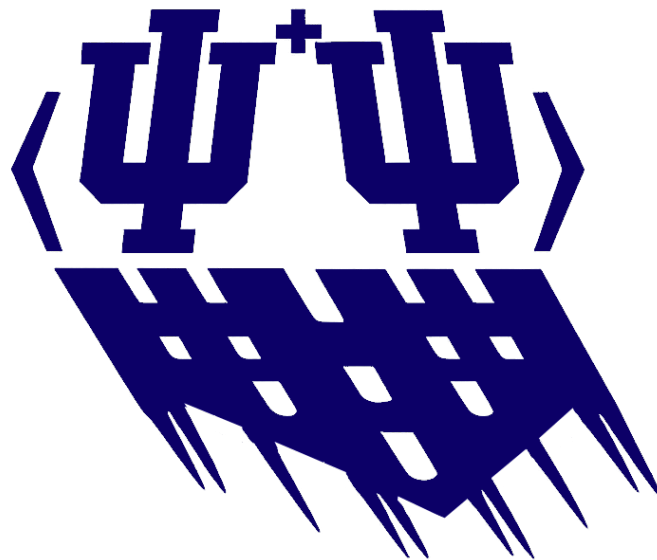


RPMBT23



**23rd International Conference on
Recent Progress in Many-Body Theories**

Milan, Italy, 14-18 September 2026

BOOK OF ABSTRACTS

PROGRAM -- 23rd Conference on Recent Progress in Many-Body Theories (RPMBT-23)

Sunday 13 September	Monday 14 September	Tuesday 15 September	Wednesday 16 September	Thursday 17 September	Friday 18 September
Participants arrival	08:30 Registration				
	09:30 Opening speech	09:00 Whaley	09:00 Gezerlis	09:00 Feenberg and Kümmel awards ceremony	09:00 Perali
	09:45 Zhang	09:30 Del Maestro	09:30 Porro		09:30 Sangalli
	10:15 Barthel	09:55 Barison	09:55 Herko		09:55 Arrigoni
	10:40 Rizzi	10:20 Green	10:20 Zurek	09:20 Soejima	10:20 Coffee break
	11:05 Coffee break	10:45 Coffee break	10:45 Coffee break	10:05 Kane	10:50 Quader
	11:35 Verstraete	11:15 Motta	11:15 Vitali	10:50 Coffee break	11:15 Pascucci
	12:05 Aligia	11:45 Negishi	11:45 Śliwiński	11:20 Glazman	11:45 Pisani
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	12:55 -- 14:40 Midday break (01:45)	12:35 -- 14:30 Midday break (01:55)	12:35 -- 14:30 Midday break (01:55)	12:50 -- 14:30 Midday break (01:40)	12:35 -- 14:30 Midday break (01:55)
18:00 -- 21:30 Welcome reception and registration	14:40 Lee	14:30 Rios	14:30 Martinazzo	14:30 Hatsuda	14:30 Colò
	15:10 Marino	15:00 Morales Silva	15:00 Nibbi	15:00 Sordi	15:00 Naito
	15:40 Brolli	15:30 Gaggioli	15:25 Taioli	15:25 Vranjes Markic	15:25 Sedrakian
	16:05 Hu	15:55 Wagner	15:50 -- 16:45 Free time (00:55)	15:50 Coffee break	15:50 RPMBT23 ends
	16:30 Coffee break	16:20 Coffee break		16:20 Huang	
	17:00 Romaniello	16:50 Levinsen		16:50 Dalmonte	
	17:30 Sa de Melo	17:20 Parish	16:45 (A) Visits to Cenacolo Vinciano (4 entrance slots)	17:20 Lerose	
	18:00 Urban	17:45 Han	17:45 (B)	17:45 -- 19:30 Free time (01:45)	
	18:25	Free time (0:25)	18:00 (C)		
		18:30 -- 22:00 Poster session reception	18:30 (D)		
				19:30 -- 23:00 Social dinner	

Invited presentations: 25 + 5 min
Oral contributions: 20 + 5 min

Color code:

Scientific program
Events on site
Events at other sites
Free time

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Forewords

It is our great pleasure to welcome you to Milan for the *23rd International Conference on Recent Progress in Many-Body Theories*. The RPMBT series began in Trieste in 1978, and this meeting marks its return to Italy for the first time in forty-eight years. We are honoured to host a conference with such a long and distinguished history, and we hope that Milan will provide a welcoming setting in which to continue its tradition of scientific exchange and collaboration.

Over nearly five decades, many-body theory has grown remarkably in both scope and reach. Advances in analytical methods and computational power have opened new directions across many areas of physics, while machine learning, artificial intelligence, and quantum technologies are becoming increasingly important parts of our scientific landscape. These developments bring new opportunities, but also new questions and challenges for our community.

With this in mind, RPMBT-23 was preceded by a satellite *School on Quantum Simulation*. The School offered advanced training designed to guide participants through the full process of simulating many-body Schrödinger dynamics on quantum hardware, from the theoretical formulation to practical implementation. Its lectures and hands-on sessions brought together 69 students and early-career researchers, some from the local community and many from abroad. Their enthusiasm, curiosity, and willingness to engage made the School a particularly rewarding experience. We are grateful to the lecturers and to everyone who contributed to its success, and we hope that it provided the participants with useful tools and new perspectives for their future work.

