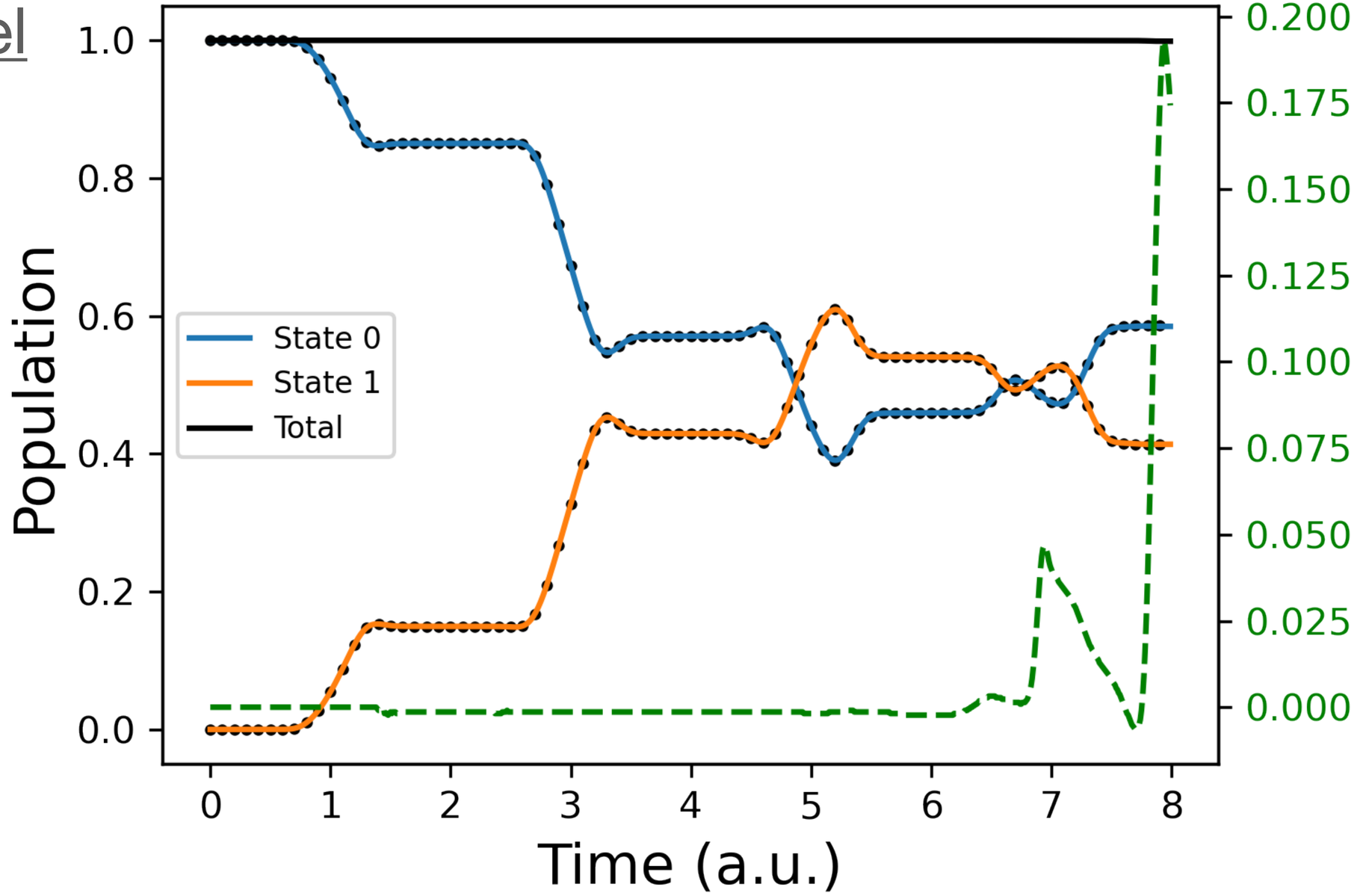


Single Avoided Crossing

ψ_0

Q_0 = -5.0
P_0 = 10.0
A_0 = 2.0
S_0 = 0.0

Potential

A = 0.01 E_h B = 1.147 a_0^{-1}
C = 0.005 E_h D = 1.0 a_0^{-2}

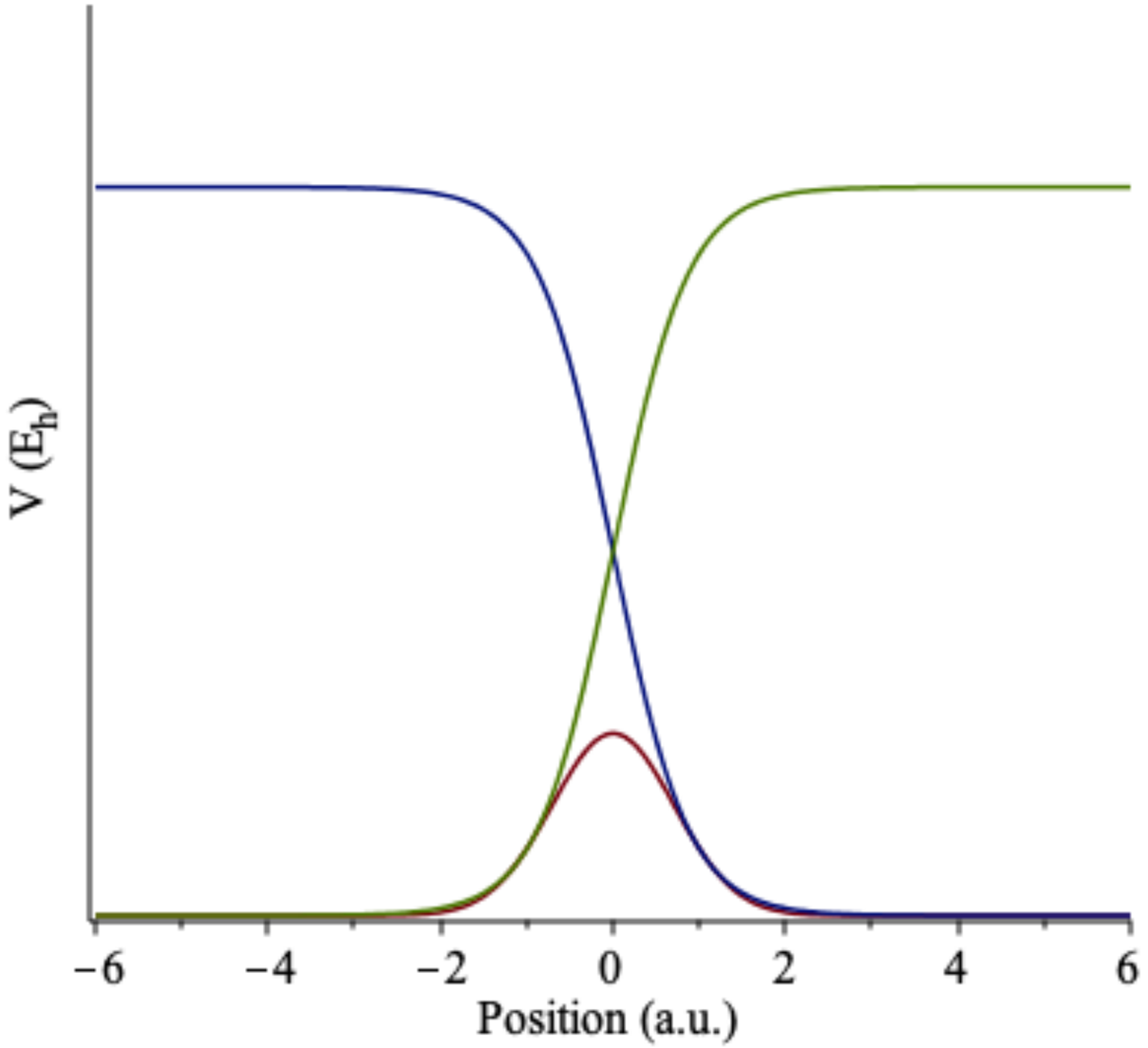
Parameters

Potential Approx. — BAT
Trajectories — 35
Width Scale — 15.0
Mass — 2000.0 a.u.
Decpl. Pop. — 0.1
dt — 1.0

$$V_{11} = A(1 + \tanh(Bx))$$

$$V_{22} = A(1 - \tanh(Bx))$$

$$V_{12} = Ce^{-Dx^2}$$



Avoided Crossing

ψ_0

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P_0 = 10.0
A_0 = 2.0
S_0 = 0.0

