Novelty Assessment Report

Paper: Orbital Transformers for Predicting Wavefunctions in Time-Dependent Density Functional Theory
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Abstract

We aim to learn wavefunctions simulated by time-dependent density functional theory (TDDFT), which can be efficiently represented as linear combination coefficients of atomic orbitals. In real-time TDDFT, the electronic wavefunctions of a molecule evolve over time in response to an external excitation, enabling first-principles predictions of physical properties such as optical absorption, electron dynamics, and high-order response. However, conventional real-time TDDFT relies on time-consuming propagation of all occupied states with fine time steps. In this work, we propose OrbEvo, which is based on an equivariant graph transformer architecture and learns to evolve the full electronic wavefunction coefficients across time steps. First, to account for external field, we design an equivariant conditioning to encode both strength and direction of external electric field and break the symmetry from SO(3) to SO(2). Furthermore, we design two OrbEvo models, OrbEvo-WF and OrbEvo-DM, using wavefunction pooling and density matrix as interaction method, respectively. Motivated by the central role of the density functional in TDDFT, OrbEvo-DM encodes the density matrix aggregated from all occupied electronic states into feature vectors via tensor contraction, providing a more intuitive approach to learn the time evolution operator. We adopt a training strategy specifically tailored to limit the error accumulation of time-dependent wavefunctions over autoregressive rollout. To evaluate our approach, we generate TDDFT datasets consisting of 5,000 different molecules in the QM9 dataset and 1,500 molecular configurations of the malonaldehyde molecule in the MD17 dataset. Results show that our OrbEvo model accurately captures quantum dynamics of excited states under external field, including time-dependent wavefunctions, time-dependent dipole moment, and optical absorption spectra characterized by dipole oscillator strength. It also shows strong generalization capability on the diverse molecules in the QM9 dataset.

Core Task Landscape

This paper addresses: **Predicting Time-Dependent Wavefunctions in Molecular Systems**

A total of **50 papers** were analyzed and organized into a taxonomy with **16 categories**.

Taxonomy Overview

The research landscape has been organized into the following main categories:

- **Time-Dependent Density Functional Theory Methods**
- **Wavefunction-Based Quantum Dynamics Methods**
- **Nonadiabatic and Mixed Quantum-Classical Dynamics**
- **Machine Learning and Data-Driven Approaches**
- **On-the-Fly and Adaptive Potential Energy Surface Methods**
- **Photochemistry and Excited State Applications**
- **Specialized Applications and Multiscale Modeling**

Complete Taxonomy Tree

- Predicting Time-Dependent Wavefunctions in Molecular Systems Survey Taxonomy
- Time-Dependent Density Functional Theory Methods
  - Real-Time TDDFT Propagation (3 papers)
  - [6] Realâtime timeâdependent electronic structure theory (Xiaosong Li, 2018) View paper
  - [40] Real-time, local basis-set implementation of time-dependent density functional theory for excited state dynamics simulations (Sheng Meng, 2008) View paper
  - [42] Machine Learning Time Propagators for Time-Dependent Density Functional Theory Simulations (Shah, 2025) View paper
  - Linear-Response and Frequency-Domain TDDFT (6 papers)
  - [7] Progress in time-dependent density-functional theory (E, 2012) View paper
  - [12] Implementation of time-dependent density functional response equations (SJA Van Gisbergen, 1999) View paper
  - [21] Time-dependent density functional theory (Chaoyuan Zhu, 2004) View paper
  - [22] Computational approaches for XANES, VtC-XES, and RIXS using linear-response time-dependent density functional theory based methods. (D. R. Nascimento, 2022) View paper
  - [48] Time-dependent density-functional theory in the projector augmented-wave method (Michael Walter, 2008) View paper
  - [49] Real-time time-dependent density functional theory approach for frequency-dependent nonlinear optical response in photonic molecules (Y Takimoto, 2007) View paper
  - Hybrid Functional and Acceleration Techniques for TDDFT (3 papers)
  - [2] Screened optimally tuned range separated hybrid functional for solvated low bandgap molecular systems. (Reinaldo V Dantas Filho, 2024) View paper
  - [4] Projected wave function extrapolation scheme to accelerate plane-wave hybrid functional-based bornâoppenheimer molecular dynamics simulations (S Jiao, 2025) View paper
  - [14] Low-rank approximations to accelerate hybrid functional enabled real-time time-dependent density functional theory within plane waves (Jielan Li, 2023) View paper

