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# ABSTRACT

327 | COMPUTATIONAL & MATHEMATICAL PHYSICS (CP) / PLASMA PHYSICS (PL)

# Interlayer Self-Doping Multiferroics

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## Abstract

Multiferroic materials are noteworthy for their simultaneous possession of two or more ferroelectric properties, such as ferroelectricity and ferromagnetism. Based on first-principles calculations and utilizing orbital interactions, we demonstrated the anomalous phenomenon of carrier doping-enhanced polarization in a class of layered ferroelectric systems, and designed a class of two-dimensional multiferroic material systems based on this. In our latest research, we theoretically predicted and experimentally confirmed two-dimensional multiferroic metallic systems caused by the splitting difference in interlayer orbital energy levels, and also demonstrated the coupling effect of ferroelastic and antiferromagnetic order caused by orbital interactions in staggered magnets. These principles provide new insights for the development of next-generation ferroic quantum devices.

**REFERENCE STYLE**

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[2] Interlayer self-doping multiferroics, *Phys. Rev. Lett.* Accepted, 2026, S. Zhong, et al

**KEYWORDS**
Interlayer, 2D layers, charge transfer, altermagnetism

# Statistical Mechanics of Disordered Systems:

# Directed Polymers in Random Media and Anderson Transitions

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**ABSTRACT**

We will discuss two topics in the statistical mechanics of disordered systems. First, we revisit the transfer-matrix formulation of directed polymers in random media and show that a single ensemble of random transfer-matrix products provides a unified framework for the canonical one-point fluctuation laws of Kardar-Parisi-Zhang (KPZ) universality class in 1+1 dimensions. Different contractions of the same product matrix reproduce the standard KPZ subclasses. This matrix-based viewpoint not only organizes the known geometry-dependent subclasses in a common framework but also suggests new observables intrinsic to the transfer matrix itself, such as the leading eigenvalue, whose fluctuations display the KPZ scaling while remaining distinct from the canonical KPZ distributions over the accessible range. Second, we turn to disorder-driven quantum criticality at the Anderson metal-insulator transition. Using large-scale numerical simulations of the Chalker-Coddington network model for the integer quantum Hall transition, we examine multifractal spectra and scaling relations at criticality. Our results show excellent quantitative agreement with predictions from the conformal field theory, providing strong evidence that conformal symmetry constrains Anderson criticality in this setting. Together, these two topics highlight how disorder gives rise to universal fluctuation and scaling phenomena.

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S. Mu, A. A. Saberi, and M. Zirnbauer.

**KEYWORDS**

Disordered systems, Directed polymers, KPZ universality class, Anderson localization and transition, Conformal symmetry.

# Cross Machine Tokamak Disruption Prediction: A Systematic Framework Driven by Physics-Guided Transfer Learning

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## ABSTRACT

Realizing fusion energy requires not only high-performance plasmas but also the ability to maintain stable operation. In tokamaks, major disruptions are rapid terminations of plasma confinement, typically involving thermal quench and current quench, remain one of the main obstacles to safe tokamak operation. They can cause severe damage, long interruptions of operation, and major economic losses. Reliable early warning is therefore required for disruption mitigation and, where possible, avoidance in future devices. Data-driven predictors have shown strong performance, but their extension to large, high-parameter devices is limited by the scarcity of target-machine disruption data. Disruption data on large, high-parameter tokamaks are inherently scarce because deliberately accumulating disruptive shots to train a predictor risks severe damage to the machine. We present a systematic framework addressing this challenge through physics-guided transfer learning, using J-TEXT as the source platform, EAST for small-to-large-device transfer, and HL-2A for cross-regime studies at higher parameters. We developed single-device disruption predictors using both physics-guided feature extraction and deep architectures, demonstrating real-time density-limit disruption avoidance. We then studied transfer from J-TEXT to EAST, an ITER-like fully superconducting long-pulse tokamak, we studied transfer under deliberately limited target-machine data to simulate the conditions future large-device predictors will face, and extended this to adaptive prediction from the very first plasma discharge. On HL-2A, cross-regime transfer revealed that disruption precursor patterns are not universal. High-performance operational regimes exhibit distinct precursor signatures, requiring regime-aware transfer strategies rather than naive pooling of data from different regimes. Interpretability is used here not mainly to explain model outputs after training, but to study disruption physics from data, identify physically meaningful and transferable precursor information, and motivate physics constraints for prediction on data-scarce new tokamaks. Taken

together, these studies support a practical route toward transferable disruption prediction under the data constraints expected in future tokamaks.