Parameters

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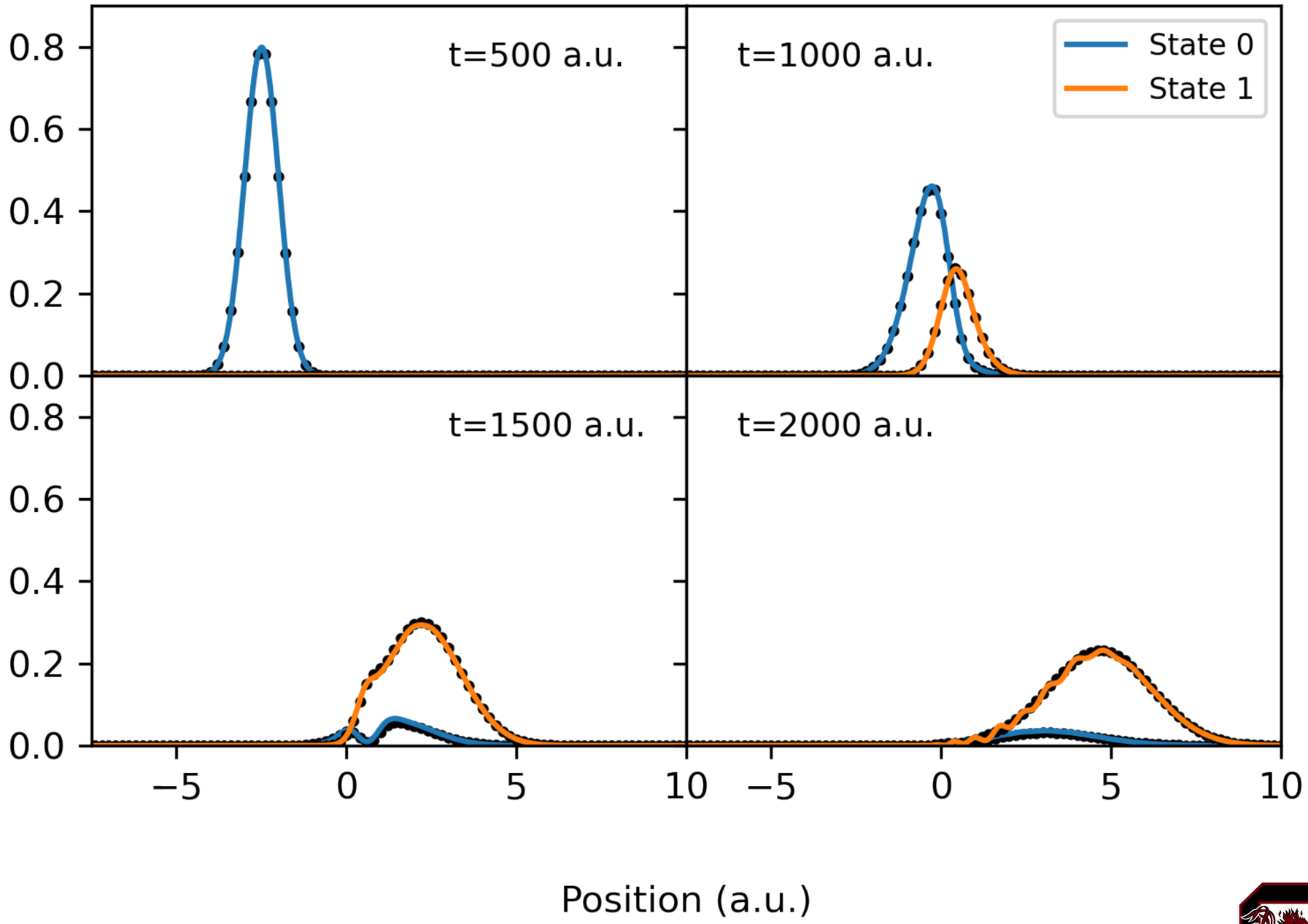
Mass — 2000.0 a.u.
Decpl. Pop. — 0.1
dt — 1.0