A cherished tradition of the RPMBT series is the presentation of the *Eugene Feenberg Memorial Medal* and the *Hermann Kümmel Early Achievement Award*. The distinction associated with the Feenberg Medal is reflected in the remarkable record of its recipients: Walter Kohn and Anthony Leggett received the medal before later being awarded Nobel Prizes. This year, the Feenberg Medal is jointly awarded to Matthew Fisher, Leonid Glazman, and Charles Kane, “for transformative contributions to the many-body theory of interacting electrons, establishing the modern understanding of one-dimensional conductors, quantum Hall transport, and topological quantum phenomena.” The Kümmel Early Achievement Award is presented to Tomohiro Soejima, “for the development of novel forms of the Density Matrix Renormalization Group and their use in discovering new quantum phases.” We warmly congratulate all four awardees.

We received more than one hundred proposals for contributed presentations, of consistently high quality. Selecting among them was a demanding task, and we sincerely thank all those who submitted their work. The resulting programme comprises 57 oral presentations and 52 posters, covering a broad and vibrant range of topics. We hope that it will encourage lively discussions, unexpected connections, and lasting collaborations—and that every participant will make the most of the scientific and personal opportunities offered by RPMBT-23.

Finally, we gratefully acknowledge our many sponsors and supporting institutions. Without their generous assistance, neither the School nor the Conference would have been possible.

Thank you for joining us in Milan. We wish you an enjoyable, stimulating, and rewarding RPMBT-23.

With best regards,

The Local Organizing Committee

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ORAL CONTRIBUTIONS

RPMBT23

Recent progress in computational studies of the Hubbard model

Shiwei Zhang¹

¹*Center for Computational Quantum Physics (CCQ)
Flatiron Institute*

The Hubbard model is an iconic model in quantum many-body physics. Its properties have proved highly challenging to determine, as they are often the outcome of a delicate balancing act between multiple competing or co-existing tendencies. Robust predictions are difficult to obtain. Recently, significant progress has been made via advances in computational methods, and the combined use of complementary methods through collaborative efforts. I will share some of the lessons learned and insights gained, and what these computations have revealed about the properties of the Hubbard model. I will highlight how, together with exciting experimental progress in neutral atom quantum simulations, this presents us with unique opportunities for a new level of synergy to address a variety of long-standing questions in quantum matter. I will also discuss how the methodological advances generalize to realistic correlated materials in condensed matter, transition metal quantum chemistry, and beyond.

Tensor network simulation of quantum scattering in $D > 1$ spatial dimensions

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Tensor network states are an indispensable tool for the simulation of strongly correlated quantum many-body systems. In recent years, tree tensor network states (TTNS) have been successfully used for two-dimensional systems and to benchmark quantum simulation approaches for condensed matter, nuclear, and particle physics. In comparison to the more traditional approach based on matrix product states (MPS), the graph distance of physical degrees of freedom can be drastically reduced in TTNS. In extension of corresponding results for MPS [1, 2], I will show how to bound TTNS approximation errors using Rényi entanglement entropies of the target state. Conversely, one obtains bounds on tensor-network bond dimensions needed to achieve a specific approximation accuracy [3]. Surprisingly, it turns out that, for large systems in $D > 1$ spatial dimensions, MPS simulations of low-energy states are more efficient than TTNS simulations. We will discuss the scaling of computational costs for different boundary conditions under the assumption that the system obeys an entanglement (log-)area law, implying that bond dimensions scale exponentially in the surface area of the associated subsystems [4]. The ultimate goal of this project is the investigation of quantum scattering events. I will discuss corresponding results for lattice gauge theories and comment on the use of helical boundary conditions as well as a novel gauge-fixing scheme for the tensor-network excitation ansatz.

- [1] F. Verstraete and J. I. Cirac, *Matrix product states represent ground states faithfully*, [Phys. Rev. B **73**, 094423 \(2006\)](#).
- [2] N. Schuch, M. M. Wolf, F. Verstraete, and J. I. Cirac, *Entropy scaling and simulability by matrix product states*, [Phys. Rev. Lett. **100**, 030504 \(2008\)](#).
- [3] T. Barthel, *Tree tensor network states represent low-energy states faithfully*, [arXiv:2512.20215 \(2025\)](#).
- [4] T. Barthel, *Cost scaling of MPS and TTNS simulations for 2D and 3D systems with area-law entanglement*, [arXiv:2601.08132 \(2026\)](#).