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## KEYWORDS

fusion energy, disruption prediction, transfer learning, interpretability, physics priors

Title:
Correlation analysis of protein condensate

Abstract：
Collective behavior is ubiquitous across biological scales—from protein folding and allostery to the recently highlighted liquid–liquid phase separation (LLPS) and condensate formation. We developed correlation–statistics analysis method and used molecular dynamics simulation to investigate the emergent correlation behavior inside protein condensates and intrinsically disordered protein (IDP). We identified spatial correlations between DOPA and positively charged residues in mussel adhesive proteins, scale-free long-range correlations in both IDP conformational fluctuations and conformational evolution within protein condensate

Bio:
Professor Jingyuan Li received his Bachelor (2002) and Ph.D. degree (2007) from Zhejiang University. After completing postdoctoral research at Columbia University, he joined the Institute of High Energy Physics, CAS as a professor in the multi-disciplinary research division (2011). In 2017, he joined Zhejiang University as a professor in the Department of Physics. He was selected for the “Hundred Talents Program” of CAS and received funding from NSFC's "Excellent Youth Science Fund". He is vice president of Zhejiang Physical Society. His research focuses on computational live matter physics with emphasis on the protein condensate and intrinsically disordered protein, i.e. to characterize, understand and predict the conformation and biological function of protein condensate and IDP..

# Novel Quantum Liquids: Spin-Charge separation, FFLO Pairing, Luther-Emery Liquid

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Low-energy excitations in one-dimensional (1D) repulsive ultracold atomic Fermi gases (Yang–Gaudin model) separate into two collective modes carrying solely spin or charge degrees of freedom-the hallmark of spin-charge separation unique to 1D systems. By contrast, attractive 1D fermionic systems host novel polarization-dependent BCS pairing states, including the Fulde-Ferrell-Larkin-Ovchinnikov pairing state and Luther–Emery liquid (LEL). The latter is a fully paired state with gapped spin excitations yet gapless charge excitations. Direct experimental detection and theoretical understanding of such exotic quantum liquids have long remained challenging and incomplete.

Using the Bethe ansatz and bosonization, this talk explores the microscopic mechanisms and experimental realization of these distinct properties in 1D interacting fermions. We tune a $^6$Li system via Feshbach resonance across repulsive and attractive regimes, and measure dynamic spin and charge structure factors using Bragg spectroscopy. Spin-charge separation is clearly resolved, with results in excellent agreement with nonlinear Luttinger liquid theory. Finally, we discuss the observation of the LEL. In attractive fermions, unlike repulsive systems, spin waves propagate faster than charge density waves, revealing the pair-breaking character of spin excitations and a reversal of conventional spin-charge separation. These results establish an important basis for understanding collective motions in low dimensions.

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2. Low Energy Excitations of a 1D Fermi Gas with Attractive Interactions, arXiv:2512.08866, 2025, A Kafle,…, X Guan, R Hulet
3. Tomonaga-Luttinger liquid theory for one-dimensional attractive Fermi gases, arXiv:2603.13958, 2026, H Cui, Y Yeh, R Hullet, H Pu, T Giamarchi, X Guan