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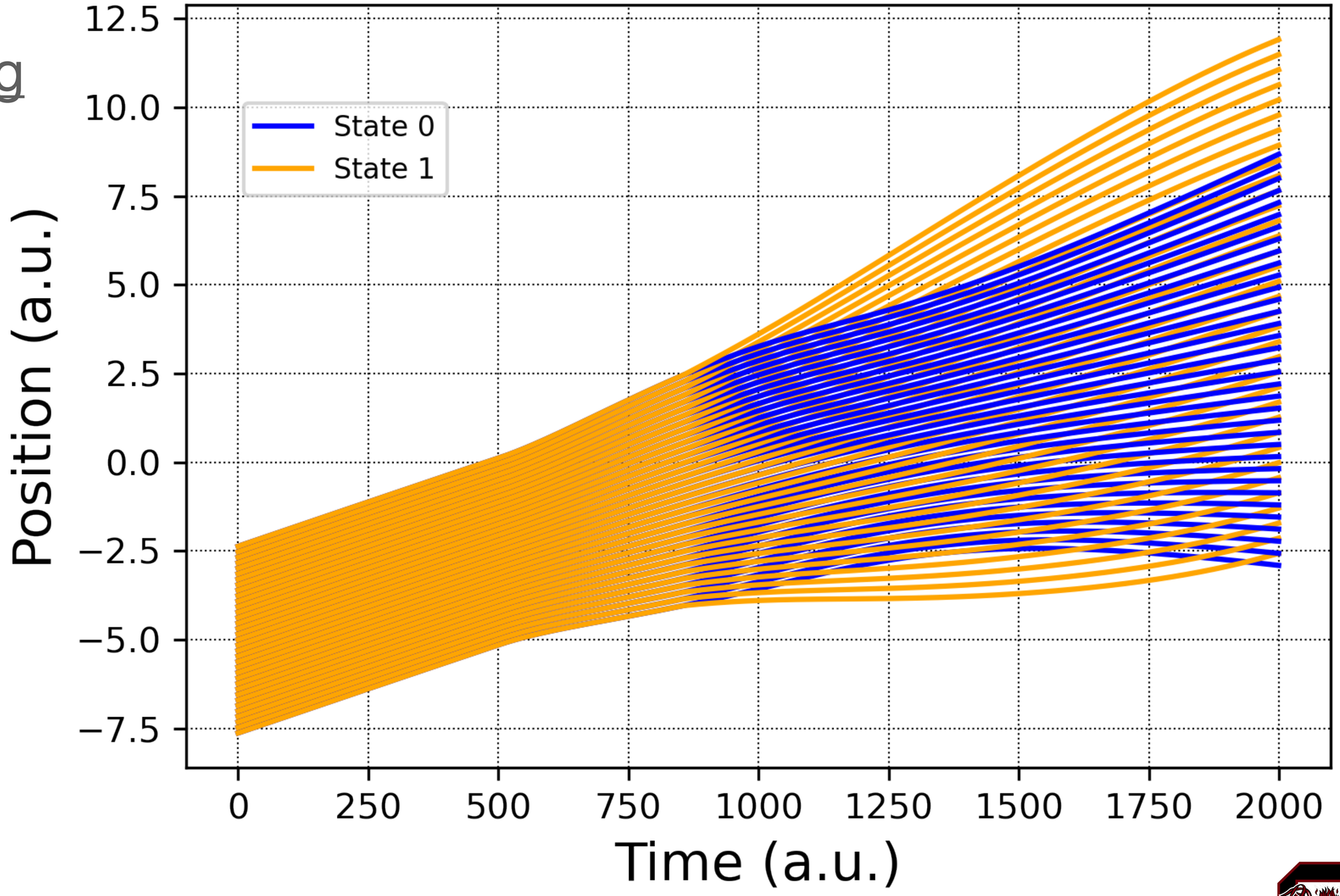

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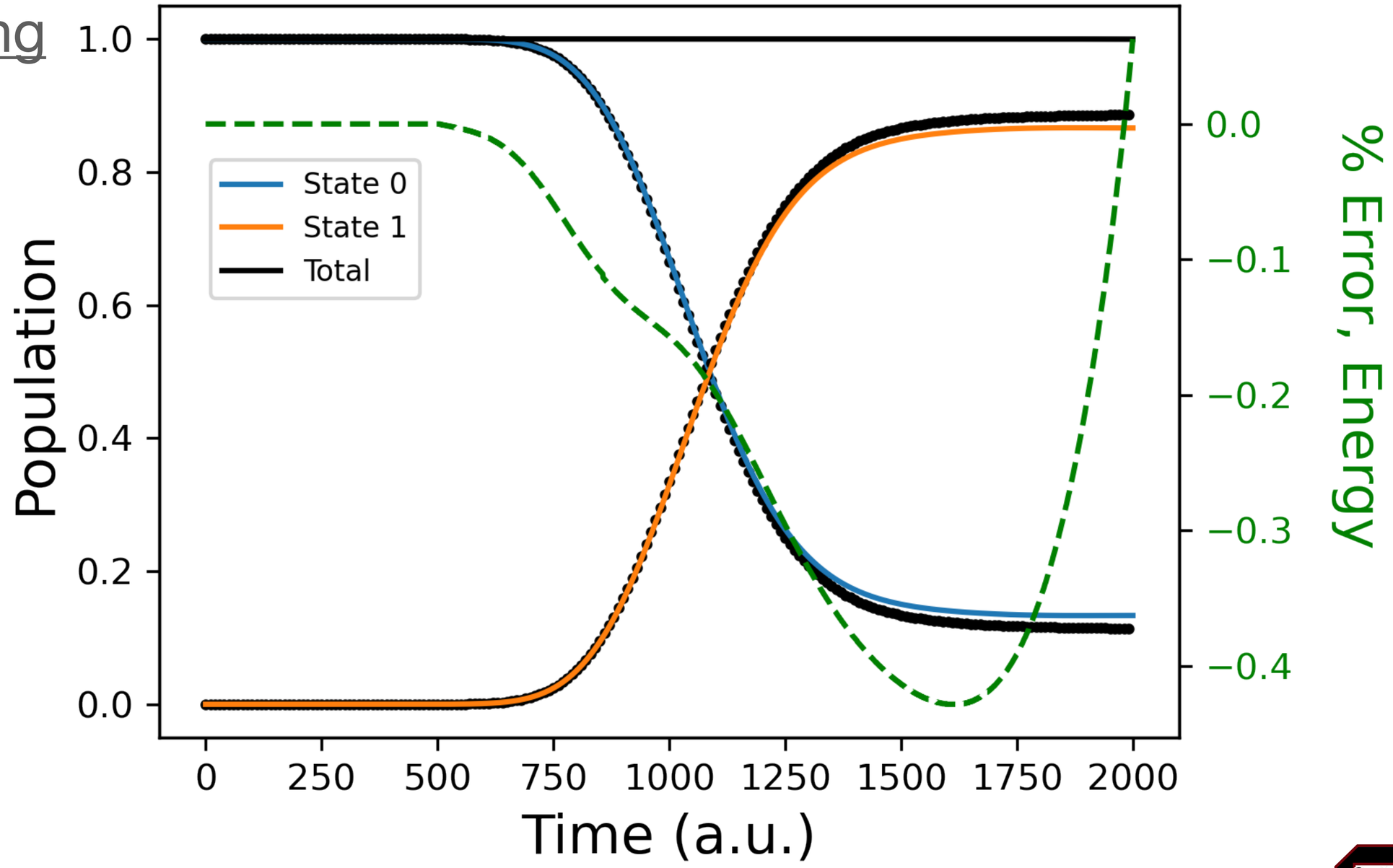