Ground state search and real-time evolution with variational finite Projected Entangled-Pair States

M. Rizzi^{1,2}, et al.

¹ *Institute of Theoretical Physics, University of Cologne, Germany*

² *Institute for Quantum Control (PGI-8), Forschungszentrum Jülich GmbH, Germany*

Projected entangled pair states (PEPS) on finite two-dimensional lattices are a natural ansatz for representing ground states of local many-body Hamiltonians, as they inherently satisfy the boundary law of entanglement entropy. Here, we propose the optimization of PEPS via an improved formulation of the time-dependent variational principle (TDVP), namely the minimum-step stochastic-reconfiguration (minSR) scheme recently introduced for neural quantum states [1]. We further discuss possible numerical issues that might arise in such a sampling-based approach, including an entanglement phase transition for random PEPS. To demonstrate the power of the framework, we apply it to frustrated models giving rise to notoriously challenging chiral spin liquids. We also exhibit our approach's capability to naturally handle long-range interactions without truncation by exploring the phase diagram of Rydberg atom arrays and dipolar systems. Additionally, we demonstrate the feasibility of reduced basis surrogate methods, which allow for faithful reconstruction of the phase diagram out of a few PEPS snapshots. We also offer some considerations about real-time evolution within the same framework, benchmarking it for the non-equilibrium dynamics of the Ising model and comparing it to some recent works of ours via Tree Tensor Networks [2]. Parallelized easy-to-use code is made available [3].

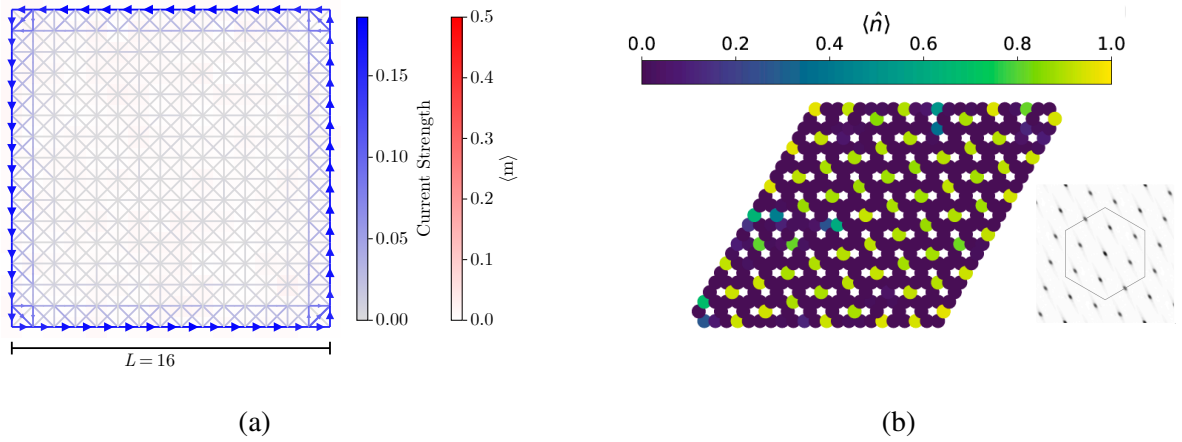


Figure 1: (a): Vanishing local magnetization ($m^2 \lesssim 10^{-4}$) and chiral spin current localized at the edge for a $J_1 - J_2$ model enriched by cyclic permutation terms on the plaquettes (data are from 16×16 square lattice). (b): Local Rydberg excitation density on a $(12 \times 12 \times 3)$ Kagome lattice in the so-called staggered phase, and the corresponding structure factor.

- [1] D. Alcalde Puente, E.L. Weerda, K. Schröder, M. Rizzi, Phys. Rev. B **111**, 195120 (2025);
- [2] W. Krinitsin, N. Tausendpfund, M. Rizzi, M. Heyl, M. Schmitt Phys. Rev. Lett. **134**, 240402 (2025).
- [3] D. Alcalde Puente, E.L. Weerda, K. Schröder, M. Rizzi, QuantumNaturalfPEPS.jl (2025),
<https://github.com/NeTeNeSyQuMa/QuantumNaturalfPEPS.jl>

Entanglement and DMRG in the generalized Landau paradigm

F. Verstraete¹

¹*Cambridge, UK*

Landau's paradigm teaches us to understand phases of matter in terms of symmetry breaking and local order parameters. Quantum mechanics, however, allows for phases whose essential structure is encoded in patterns of entanglement. I will discuss how DMRG and tensor networks provide a natural computational framework for this generalized Landau paradigm. In one dimension, matrix product states make the relation between entanglement, symmetry and efficient simulation particularly transparent, allowing symmetry-breaking phases, symmetry-protected phases and critical points to be treated within a common language. More generally, the success of DMRG can itself be understood as a consequence of the restricted entanglement structure of physically relevant quantum states. I will discuss how these ideas turn entanglement from a diagnostic into an organizing principle for quantum matter, and what they suggest for extending DMRG beyond its traditional setting.