**Key words:** Yang-Gaudin model, Spin-charge separation, FFLO pairing, Luther-Emery liquid

# SOLUTIONS OF MULTI-ELECTRON SYSTEMS USING HYPERSPHERICAL COORDINATES AND 1-D BASIS FUNCTIONS

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**ABSTRACT**

We present integrated numerical approaches for solving the many-electron Schrödinger equation that circumvent limitations of conventional Hartree-Fock and DFT methods. Our methodologies combine hyperspherical coordinates, one-dimensional basis functions, and nonlinear coordinate transformations with advanced iterative algorithms. In the hyperspherical approach, wave functions are expanded into orthonormal basis sets of hyperspherical harmonics and generalized Laguerre polynomials, reducing the many-body problem to a secular equation that accurately describes electron correlation in He atoms and charged excitons. The 1-D basis function method constructs three-dimensional wave functions from linear combinations of one-dimensional hydrogenic functions along Cartesian axes. Implemented on uniform real-space grids with finite-difference discretization, this approach utilizes the Residual Minimization Method-Direct Inversion in the Iterative Subspace (RMM-DIIS) to minimize the Rayleigh quotient variationally. The method captures electron correlation explicitly, achieving virial ratios of $-V/T \approx 2.0$ and energies comparable to Hylleraas variational results for He and $H_2$. For molecular systems, we employ a sign square-root coordinate transformation that concentrates grid points near nuclei while maintaining uniform grids in transformed space. This yields a Hamiltonian with faster potential decay and reduced kinetic energy, enabling accurate treatment of nuclear cusps and electron correlation using minimal grid points. To accelerate convergence, we developed Residual Direct Inversion in the Iterative Subspace (RDIIS) and Residual Vector Correction (RVC) algorithms that eliminate cubic scaling. These methods have been validated across hydrogen-like atoms, two-electron systems, and small molecules, demonstrating explicit treatment of electron correlation with favorable computational scaling.

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**KEYWORDS**
Multi-electron systems, Schrödinger equation, Hyperspherical coordinates, 1-D basis functions, Electron correlation

# Moiré Excitons in van der Waals Materials

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**ABSTRACT**
Understanding excited state phenomena is at the heart of many important materials problems, such as photovoltaics, photocatalysis, plasmonics and quantum information. In this talk, I will highlight our recent progress in developing accurate and efficient first-principles methods that enable us to probe electronic excitations in emerging materials. In particular, I'll focus on a linear-response time-dependent density functional theory (LR-TDDFT) method with optimally tuned, screened and range-separated hybrid (OT-SRSH) exchange-correlation functional that can compute exciton band structure, exciton charge density, excited state forces, and exciton-phonon coupling matrix accurately for large-scale extended systems. Formulated with spinor wavefunctions, the LR-TDDFT method enables calculations of noncollinear magnetism and spin-orbit coupling and can be combined with non-adiabatic molecular dynamics to explore exciton dynamics. Using this method, we have examined electron excitations in 2D van der Waals materials, including moiré excitons, moiré magnetism, exciton dynamics, and Bose-Einstein condensation of moiré excitons.

# Ab initio spin wave dynamics: DFPT and adiabatic theory

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**ABSTRACT**
Density Functional Perturbation Theory (DFPT) provides a rigorous theoretical and computational framework for studying the linear response properties of many-electron systems in real materials. We have developed a DFPT implementation based on the Projector Augmented-Wave (PAW) method, enabling self-consistent calculations of charge-spin density response functions and four-component polarizabilities under electromagnetic fields. This computational toolkit allows for first-principles calculation of spin-wave excitation spectra without relying on empirical models or adjustable parameters.[1] However, brute-force DFPT calculations of spin-wave dynamics can be computationally prohibitive. To address this challenge, we leverage first-order wavefunctions and density responses from DFPT calculations to solve the Niu-Kleinman adiabatic spin dynamics equation, establishing an efficient and universal method for obtaining spin-wave dispersion relations and eigenmode collective excitations.[2] Finally, I will discuss theoretical approaches for investigating geometric phases and topological properties of spin-wave excited states within the DFPT framework.[3]

**REFERENCE STYLE**
[1] Implementation of the density functional perturbation theory for generalized susceptibility in the projector augmented wave framework. *Physical Review B* 108 (9), 094405, 2023. X. Liu, Y. Lin, J. Feng
[2] Assessing the atomic moment picture of spin dynamics with ab initio magnon wavefunctions. *Physical Review B* 111, 054419, 2025. Y. Lin, X. Liu, J. Feng.
[3] Fully first-principles approach in studying topological magnons. *Physical Review B* (2026, accepted). X. Liu, J. Feng, Z. Qiao, Q. Niu.