Dual Avoided Crossing

ψ_0

$Q_0 = -5.0$
$P_0 = 10.0$
$A_0 = 2.0$
$S_0 = 0.0$

Potential

$A = 0.1\ E_h$ $B = 0.28\ a_0^{-2}$
$C = 0.015\ E_h$ $D = 0.06\ a_0^{-2}$
$E_0 = 0.05\ E_h$

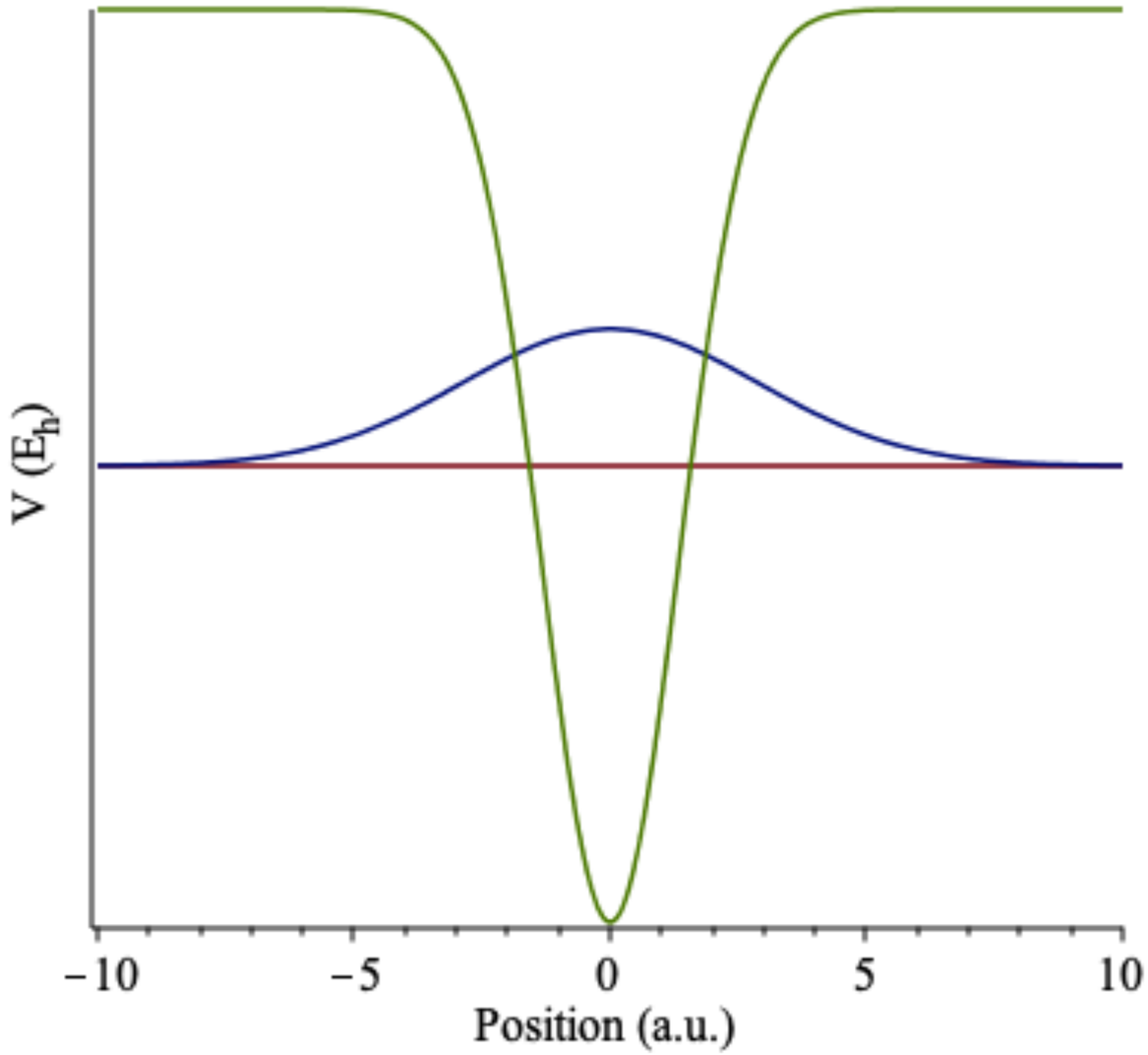
Parameters

Potential Approx. — BAT