    - Simplified and Approximate TDDFT Frameworks (2 papers)
    - [1] The symmetric quasi-classical model using on-the-fly time-dependent density functional theory within the Tammâ□□Dancoff approximation (Justin J. Talbot, 2022) View paper
    - [37] Approximate time-dependent density functional theory (Niehaus, 2009) View paper
    - TDDFT for Spectroscopy and Multiscale Applications (4 papers)
    - [23] Time-dependent quantum/continuum modeling of plasmon-enhanced electronic circular dichroism. (P. Dâ□□Antoni, 2024) View paper
    - [36] Assessment of the time correlation function-based approach for absorption spectrum calculations using time-dependent density functional theory and molecular dynamics simulations. (Saito Shinji, 2025) View paper
    - [43] Automatized protocol and interface to simulate QM/MM timeâ□□resolved transient absorption at TDâ□□DFT level with COBRAMM (Davide Avagliano, 2022) View paper
    - [46] Resonant Inelastic X-ray Scattering Calculations of Transition Metal Complexes Within a Simplified Time-Dependent Density Functional Theory Framework. (D. R. Nascimento, 2021) View paper
- Wavefunction-Based Quantum Dynamics Methods
    - Variational and Configuration Interaction Approaches (3 papers)
    - [3] Ab-initio variational wave functions for the time-dependent many-electron SchrÃ¶dinger equation (J. Nys, 2024) View paper
    - [27] Many-electron dynamics in laser-driven molecules: Wavefunction theory vs. density functional theory (Florian Bedurke, 2021) View paper
    - [41] Sequential double ionization of molecules by strong laser fields simulated with time-dependent configuration interaction. (Paul Hoerner, 2021) View paper
    - Tensor Network and Multi-Configuration Methods (3 papers)
    - [9] Optimal tree tensor network operators for tensor network simulations: Applications to open quantum systems. (Li, 2024) View paper
    - [16] Multiconfigurational time-dependent Hartree approaches for indistinguishable particles (Lode, 2019) View paper
    - [18] Timeâ□□dependent density matrix renormalization group method for quantum dynamics in complex systems (Jiajun Ren, 2022) View paper
    - Semiclassical and Coherent State Methods (2 papers)
    - [28] Coherent state based solutions of the time-dependent SchrÃ¶dinger equation: hierarchy of approximations to the variational principle (Michael Werther, 2021) View paper
    - [50] Timeâ□□dependent approach to semiclassical dynamics (Eric J. Heller, 1975) View paper
    - Direct Wavepacket Propagation and Numerical Methods (3 papers)
    - [17] A Fourier method solution for the time dependent SchrÃ¶dinger equation as a tool in molecular dynamics (D. Kosloff, 1983) View paper
    - [44] Time-dependent quantum-mechanical methods for molecular dynamics (Ronnie Kosloff, 1988) View paper
    - [45] Time-dependent quantum mechanical wave packet dynamics (Narayanasami Sathyamurthy, 2021) View paper
- Nonadiabatic and Mixed Quantum-Classical Dynamics
    - Exact Factorization and Coupled Trajectory Methods (3 papers)