**KEYWORDS**
DFPT, spin wave, magnon, adiabatic dynamics, excited states

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# Single-layer Framework of Variational Tensor Network States

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## ABSTRACT

In the tensor-network framework, the expectation values of two-dimensional quantum states are evaluated by contracting a double-layer tensor network constructed from initial and final tensor-network states. The computational cost of carrying out this contraction is generally very high, which limits the largest bond dimension of tensor-network states that can be accurately studied to a relatively small value. In the nested tensor network method [1], we propose to solve this problem by mapping the double-layer tensor network onto an intersected single-layer tensor network. This reduces greatly the bond dimensions of local tensors to be contracted and improves dramatically the efficiency and accuracy of the evaluation of expectation values of tensor-network states. Furthermore, by combining this with the automatic differentiation technique [2], our approach can reduce the computational cost by three orders of magnitude in bond dimension, and therefore enables highly efficient variational ground-state calculations [3]. Even without GPU acceleration or symmetry implementation, we have achieved a bond dimension of nine and obtained accurate ground-state energy and consistent order parameters compared to prior studies on tested interesting models. Our work provides a promising route for large-scale tensor network calculations of two-dimensional quantum systems.

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## KEYWORDS

tensor networks, single-layer framework, variational calculation, automatic differentiation

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# Probing Deconfined Quantum Criticality via Entanglement Entropy

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## ABSTRACT

Scaling behavior of entanglement entropy serves as a powerful tool for investigating the ground states and low-energy excitations of quantum many-body systems. In particular, for systems exhibiting spontaneous breaking of continuous symmetry, the scaling behavior of entanglement entropy can reflect the number of Goldstone modes. By analyzing the scaling behavior of entanglement entropy with finite-size corrections, this number can be determined with considerable accuracy in practical numerical simulations. This talk will present our application of this tool to study the properties of lattice models realizing deconfined quantum criticality. We provide evidence for the presence of an emergent O(5) symmetry at the AFM-CVBS transition point and reveal that the phase transition is first-order. For the AFM-PSS (plaquette-singlet solid) transition, we observe the emergence of a specific coplanar order at the transition point and propose a novel emergent frustration mechanism responsible for inducing this coplanar order.

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2. Coplanar order induced by emergent frustration, arXiv: 2504.13555, Zehui Deng, Lu Liu, Wenan Guo, and Hai-Qing Lin.

## KEYWORDS

Deconfined Criticality, Entanglement entropy, Scaling behavior, Emergent symmetry, Emergent frustration

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# NEAR-OPTIMAL PARAMETER TUNING OF LEVEL-1 QAOA FOR ISING MODELS

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## ABSTRACT

Variational quantum algorithms are widely viewed as one of the most promising routes to useful computation on near-term quantum hardware, with the Quantum Approximate Optimisation Algorithm (QAOA) emerging as a leading framework for combinatorial optimisation. Yet even in its shallowest and most experimentally accessible regime, level-1 QAOA, a fundamental obstacle persists: how can globally optimal or provably near-optimal variational parameters be identified efficiently and reliably for realistic weighted problem instances? We show that this problem is considerably more intricate than conventional intuition suggests. For general Ising formulations of optimisation tasks, the level-1 QAOA landscape is not a simple smooth surface, but can instead develop rapid oscillations whose fine structure becomes increasingly pronounced with growing system size, graph density, and coupling strength. As a result, coarse parameter scans—the standard approach in many studies—can significantly misrepresent the landscape and fail to locate the true optimum. To address this, we develop a principled framework based on a Fourier analysis of the QAOA objective. This allows us to derive closed-form bounds on the highest relevant frequencies in the landscape, determine the sampling resolution required to resolve them faithfully, and reduce the original two-parameter optimisation problem to a one-dimensional search with the second parameter obtained analytically. We further prove that for regular graphs, the first local optimum near zero is, on average, already globally optimal, providing a rigorous explanation for a striking empirical phenomenon and a firm foundation for simple optimisation strategies. When integrated into Recursive QAOA, our method yields substantial performance gains and enables it to outperform both coarse tuning methods and semidefinite-programming baselines on large weighted Ising instances. These results provide new theoretical insight into shallow variational quantum algorithms and a practical route toward scalable quantum optimisation.