Trajectories — 35
Width Scale — 25.0
Mass — 2000.0 a.u.
Decpl. Pop. — 0.01
dt — 1.0

$$V_{11} = 0$$

$$V_{22} = -Ae^{-Bx^2} + E_0$$

$$V_{12} = Ce^{-Dx^2}$$



Dual Avoided Crossing

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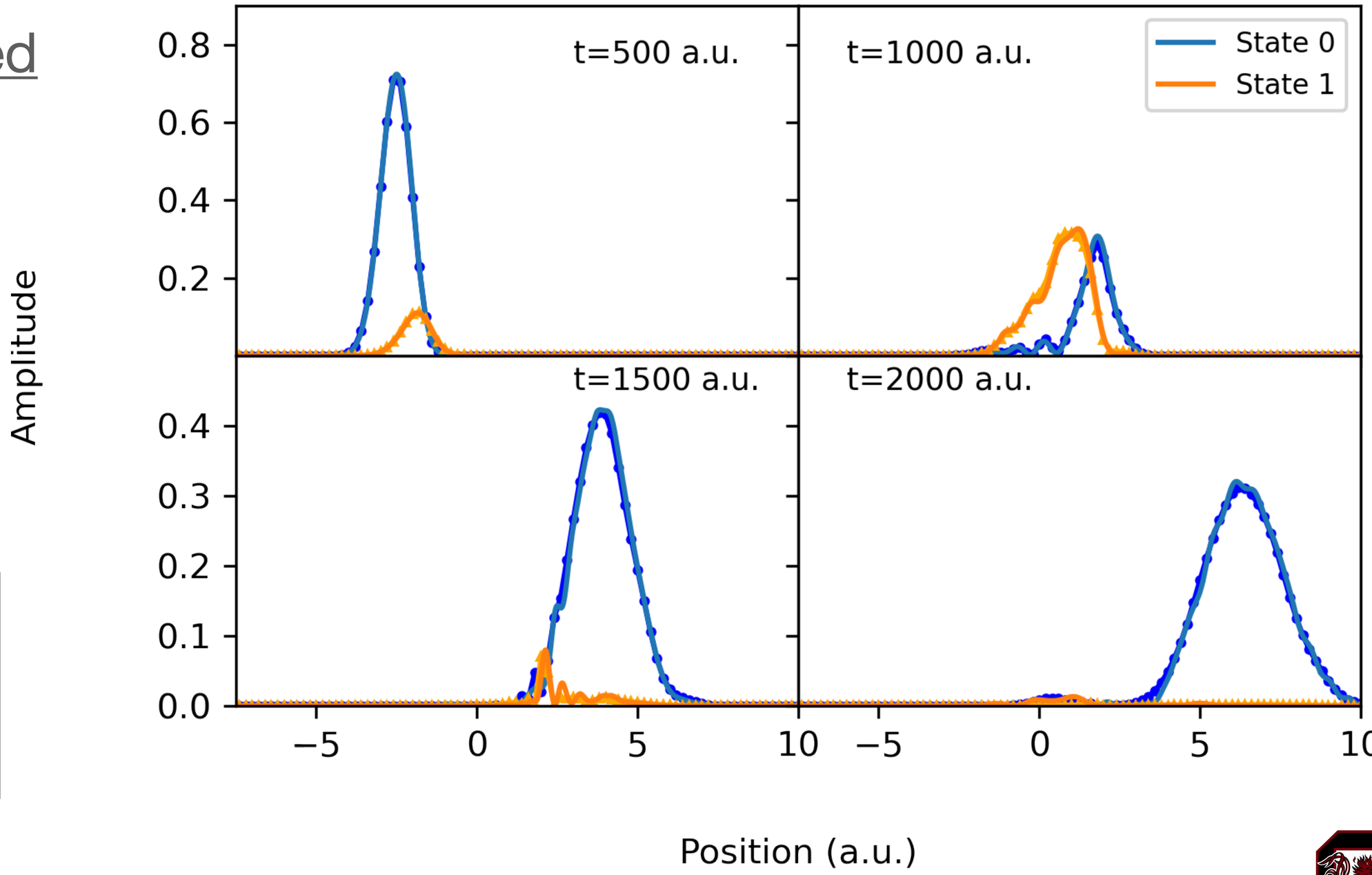