    - [8] Numerical analysis of the exact factorization of molecular time-dependent SchrÃ¶dinger wavefunctions (Emmanuel Lorin, 2021) View paper
    - [19] Electron-nuclear entanglement in the time-dependent molecular wavefunction (Federica Agostini, 2019) View paper
    - [35] Describing the photo-isomerization of a retinal chromophore model with coupled and quantum trajectories (Francesco Talotta, 2022) View paper
    - Trajectory Surface Hopping and Mixed Dynamics (3 papers)
    - [24] Time-dependent theoretical treatments of the dynamics of electrons and nuclei in molecular systems (E. Deumens, 1994) View paper
    - [26] Different flavors of nonadiabatic molecular dynamics (F. Agostini, 2019) View paper
    - [34] Time-Dependent Nonadiabatic Molecular Dynamics (Zhu, 2024) View paper
    - General Time-Dependent Quantum Methods for Large Systems (2 papers)
    - [15] Time-dependent quantum methods for large systems (Nancy Makri, 1999) View paper
    - [39] Stationary and time-dependent wave-operator formulation in molecular dynamics (G. Jolicard, 1991) View paper
- Machine Learning and Data-Driven Approaches ★ (4 papers)
    - [0] Orbital Transformers for Predicting Wavefunctions in Time-Dependent Density Functional Theory (Anon et al., 2026) View paper
    - [5] Machine learning enables long time scale molecular photodynamics simulations (Westermayr, 2019) View paper
    - [29] Molecular excited states through a machine learning lens (Pavlo O. Dral, 2021) View paper
    - [30] Scalable learning of potentials to predict time-dependent Hartreeâ□□Fock dynamics (Gupta Prachi, 2024) View paper
- On-the-Fly and Adaptive Potential Energy Surface Methods (2 papers)
    - [10] Quasi-direct quantum molecular dynamics: The time-dependent adaptive density-guided approach for potential energy surface construction (Nicolai Machholdt HÃ¸yer, 2024) View paper
    - [33] Solving the time-dependent SchrÃ¶dinger equation for nuclear motion in one step: direct dynamics of non-adiabatic systems (Graham A. Worth, 2008) View paper
- Photochemistry and Excited State Applications (3 papers)
    - [31] Making optical excitations visibleâ□□An exciton wavefunction extension to the time-dependent configuration interaction method (Fabian Langkabel, 2022) View paper
    - [38] Molecular photochemistry: recent developments in theory (S. Mai, 2020) View paper
    - [47] Time-dependent ab initio approaches for high-harmonic generation spectroscopy (Emanuele Coccia, 2021) View paper
- Specialized Applications and Multiscale Modeling (5 papers)
    - [11] Multiplex movie of concerted rotation of molecules on a 2D material (Reuner, 2023) View paper
    - [13] MDâ□□Ligandâ□□Receptor: A High-Performance Computing Tool for Characterizing Ligandâ□□Receptor Binding Interactions in Molecular Dynamics Trajectories (Michele Pieroni, 2023) View paper
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    - [25] Introduction to Time-Dependent Quantum Mechanics with Python (Atanu Bhattacharya, 2023) View paper
    - [32] Time-dependent surface-enhanced Raman scattering: A theoretical approach. (Corni Stefano, 2024) View paper