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**REFERENCE STYLE**
Near-Optimal Parameter Tuning of Level-1 QAOA for Ising Models, arXiv preprint, arXiv:2501.16419, 2025, V. Vijendran, D.E. Koh, E. Bae, H. Kwon, P.K. Lam, S.M. Assad.

**KEYWORDS**
Variational Quantum Algorithms, Combinatorial Optimisation, Quantum Optimisation, Ising Models, Parameter Tuning

# Advances in Close-Coupling Methods for Electron-Atom Collisions in Plasma Environments

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**ABSTRACT**

Understanding the detailed dynamics of electron-atom/ion interactions is crucial for diverse plasma applications in fields such as astrophysics, fusion research, and semiconductor lithography. For atoms embedded in plasma environments, their structures and properties will be significantly altered due to the complicated many-body interactions with the surrounding plasmas, which pose a significant challenge in calculation these structure and dynamical properties.

In this talk, I'll present our recent progress on close-coupling (CC) computational methods for electron-atom collisions across diverse plasma environments. We developed a specialized CC method for highly charged ions with strong radiative damping [1,2]. By investigating J=1/2→1/2 transitions in $Pb^{78+}$, we demonstrate that x-ray polarization arises from distinct quantum interference, leading to unexpectedly large polarization even in nearly symmetric Fano profiles [1]. We also developed a CC framework for general screened potentials. By developing a numerical method to compute asymptotic regular and irregular wavefunctions efficiently, this approach resolves the technical challenge of extracting short-range scattering phase shifts under screened Coulomb interactions. The method ensures that scattering matrices remain invariant with respect to the matching point in the asymptotic region, providing a robust tool for calculating collision processes in warm dense plasmas [3]. We applied this plasma-screened CC theory to spectral line shape calculations. Systematic investigations of hydrogenic radiators reveal distinct patterns of line-broadening dependence on plasma conditions [4]. These works provide a comprehensive theoretical foundation for modelling of complex atomic systems in high-density plasma environments.

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**KEYWORDS**
Electron-atom Collision, Close-Coupling Methods, R-matrix Method, Plasma Environments

# SIMULATION OF PLASMA DETACHMENT IN TCV USING HERMES-3

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## ABSTRACT

Achieving plasma detachment is essential for managing divertor heat loads in magnetic confinement fusion devices. In this work, we investigate detachment physics in configurations relevant to a lower single-null Tokamak à Configuration Variable **(**TCV**)** using the 2D simulations with the HERMES-3 code. By scanning a range of upstream densities, we identify the onset and evolution of detachment within TCV geometry. The model incorporates self-consistent plasma-neutral interactions, including ionization, recombination, and charge-exchange process, enabling detailed analysis of momentum and power balance in the divertor region. Our result captures the characteristic ion flux "rollover", marking the transition from attached to detached regimes characterized by strong volumetric power losses, reduction of target ion flux, and the formation of a cold, dense plasma region near the divertor plates. These results provide insight into the mechanisms governing detachment in TCV configurations and offer guidance for experimental scenarios and future predictive modeling of divertor operation in next-step devices.

This research is supported by the National Research Foundation, Singapore. The computational work for this research was fully performed on resources of the National Supercomputing Centre, Singapore. This research is prepared in part by LLNL under Contract DE-AC52-07NA27344.

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Divertor plasma detachment, *Physics of Plasmas*, 23, 055602, 2016, S. I. Krasheninnikov, A. S. Kukushkin and A. A. Pshenov.