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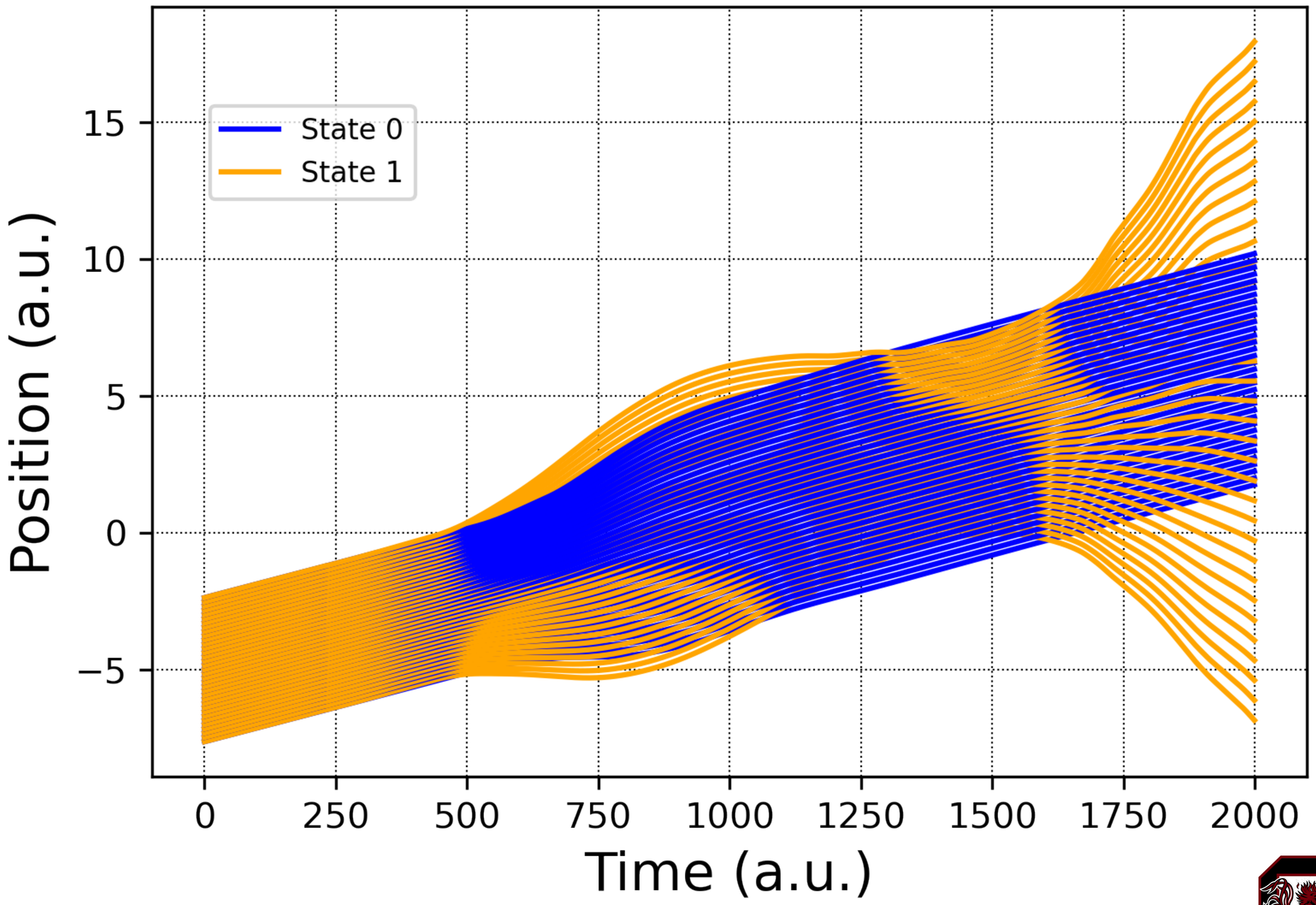