Narrative

Core task: predicting time-dependent wavefunctions in molecular systems. This field encompasses a diverse set of computational strategies for capturing how electronic and nuclear degrees of freedom evolve under external perturbations or during photochemical events. The taxonomy reflects several major branches: Time-Dependent Density Functional Theory Methods (TDDFT) offer a balance between accuracy and computational cost for many-electron systems, with foundational implementations like TDDFT Response Implementation[12] and ongoing refinements such as Symmetric Quasiclassical TDDFT[1] and Low-Rank Hybrid TDDFT[14]. Wavefunction-Based Quantum Dynamics Methods provide high-accuracy treatments through approaches like Multiconfigurational MCTDH[16] and Time-Dependent DMRG[18], while Nonadiabatic and Mixed Quantum-Classical Dynamics address coupled electronic-nuclear motion via methods exemplified by Direct Nonadiabatic Dynamics[33] and Exact Factorization Analysis[8]. Machine Learning and Data-Driven Approaches represent an emerging direction that leverages neural architectures to accelerate or replace traditional quantum propagation. On-the-Fly and Adaptive Potential Energy Surface Methods enable dynamics without precomputed surfaces, and specialized branches focus on Photochemistry and Excited State Applications as well as Multiscale Modeling for complex environments.

Within the Machine Learning and Data-Driven Approaches branch, a small handful of works explore how neural networks can learn quantum dynamics directly from data. Machine Learning Photodynamics[5] and Machine Learning Excited States[29] demonstrate early efforts to predict excited-state properties and nonadiabatic trajectories using data-driven models, while Scalable Hartree-Fock Learning[30] targets efficient representations of electronic structure. Orbital Transformers[0] sits naturally in this cluster, employing transformer architectures to predict time-evolved molecular orbitals and wavefunctions, thereby bypassing expensive iterative solvers. Compared to Machine Learning Photodynamics[5], which focuses on trajectory-level predictions, Orbital Transformers[0] emphasizes direct wavefunction propagation at the orbital level. This distinction highlights a key trade-off in the field: whether to learn coarse-grained dynamics or fine-grained quantum amplitudes, with the former offering broader applicability and the latter promising higher fidelity for systems where explicit wavefunction detail is essential.

Related Works in Same Category

The following **3 sibling papers** share the same taxonomy leaf node with the original paper:

1. Machine learning enables long time scale molecular photodynamics simulations

Authors: Westermayr, Julia, Gastegger, Michael, Menger, et al. (9 authors total) | **Year/Venue**: 2019 | **URL**: View paper

Abstract

Photo-induced processes are fundamental in nature but accurate simulations of their dynamics are seriously limited by the cost of the underlying quantum chemical calculations, hampering their application for long time scales. Here we introduce a method based on machine learning to overcome this bottleneck and enable accurate photodynamics on nanosecond time scales, which are otherwise out of reach with contemporary approaches. Instead of expensive quantum chemistry during molecular dynamics simu...

Relationship Analysis

Both papers belong to the Machine Learning and Data-Driven Approaches category, using neural networks to accelerate quantum dynamics simulations for molecular systems. The original paper (Orbital Transformers) focuses on learning time-dependent wavefunction coefficients in real-time TDDFT under external electric fields using equivariant graph transformers with SO(2) symmetry, while the candidate paper uses deep neural networks to learn potential energy surfaces, couplings, and other properties for nonadiabatic excited-state dynamics simulations via surface hopping. The key difference is that the original paper directly predicts wavefunction evolution in TDDFT, whereas the candidate paper learns PESs and couplings to enable trajectory-based photodynamics on nanosecond timescales.

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2. Molecular excited states through a machine learning lens

Authors: Pavlo O. Dral, M. Barbatti, Mario Barbatti | **Year/Venue**: 2021 | **URL**: View paper

Abstract

â¦ molecule evolves with time 16,17 . We may also be interested in statistical treatments, for example, for the prediction â¦ themselves, even by learning the wavefunctions 23,65 . For exampleâ¦

Relationship Analysis

Both papers belong to the Machine Learning and Data-Driven Approaches category, focusing on using machine learning to predict or accelerate quantum dynamics simulations for molecular excited states. The original paper (Orbital Transformers) develops a specific equivariant graph transformer architecture to directly learn time-dependent wavefunction coefficients in real-time TDDFT simulations under external electric fields, while the candidate paper (Molecular excited states through a machine learning lens) is a comprehensive review article surveying the broader landscape of ML applications in excited-state research, including property prediction, spectrum simulation, and materials design. The key difference is that the original paper presents a novel technical method for wavefunction evolution, whereas the candidate paper provides a systematic overview of the entire field without proposing a specific new method.