**KEYWORDS**
Magnetic confinement fusion, plasma detachment, radiation, plasma-neutral interaction, plasma simulation

# A PENALTY-FREE QUANTUM ALGORITHM TO FIND ENERGY EIGENSTATES

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**ABSTRACT**

**FINDING EIGENSTATES OF A GIVEN MANY-BODY HAMILTONIAN IS A LONG-STANDING CHALLENGE DUE TO THE PERCEIVED COMPUTATIONAL COMPLEXITY. LEVERAGING ON THE HARDWARE OF A QUANTUM COMPUTER ACCOMMODATING THE EXPONENTIAL GROWTH OF THE HILBERT SPACE SIZE WITH THE NUMBER OF QUBITS, MORE QUANTUM ALGORITHMS TO FIND THE EIGENSTATES OF MANY-BODY HAMILTONIANS WILL BE OF WIDE INTEREST WITH PROFOUND IMPLICATIONS AND APPLICATIONS. IN THIS WORK, WE ADVOCATE A QUANTUM ALGORITHM TO FIND THE GROUND STATE AND EXCITED STATES OF MANY-BODY SYSTEMS, WITHOUT ANY PENALTY FUNCTIONS, VARIATIONAL STEPS OR HYBRID QUANTUM-CLASSICAL STEPS. OUR FULLY QUANTUM ALGORITHM WILL BE AN IMPORTANT ADDITION TO THE QUANTUM COMPUTATIONAL TOOLBOX TO TACKLE PROBLEMS INTRACTABLE ON CLASSICAL MACHINES.**

**REFERENCE STYLE**

A penalty-free quantum algorithm to find energy eigenstates, Physical Review A, in press, 2026, Ma, N., Dai, H., & Gong, J.

**KEYWORDS**

Ground state, penalty-free, quantum circuit.

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# Topological Physics in Quantum Critical Systems

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**ABSTRACT**
Topology forms a cornerstone in modern condensed matter and statistical physics, offering a new framework to classify the phases and phase transitions beyond the traditional Landau paradigm. However, it is widely believed that topological properties are destroyed when the bulk energy gap closes, making it highly nontrivial to consider topology in gapless quantum critical systems. To address these challenges, recent advancements have sought to generalize the notion of topology to systems without a bulk energy gap, including quantum critical points and critical phases, collectively referred to as gapless symmetry-protected topological states. Extending topology to gapless quantum critical systems challenges the traditional belief in condensed matter physics that topological edge states are typically tied to the presence of a bulk energy gap. Furthermore, it suggests that topology plays a crucial role in classifying quantum phase transitions even if they belong to the same universality class, fundamentally enriching the textbook understanding of phase transitions. Given its importance, here we give a pedagogical review of the current progress of topological physics in quantum critical systems. We introduce the topological properties of quantum critical points and generalize them to stable critical phases, both for noninteracting and interacting systems. Additionally, we discuss further generalizations and future directions, including higher dimensions, nonequilibrium phase transitions, and realizations in modern experiments.

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**KEYWORDS**
Quantum phase transition, Gapless systems, Topological phases, Quantum entanglement, Conformal field theory

# Study of the Effect of Interchange and Adiabaticity in Turbulence Spreading with 2-Fields Fluid Simulations

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**ABSTRACT**

Turbulence spreading is a fundamental nonlocal process in which fluctuation energy propagates from unstable into weakly unstable or stable regions through nonlinear mode coupling. Its properties depend heavily on the underlying turbulence regime. In particular, drift-wave and interchange turbulence are characterized by different instability drives, mode structures, and transports, all of which can affect the radial propagation of turbulence intensity. In this work, turbulence spreading is investigated using two-dimensional drift-reduced two-field fluid simulations with TOKAM2D. The model evolves the density and vorticity fields and allows systematic variation of the interchange forcing parameter, $\boldsymbol{g}$, and the adiabaticity parameter, $\boldsymbol{C}$. This provides a controlled framework for examining how turbulence spreading changes across regimes ranging from drift-wave-dominated to interchange-dominated dynamics. The study helps clarify the regime dependence of turbulence spreading and offers a reduced-fluid perspective on the mechanisms governing its propagation.

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**KEYWORDS**

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Tokamak, turbulence spreading, TOKAM2D, drift-wave instability, interchange instability.