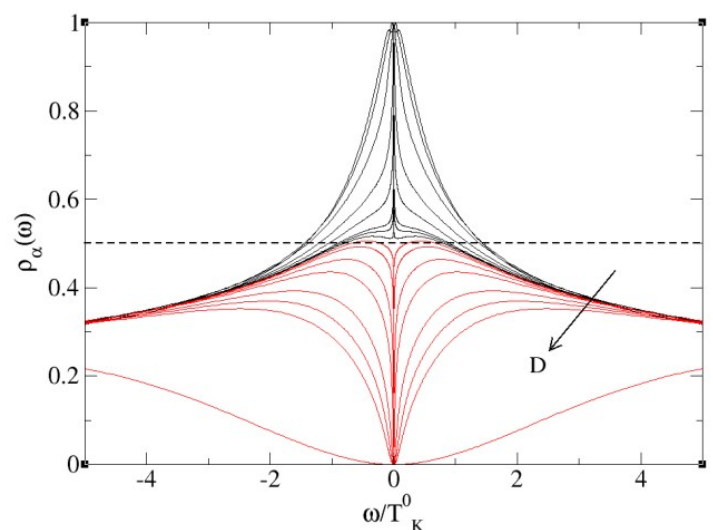
Topological transition to a “non-Landau” Fermi liquid in a two-channel spin-1 anisotropic Kondo model and its experimental relevance

A. A. Aligia¹

¹*Instituto de Nanociencia y Nanotecnología, CNEA-CONICET, Bariloche, Argentina*

The Kondo problem is one of the paradigms of strongly correlated systems. A recent realization consist of magnetic molecules on noble metal surfaces. We present a numerical-renormalization group study of a spin-1 two-channel Kondo model with anisotropy $D(S_z)^2$. We find a topological quantum phase transition in which the Kondo peak in the spectral density is suddenly turned to a dip with increasing D (see figure below) [1]. For large D the system is in a “non-Landau” Fermi liquid phase (i.e. with no adiabatic connection with a non-interacting system). Extending the theory to non-equivalent orbitals and non-zero magnetic field we can explain several relevant experiments in the system of Fe phthalocyanine on Au(111) [2]. The model is also relevant for similar systems, like Mn phthalocyanine on Au(111) and nickelocene on Cu(100) [3]. In the latter case, two types of behavior are observed, depending on the details of the geometry of the absorption of the molecule, a continuous transition to the non-Landau phase (which we can explain in terms of the effects of intermediate valence in the corresponding Anderson impurity model) and an abrupt transition, which can be understood from the effects of relaxation of the position of the molecule [4]. In addition, for Fe atoms on MoS₂/Au(111) three different behaviors depending on the spectral density of the substrate: one dominated by a single ion anisotropy, one by the Kondo effect, and an intermediate one [5]. We show that the different behaviors can be explained in a unified fashion with our theory [6]. Other experiments and relation with other impurity models are discussed [7].

Figure 1: Spectral density as a function of energy for several values of the anisotropy.



- [1] G. G. Blesio, L. O. Manuel, P. Roura-Bas, and A. A. Aligia, Phys. Rev. B 98, 195435 (2018), Phys. Rev. B 100, 075434 (2019).
- [2] R. Žitko, G. G. Blesio, L. O. Manuel, and A. A. Aligia, Nature Commun. 12, 6027 (2021).
- [3] M. Ormaza *et al.*, Nature Commun. 8, 1974 (2017), M. Mohr *et al.*, Phys. Rev. B 101, 075414 (2020).
- [4] G. G. Blesio, R. Žitko, L. O. Manuel, and A. A. Aligia, SciPost Phys. 14, 042 (2023).
- [5] Trishin *et al.*, Phys. Rev. Lett. 127, 236801 (2021).
- [6] G. G. Blesio and A. A. Aligia, Phys. Rev. B 108, 045113 (2023).
- [7] G. Blesio, L. O. Manuel, and A. A. Aligia, Mater. Quantum Technol. 4, 042001 (2024).

Recent Progress on Ultrafast Laser Physics with Strongly Correlated Systems

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Castelldefels (Barcelona) 08860, Spain*

Ultrafast laser physics (ULP) has undergone spectacular developments and achievements in recent years, crowned with the Nobel Prize for ultrastrong table-top lasers [1, 2], and attosecond physics [3, 4, 5]. Only recently, however, have the methods and techniques of ULP begun to be applied to the analysis of properties of strongly correlated quantum systems. In this report, we review the efforts of the Quantum Optics theory Group in this field over the past few years.

The report covers three sub-areas: i) Applications of High Harmonic Generation (HHG) by strong, ultrashort laser pulses to search for signatures of strong correlations and phase transitions in correlated materials, like high T_c superconductors [6] and Charge Density Waves (CDW) [7, 8]; ii) Applications of HHG to topological and strongly correlated 1D systems [9, 10, 11, 12]; iii) Laser induced phase transitions and state control in strongly correlated materials [13, 14, 15].

All of these sub-areas call for new progress in many-body theory, creatively mixing and combining whatever is accessible in condensed matter and atomic physics, quantum optics, and quantum information, from mean-field and pairing theories, to exact diagonalization, quantum Monte Carlo, and tensor network methods.