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3. Scalable learning of potentials to predict time-dependent Hartreeâ□□Fock dynamics

Authors: Gupta Prachi, Isborn, Christine | **Year/Venue**: 2024 • APL Machine Learning | **URL**: View paper

Abstract

We propose a framework to learn the time-dependent Hartreeâ□□Fock (TDHF) inter-electronic potential of a molecule from its electron density dynamics. Although the entire TDHF Hamiltonian, including the inter-electronic potential, can be computed from first principles, we use this problem as a testbed to develop strategies that can be applied to learn a priori unknown terms that arise in other methods/approaches to quantum dynamics, e.g., emerging problems such as learning exchangeâ□□correlation ...

Relationship Analysis

Both papers belong to the Machine Learning and Data-Driven Approaches category, using neural networks to accelerate quantum dynamics simulations by learning time-dependent electronic structure evolution. They overlap in addressing the core task of predicting time-dependent wavefunctions in molecular systems under external perturbations, with both employing data-driven methods to bypass expensive iterative quantum calculations. The key difference is that the original paper (OrbEvo) focuses on learning TDDFT wavefunction coefficients using equivariant graph transformers with SO(2) symmetry for external field conditioning, while the candidate paper learns the time-dependent Hartree-Fock inter-electronic potential using tensor-parameterized models with eight-fold permutation symmetry, serving as a testbed for learning unknown potential terms in quantum dynamics methods.

Contributions Analysis

Overall novelty summary. The paper introduces OrbEvo, a machine learning model that learns to propagate time-dependent electronic wavefunction coefficients in real-time TDDFT simulations. It resides in the 'Machine Learning and Data-Driven Approaches' leaf of the taxonomy, which contains only four papers total. This is a notably sparse research direction compared to the more established TDDFT and wavefunction-based branches, suggesting that direct ML-based wavefunction evolution remains an emerging and relatively unexplored area within the broader field of time-dependent quantum dynamics.

The taxonomy reveals that OrbEvo's immediate neighbors focus on related but distinct ML strategies: one sibling targets photodynamics trajectories, another addresses excited-state property prediction, and a third explores Hartree-Fock representations. The broader TDDFT branch (containing real-time propagation, linear-response, and hybrid functional methods) represents the traditional computational paradigm that OrbEvo aims to accelerate. By bridging the ML leaf with the real-time TDDFT subcategory, OrbEvo occupies a boundary position—applying data-driven techniques to a problem historically dominated by iterative numerical solvers.

Among 18 candidate papers examined across three contributions, none were flagged as clearly refuting the work. The core OrbEvo model examined 10 candidates with no refutations, the SO(2)-equivariant conditioning examined zero candidates, and the dual interaction methods (wavefunction pooling and density matrix) examined 8 candidates with no refutations. This limited search scope—covering top-K semantic matches and citation expansion—suggests that within the examined literature, no prior work directly overlaps with OrbEvo's specific combination of equivariant graph transformers, external field conditioning, and dual wavefunction-density matrix interaction schemes for TDDFT propagation.

Given the sparse ML-for-TDDFT landscape and the absence of refutations among 18 examined candidates, the work appears to occupy a relatively novel niche. However, the small search scale means the analysis cannot rule out relevant prior work outside the top-K semantic neighborhood or in adjacent subfields. The taxonomy structure indicates that while ML approaches to quantum dynamics are growing, direct wavefunction evolution via transformers remains less crowded than traditional TDDFT or nonadiabatic methods.

This paper presents **3 main contributions**, each analyzed against relevant prior work:

Contribution 1: OrbEvo model for learning time-dependent wavefunction evolution in TDDFT

Description: The authors introduce OrbEvo, a machine learning model that uses an equivariant graph transformer to predict the temporal evolution of electronic wavefunction coefficients in real-time time-dependent density functional theory. The model learns to propagate wavefunctions under external electric fields, enabling efficient prediction of quantum dynamics.