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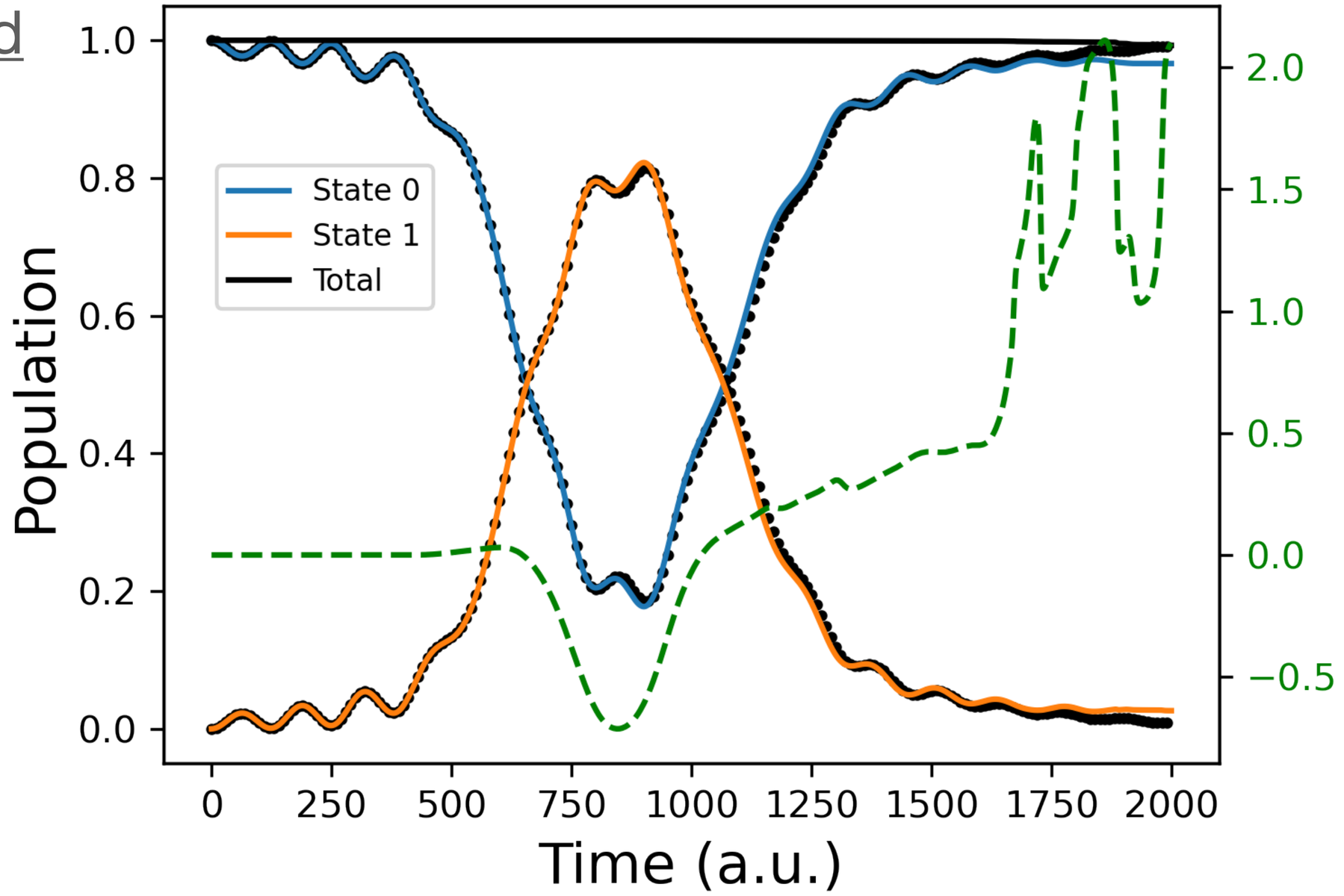

Gaussian parameters are consistent with Bohmian trajectories

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Nonadiabatic dynamics requires minor matrix modifications

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Trajectories in the nonadiabatic picture still evolve on single surfaces*

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Proof-of-concept models look promising in low dimension

Thank You!

Prof. Sophya Garashchuk
Prof. Alexey Akimov