- [1] G. Mourou, Extreme light physics and application, *Rev. Mod. Phys.* **91**, 030501 (2019).
- [2] D. Strickland, Generating high-intensity ultrashort optical pulses, *Rev. Mod. Phys.* **91**, 030502 (2019).
- [3] A. L'Huillier, The route to attosecond pulses, *Rev. Mod. Phys.* **96**, 030503 (2024).
- [4] F. Krausz, Sub-atomic motions, *Rev. Mod. Phys.* **96**, 030502 (2024).
- [5] P. Agostini, Genesis and applications of attosecond pulse trains, *Rev. Mod. Phys.* **96**, 030501 (2024).
- [6] J. Alcalà *et al.*, High-harmonic spectroscopy of quantum phase transitions in a high- T_c superconductor, *Proc. Nat. Acad. Sci.* **119**, e2207766119 (2022).
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- [8] L. Zhang *et al.*, Revealing the anisotropic charge-density-wave order of TiSe_2 through high harmonic generation, *Phys. Rev. B* **112**, 085147 (2025).
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Evidence for multimodal superfluidity of neutrons

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I present theoretical and experimental evidence for a new phase of matter in neutron-rich systems called multimodal superfluidity. Using ab initio lattice calculations, our team has shown that the condensate consists of coexisting S-wave pairs, P-wave pairs, and quartets composed of bound states of two S-wave pairs. We identify multimodal superfluidity as a general feature of two-component fermionic systems with attractive S-wave and P-wave interactions, provided the system is stable against collapse into a dense droplet. Beyond neutrons at sub-saturation densities, we demonstrate that this phase appears in generalized attractive Hubbard models across 1D, 2D, and 3D. We elucidate the mechanism for this coexistence using self-consistent few-body Cooper models and make comparisons and contrasts with standard Bardeen-Cooper-Schrieffer theory. Finally, we analyze experimental data to show that P-wave pair gaps and quartet gaps are present in atomic nuclei, and we discuss the consequences of this new phase for neutron star crusts and cooling.

Green's functions investigation of nuclear matter from low to high densities

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Infinite nuclear matter is subject to intense investigations, thanks to its key role in describing neutron stars, its connections with the physics of finite nuclei (e.g., neutron skins and collective electromagnetic excitations), and its similarity (at very low densities) with the unitary Fermi gas [1, 2]. As nuclear matter is not directly observable, nuclear ab initio theory, which combines sophisticated many-body techniques with realistic models of the nuclear interaction rooted in QCD, is important to achieve accurate, unbiased predictions.

In this contribution, we exploit our recently developed Self-consistent Green's functions (SCGF) approach [3, 4] to provide a comprehensive picture of nuclear matter. We first summarize the key features of our method [4], which is based on Gorkov superfluid theory, and show how its accuracy can be enhanced by incorporating coupled-cluster amplitudes in the self-energy. We discuss predictions for the equation of state (EOS) across densities and isospin asymmetries obtained with modern chiral interactions, benchmarking our method [3, 5] and providing estimates of the empirical parameters of the EOS around saturation.

Then, we exploit the unique capabilities of Gorkov SCGF to investigate the low-density region, where neutron matter enters the superfluid regime [6]. We predict the EOS, momentum distributions, spectral functions, and, crucially, pairing gaps consistently within the same theoretical framework, and discuss the relevance of these results for our understanding of pairing properties in both nuclear matter and finite nuclei.

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Time-ordered diagrammatic Monte Carlo and next generation emulators

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Within *ab initio* nuclear physics, incorporating high-order diagrams in the many-body expansion is becoming increasingly important, both to match the precision of next-generation interactions and to achieve a unified description of nuclear structure and reactions. Methods capable of accurately resolving these high-order correlations in nuclei can also be naturally extended to atomic and molecular systems.

This presentation introduces a novel time-ordered diagrammatic Monte Carlo (TO-DiagMC) algorithm for finite systems at zero temperature. TO-DiagMC builds on our benchmark studies of the Richardson pairing model, which showed that diagrammatic Monte Carlo can outperform standard many-body truncation schemes in finite systems [1]. We apply TO-DiagMC to ^{16}O using a modern chiral interaction in a controlled model space [2]. By sampling time-ordered diagrams directly, TO-DiagMC avoids costly frequency integrations, reduces the dimensionality of the sampling space, and mitigates the sign problem. While existing approaches are typically limited to third-order diagrams, TO-DiagMC enables calculations up to fifth order.

Combining TO-DiagMC with fast surrogate models enables applications requiring repeated evaluations, such as uncertainty quantification and parameter optimization. I will introduce a novel emulator based on parametric matrix models (PMMs) [3]. Unlike standard approaches, PMMs are designed to learn the underlying equations of the system rather than simply interpolate training data. I will present a test application to the Richardson model, demonstrating high accuracy in reproducing the exact Green's function together with robust extrapolation capabilities. This framework opens the door to new methods for interaction optimization and uncertainty quantification, with broad impact across nuclear physics.

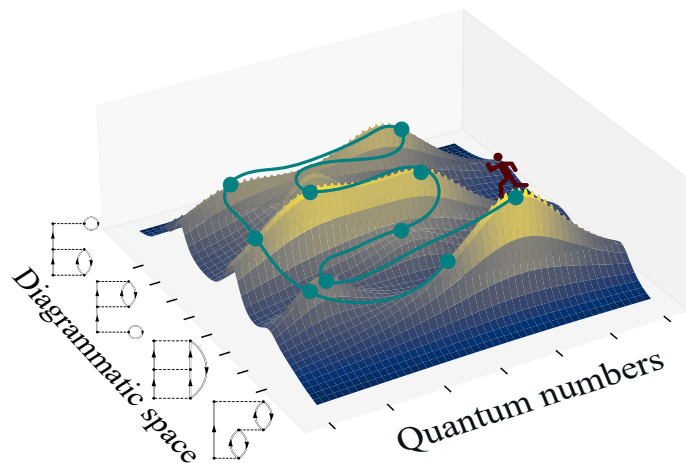


Figure 1: Visual representation of a walker sampling the diagrammatic space.