This contribution was assessed against **10 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

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1. Physics-informed neural networks for quantum propagators in Wavepacket dynamics

URL: View paper

Brief Assessment

Physics-Informed Quantum Propagators[61] focuses on learning quantum propagators using linear fully connected neural networks for the time-dependent Schrödinger equation and related quantum dynamics equations. This differs from OrbEvo's equivariant graph transformer architecture for TDDFT wavefunction coefficient evolution under external electric fields in molecular systems.

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2. Many-body dynamics with explicitly time-dependent neural quantum states

URL: View paper

Brief Assessment

Time-Dependent Neural States[59] focuses on many-body quantum systems using neural quantum states for the time-dependent Schrödinger equation, not on TDDFT electronic structure calculations with atomic orbital basis sets under external electric fields.

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3. Photocatalytic activity of dual defect modified graphitic carbon nitride is robust to tautomerism: machine learning assisted ab initio quantum dynamics.

URL: View paper

Brief Assessment

Photocatalytic Machine Learning[62] focuses on combining TDDFT with nonadiabatic molecular dynamics and machine learning to study photocatalytic processes in graphitic carbon nitride over nanosecond timescales. This differs from OrbEvo's focus on learning wavefunction coefficient evolution in real-time TDDFT using equivariant graph transformers.

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4. Accelerating wavepacket propagation with machine learning

URL: View paper

Brief Assessment

Machine Learning Wavepacket[65] focuses on solving the time-dependent Schrödinger equation using Fourier neural operators for wavepacket propagation in quantum systems, not on learning wavefunction evolution in time-dependent density functional theory (TDDFT) with equivariant graph transformers for molecular systems.

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5. Machine learning a molecular Hamiltonian for predicting electron dynamics

URL: View paper

Brief Assessment

Machine Learning Hamiltonian[67] learns a molecular Hamiltonian matrix from density matrix time series, not wavefunction coefficients. The candidate focuses on learning the Hamiltonian operator representation rather than directly predicting wavefunction evolution as OrbEvo does.

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6. Dual-Capability Machine Learning Models for Quantum Hamiltonian Parameter Estimation and Dynamics Prediction.

URL: View paper

Brief Assessment

Dual-Capability Hamiltonian Models[60] focuses on quantum Hamiltonian parameter estimation and dynamics prediction in quantum computing contexts (NMR and superconducting systems), not on time-dependent density functional theory or electronic wavefunction evolution in molecular systems.

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7. Discrete real-time learning of quantum-state subspace evolution of many-body systems in the presence of time-dependent control fields

URL: View paper

Brief Assessment

Discrete Real-Time Learning[68] focuses on quantum-state subspace evolution with time-dependent control fields using stochastic quantum natural gradient descent, which is a different approach from OrbEvo's equivariant graph transformer for predicting electronic wavefunction coefficients in TDDFT.

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8. Ab initio solution of the many-electron SchrÃ¶dinger equation with deep neural networks

URL: View paper

Brief Assessment

Deep Neural Schrodinger[63] focuses on variational quantum Monte Carlo for solving the time-independent many-electron Schrödinger equation using neural network ansätze, not time-dependent density functional theory or temporal wavefunction evolution under external fields.

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9. The 2025 roadmap to ultrafast dynamics: frontiers of theoretical and computational modelling

URL: View paper

Brief Assessment

Ultrafast Dynamics Roadmap[66] is a broad survey covering multiple theoretical approaches to ultrafast phenomena. While it discusses time-dependent density functional theory and various computational methods for ultrafast dynamics, it does not present a specific machine learning model for predicting wavefunction coefficient evolution like OrbEvo.

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10. Deep learning for Feynman's path integral in strong-field time-dependent dynamics

URL: View paper

Brief Assessment

Deep Learning Path Integral[64] focuses on strong-field ionization dynamics using Feynman path integrals for photoelectron spectra, not real-time TDDFT wavefunction coefficient evolution in molecular systems.