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# GENERATIVE INITIALIZATION OF GBS SIMULATIONS USING VAE-BASED LATENT FLOW MATCHING

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## ABSTRACT

High-fidelity plasma simulations based on the Global Braginskii Solver (GBS) are essential for studying edge plasma dynamics, but they are often computationally expensive, especially when simulations start from random or uniformly prescribed initial conditions. Such initializations may require long transient evolution before reaching physically meaningful plasma states, leading to a considerable waste of computational resources. To address this issue, this work develops a generative reconstruction framework that combines a variational autoencoder (VAE) with latent flow matching for GBS simulation data. The VAE first learns a compact latent representation of high-dimensional plasma fields, while the flow-matching model learns the distributional evolution in the latent space and generates physically plausible plasma states. These generated states are then decoded back to the physical field space and used as simulation initial conditions, replacing conventional random or uniform initialization strategies. By initializing GBS simulations from data-informed generated fields, the proposed approach aims to reduce the initial relaxation stage and accelerate convergence toward statistically meaningful plasma dynamics. Preliminary results show that the VAE-based latent generative model can reconstruct the dominant spatial structures of GBS fields and produce initial states that are more consistent with learned plasma patterns than manually specified initial conditions. This suggests that generative modeling can serve not only as a surrogate reconstruction tool, but also as a practical initialization strategy for accelerating physics-based plasma simulations. The proposed framework provides a promising route toward combining data-driven generative models with first-principles simulation codes for efficient plasma modeling.

## REFERENCE STYLE

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**KEYWORDS**
GBS simulation, Plasma modeling, Variational autoencoder, Flow matching, Generative initialization

# First Principles Design of Functional Materials for Energy And Optoelectronic Device Applications

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**ABSTRACT**

Materials design using first-principles techniques is one of the ultimate goals in computational materials science. Recent advances in first-principles electronic structure theory and computing power have enabled us to perform *knowledge-based* computational design of materials with unique properties that are tuned to specific energy and optoelectronic applications. This approach has now become a vital tool in accelerating scientific discovery of energy and optoelectronic materials. In this talk, selective topics from our recent studies will be discussed to illustrate how computational methods can be used to understand and design functional materials, including solar cell materials; thermoelectric materials; and transparent conducting materials.

**KEYWORDS**

Energy materials, Optoelectronic materials, First-principles calculations, Inverse Design

# *Variational tensor network operator*

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**ABSTRACT**
In this talk, I will introduce a simple and generic construction of the variational tensor network operators to study the quantum spin systems by the synergy of ideas from the imaginary-time evolution and the variational optimization of trial wave functions [1]. By applying these operators to simple initial states, accurate variational ground-state wave functions with extremely few parameters can be obtained. Furthermore, the framework can be applied to spontaneously study symmetry-breaking, symmetry-protected topological, and intrinsic topologically ordered phases, and we show that symmetries of the local tensors associated with these phases can emerge directly after the optimization without any gauge fixing. This provides a universal way to identify quantum phase transitions without prior knowledge of the system. Finally, I will show the applications to the study of anisotropic Kitaev model under magnetic fields

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**KEYWORDS**
Tensor Network, SPT, Topological Order, Anyon

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# THEORY OF QUANTUM IMAGINARY-TIME MPEMBA EFFECT

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## ABSTRACT

Quantum imaginary-time evolution (QITE) is a fundamental framework for preparing ground and thermal states, yet its computational cost scales significantly with the evolution duration $\tau$. Reducing this duration is critical for practical quantum advantage. Here, we establish a unified theoretical framework for the Mpemba effect in QITE—a counterintuitive phenomenon where a state initially farther from the ground state relaxes to it faster than one initially closer. We derive a remarkably simple necessary and sufficient condition for the occurrence of this effect, showing it is uniquely determined by the population ratios of excited states to the ground state. For practical state preparation, we introduce a rigorous sufficient condition for the finite-time Mpemba effect, ensuring the crossing occurs before reaching a prescribed proximity threshold. Furthermore, we unveil unique dynamical features, including a multiple-crossing phenomenon in multi-level systems and simultaneous intersections for collinear initial states. Our results provide criteria for identifying favorable initial states in QITE and offer deep insights into the speed limit of quantum state preparation.

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**KEYWORDS**
Imaginary-time evolution, Mpemba effect, Ground state preparation, Population ratio, Finite-time crossing