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Full configuration-interaction quantum Monte Carlo for *ab initio* nuclear structure calculations

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Quantifying high-order many-body correlations is essential for reliable *ab initio* predictions of finite nuclei and nuclear matter. We present applications of full configuration-interaction quantum Monte Carlo (FCIQMC) to both systems using chiral nuclear interactions [1, 2, 3]. By propagating signed walkers in imaginary time, FCIQMC samples the wave function in the full determinant space of a chosen single-particle basis, without an excitation-rank truncation or a fixed-node constraint. The initiator approximation and adaptive-shift correction enable large-space calculations, with residual finite-walker bias assessed through systematic convergence studies and infinite-walker extrapolations.

For finite nuclei, we compute ground-state energies and charge radii of ^4He , ^8Be , ^{12}C and ^{16}O with the chiral two-nucleon interaction $\text{N}^2\text{LO}_{\text{opt}}$, achieving estimated sub-percent many-body uncertainties. Replica sampling of reduced density matrices provides pure estimators for radii. Benchmarks reproduce deterministic full configuration interaction results in small spaces, while larger calculations access spaces beyond conventional no-core shell model. Comparisons with coupled-cluster, in-medium similarity renormalization group and many-body perturbation theory reveal the importance of high-order many-body correlations, particularly in clustering nucleus ^8Be . We also demonstrate the extension of FCIQMC to nuclear spectroscopy through the low-lying excited states calculations of ^6Li .

For nuclear matter, we calculate the equations of state of pure neutron matter and symmetric nuclear matter using chiral two- and three-nucleon interactions. Comparisons in identical model spaces show substantially stronger effects of high-order correlations in symmetric matter, especially for harder interactions and increasing density, which impacts our understanding for nuclear saturation. Together, these studies establish FCIQMC as an accurate benchmark for other nuclear many-body methods and help disentangle many-body errors from deficiencies of nuclear interactions.

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A multichannel Dyson-equation approach to theoretical spectroscopy

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In this talk, we present the multichannel Dyson equation (MCDE) as an alternative to the standard single-channel Dyson equation. [1, 2, 3, 4, 5] While the latter involves a single many-body Green's function, the MCDE employs a multichannel Green's function in which two or more many-body Green's functions are coupled to describe a particular spectroscopy. For example, by coupling the one-body and three-body Green's functions, one can calculate direct and inverse photoemission spectra. This coupling naturally places quasiparticles and satellites on an equal footing and therefore allows accurate results to be obtained from relatively simple approximations to the multichannel self-energy. We illustrate our approach by applying the MCDE to various spectroscopies, as well as to models [2, 4, 6, 7] and real systems.[8, 9]

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Topological quantum phase transitions and collective excitations in ultracold Fermi gases: Creating and detecting Weyl Bosons

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Inspired by investigations of Dirac, Majorana and Weyl fermions in the context of particle, condensed matter and atomic physics, we propose theoretical and experimental platforms to create and detect massless helical boson modes that we call Weyl bosons, the bosonic cousins of Weyl fermions [1, 2, 3]. We show that these exotic excitations arise naturally in one-dimensional interacting Fermi gases, when spin-orbit coupling and Rabi fields are present, through the mixing of charge and spin degrees of freedom [1, 2, 3]. We obtain the phase diagram of chemical potential versus Rabi fields for given spin-orbit coupling and interactions, showing regions where zero, one or two types of Weyl bosons exist. We find that, when two types of Weyl bosons emerge, they must propagate with different velocities. Furthermore, we show that the disappearance of any Weyl boson species is described by a topological quantum phase transition of the Lifshitz type, where the velocity of the disappearing Weyl boson vanishes, and the velocity of the surviving Weyl boson develops a cusp at the transition boundary. Lastly, to detect the existence of Weyl bosons, we propose measurements of the dynamic structure factor tensor (charge-charge, charge-spin and spin-spin), where the energy dispersions, spectral weights and helicities of the emergent Weyl bosons may be experimentally extracted in ultracold Fermi systems such as ^6Li , ^{40}K , ^{173}Yb and ^{87}Sr .