Contribution 2: SO(2)-equivariant conditioning for external electric field

Description: The authors develop a method to incorporate external electric field information into the model by breaking the full SO(3) rotational symmetry down to SO(2) symmetry around the field axis. This conditioning encodes both the magnitude and direction of the field while respecting the reduced symmetry constraints.

This contribution was assessed against **0 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

Contribution 3: Two interaction methods for electronic states: wavefunction pooling and density matrix

Description: The authors propose two distinct architectures for handling interactions among multiple electronic states. OrbEvo-WF uses layer-wise pooling over electronic states, while OrbEvo-DM aggregates information via density matrix features computed through tensor contraction, providing a more physically motivated approach aligned with TDDFT formalism.

This contribution was assessed against **8 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

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1. Quantum Chemical Density Matrix Renormalization Group Method Boosted by Machine Learning

URL: View paper

Brief Assessment

DMRG Machine Learning[55] focuses on enhancing quantum chemical DMRG calculations using machine learning, not on neural network architectures for electronic state interactions in TDDFT simulations.

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2. General framework for E (3)-equivariant neural network representation of density functional theory Hamiltonian

URL: View paper

Brief Assessment

Equivariant DFT Hamiltonian[52] focuses on E(3)-equivariant neural network representation of DFT Hamiltonians for materials, not on time-dependent wavefunction evolution or electronic state interaction methods like pooling and density matrix aggregation in TDDFT contexts.

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3. Machine learning electronic structure methods based on the one-electron reduced density matrix

URL: View paper

Brief Assessment

Machine Learning Density Matrix[57] focuses on learning one-electron reduced density matrices for electronic structure methods, not on neural network architectures for handling interactions among multiple electronic states in time-dependent systems as in the original paper.

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4. DEMANDE: Density Matrix Neural Density Estimation

URL: View paper

Brief Assessment

DEMANDE[58] focuses on density estimation using density matrices for probability density functions, not electronic state interactions in quantum chemistry simulations. The density matrix usage is fundamentally different from TDDFT wavefunction evolution.

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5. Neural pfaffians: Solving many many-electron schrÃ¶dinger equations

URL: View paper

Brief Assessment

Neural Pfaffians[53] focuses on enforcing fermionic antisymmetry through Pfaffian wave functions for generalized molecular systems, not on interaction methods between electronic states via wavefunction pooling or density matrix features.

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6. Neural network ansatz for periodic wave functions and the homogeneous electron gas

URL: View paper

Brief Assessment

Neural Periodic Wavefunctions[51] focuses on neural network ansätze for ground-state wave functions of the homogeneous electron gas with periodic boundary conditions, not on time-dependent density functional theory or methods for handling interactions among multiple electronic states during time evolution.

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7. Neural Mulliken Analysis: Molecular Graphs from Density Matrices for QSPR on Raw Quantum-Chemical Data

URL: View paper

Brief Assessment

Neural Mulliken Analysis[54] focuses on molecular property prediction using density matrices for molecular graph construction, not on time-dependent wavefunction evolution or electronic state interactions in TDDFT contexts.

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8. Improving density matrix electronic structure method by deep learning

URL: View paper

Brief Assessment

Deep Learning Density Matrix[56] focuses on predicting the density matrix itself as a fundamental DFT quantity, not on designing interaction architectures for multiple electronic states in time-dependent simulations. The candidate's density matrix is a static ground-state property used for charge density prediction, whereas the original paper's contribution concerns dynamic wavefunction evolution methods.

Appendix: Text Similarity Detection

No high-similarity text segments were detected across any compared papers.

References

- [0] Orbital Transformers for Predicting Wavefunctions in Time-Dependent Density Functional Theory View paper
- [1] The symmetric quasi-classical model using on-the-fly time-dependent density functional theory within the Tammâ□□Dancoff approximation View paper
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- [58] DEMANDE: Density Matrix Neural Density Estimation View paper
- [59] Many-body dynamics with explicitly time-dependent neural quantum states View paper
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