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Higher-order corrections to pairing in ultracold Fermi gases: testing many-body methods for neutron matter

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The technique of softened interactions, which can be treated in Hartree-Fock-Bogoliubov (HFB) theory with perturbative corrections, has allowed for important progress in “ab-initio” nuclear structure calculations and it has also been used to compute the equation of state of superfluid neutron matter [1], which is relevant for the modeling of neutron stars. However, the density dependence of the pairing gap in neutron matter is still very uncertain and it is difficult to be pinned down from neutron-star observations. Since neutron matter has some analogies with ultracold Fermi gases with negative scattering length, these experimentally well-studied systems provide a valuable benchmark for the many-body approaches used in the modeling of neutron matter. I will present a recent diagrammatic calculation of the pairing gap and the Hartree shift in ultracold Fermi gases from the BCS regime to the unitary limit [2], using a low-momentum interaction with a cutoff that is scaled with the Fermi momentum. Including up to third-order corrections on top of HFB, not only the Gor’kov-Melik-Barkhudarov result for the weak-coupling limit is recovered, but also leading corrections to it, e.g., from the effective mass and the quasiparticle interaction. A reasonable agreement with experiment is obtained even near unitarity. This makes us confident that it will be possible to obtain reliable predictions of the pairing gap in neutron matter with this approach.

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Non-orthogonal Quantum Eigensolvers for Strongly Correlated Systems

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Non-orthogonal quantum eigensolvers provide an attractive path to accurate calculation of ground and excited electronic states for strongly correlated molecular systems. These quantum algorithms realize efficient computation of Hamiltonian and overlap matrix elements between non-orthogonal ansatz states that incorporate both strong and weak correlation. Ansatz states expressed by either generalized UCCSD circuits (NOQE), which can be prepared in polynomial depth, or by orbital-rotated matrix product circuits (TNQE), which can be prepared in linear depth, have been developed. The quantum computations are followed by classical post-processing in which the generalized eigenvalue problem constructed from these matrix elements is solved to yield both electronic states and energies. These quantum eigensolvers possess several advantages: they have exponentially less cost than the best classical multi-reference subspace methods, have been established as computationally hard to dequantize for strongly correlated systems, and they are both variational and size consistent. Furthermore, the output states can be input to quantum phase estimation algorithms to obtain even more accurate energies with guaranteed accuracy. I shall summarize this non-orthogonal approach to quantum algorithms for molecular electronic energies and states, outlining the costs of the various components, and discuss the feasibility of applying this approach to challenging large-scale systems relevant to biocatalysis.

A quantum-chemical accurate helium-benzene interaction potential

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Light atoms such as helium adsorbed on atomically thin substrates provide a rich platform for exploring exotic quantum many-body phenomena, owing to the highly tunable and atomic-scale nature of their interactions. However, the emergent physics depends sensitively on the detailed form of the adsorbate–adsorbent potential. To advance the development of accurate adsorption interaction models for two-dimensional systems, we present a study of helium interacting with a single benzene molecule. By combining high-level coupled-cluster calculations [CCSD(T) at the complete-basis-set limit validated by CCSDT(Q)] with multi-fidelity Gaussian process regression, we construct a new potential energy surface with sub-kelvin accuracy. Quantum Monte Carlo simulations of helium clusters surrounding benzene at low temperature reveal qualitative differences in solvation structure and configuration compared with existing model potentials. We conclude by discussing the transferability of this approach to larger polycyclic aromatic hydrocarbons.

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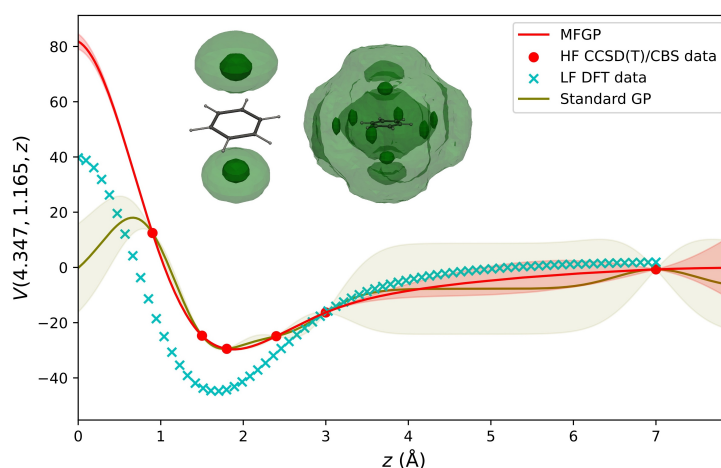


Figure 1: A multifidelity Gaussian Process (MFGP) fit to high fidelity CCSD(T)/CBS data leveraging low fidelity density functional theory results for the interaction potential between helium and benzene along a low-symmetry cut in the z -direction.

Sample-based quantum algorithms in quantum chemistry: to ground states and beyond

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Simulation of quantum physical systems is among the most compelling applications of quantum computing devices. In particular, the electronic structure problem in chemistry presents challenging use cases already at the scale of roughly one hundred qubits. Several strategies have been developed in recent years to simulate these systems on current quantum devices [1]. However, these approaches have so far been limited to small systems, due to the long timescales required for energy estimation and the depth of chemically motivated quantum circuits.

In this talk, I will present a class of hybrid quantum–classical algorithms that bypasses these limitations and have enabled the largest quantum chemical simulations to date. First, I will introduce the concept of subspace diagonalization and its quantum counterpart (Sample-based Quantum Diagonalization, or SQD) illustrating how the approach has been combined with a self-consistent error mitigation technique and high-performance computing (HPC) to scale simulations beyond 50 qubits [2]. I will then address the problem of preparing chemically motivated quantum circuits for sample-based algorithms, introducing Sample-based Krylov Diagonalization (SKQD) and Sample-based qDRIFT (SqDRIFT) [3, 4]. I will show how SqDRIFT enables practical quantum chemical SQD calculations on current devices, presenting studies of the ground states of hydrocarbons such as naphthalene and coronene, with active spaces of up to 48 qubits. Finally, I will present the case of the half-Möbius molecule, recently published in *Science*, in which a carbon ring was engineered to exhibit a nontrivial—and previously unobserved—electronic structure topology. SqDRIFT was used to validate the experimental measurements, with active spaces of up to 46 electrons in 50 orbitals, corresponding to a total of 100 qubits [5, 6]. This work marks a transition from proof-of-principle demonstrations toward practical quantum-enhanced electronic structure calculations.

However, the study of ground states alone is not exhaustive, as many important chemical phenomena involve processes such as light absorption and emission, as well as transitions between electronic states. For this reason, I will dedicate the final part of my talk to exploring opportunities for sample-based algorithms beyond ground-state studies. In particular, I will present a workflow for tailoring quantum-selected subspaces to excited states based on quantum subspace expansion [7], as well as a strategy for preparing subspaces for dynamics by implementing short-time evolution operators on a quantum device [8].

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Many-body theory of positron interactions in polyatomic molecules

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Positrons have important use in materials science, medical imaging and astrophysics, in fundamental AMO physics (including via positronium and antihydrogen), and for novel molecular spectroscopy. Proper interpretation of experiments and materials science techniques, and development of antimatter-based technologies (traps, beams, medical imaging) rely on fundamental understanding of positron interactions with atoms and molecules. These interactions are, however, characterised by strong correlations. They have an overwhelming effect, and make the description of positron-molecule interactions a challenging many-body problem. I will present the many-body theory of positron-molecule interactions developed by my group at QUB [1]. It has been used to e.g., provide the first accurate *ab initio* description of positron binding to molecules [1], extended to positron scattering on molecules [2], annihilation γ spectra [3], to predict new class of positronically-bonded molecules [4], and understand trends in binding energies across families of molecules [5]. I will also discuss recent computational developments, including successful summation of the electron-positron ladder series via diagrammatic Monte Carlo. See Figure 1.

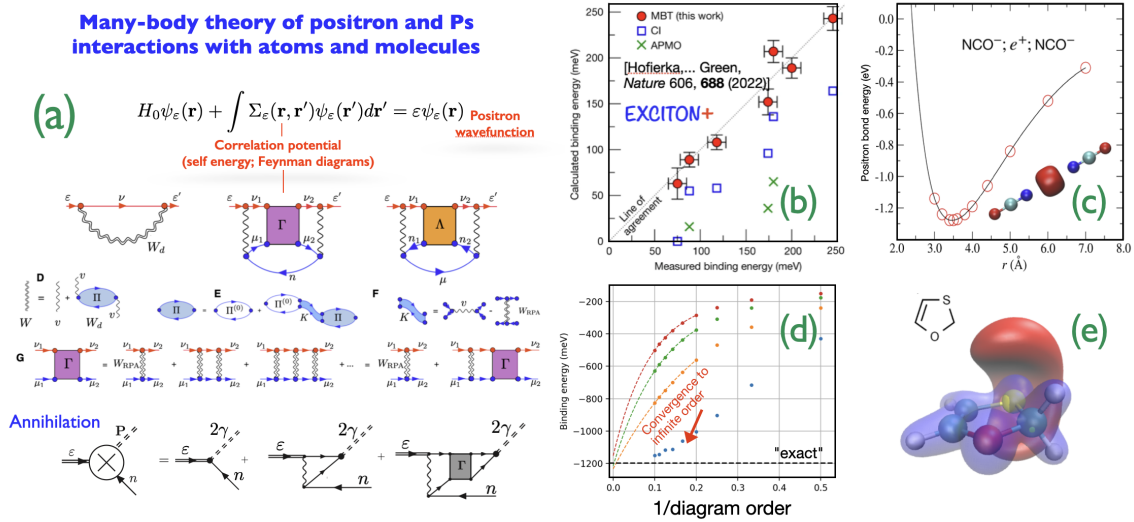


Figure 1: Positron-molecule many-body theory [1]; (a) Dyson equation with positron-molecule self energy comprised of $GW@BSE$ term and infinite electron-positron and electron-hole ladder series [1]. (b)–(e) examples of results: (b) the first accurate calculations of positron-molecule binding energies [1]; (c) prediction of new class of positronically-bonded molecule [3]; (d) diagrammatic Monte Carlo evaluation of the virtual-positronium ladder series for LiH [6]; (e) positron bound state (red lobe) from new calculations on heterocyclic molecules [3].

* This work was funded by the European Research Council, grant numbers 804383 and 101170577.

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Crossing the 12,000-atom barrier with heterogeneous quantum-classical supercomputing: quantum chemistry of protein-ligand complexes

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Ab initio wavefunction methods provide accurate molecular simulations but their computational scaling restricts applications to small systems. We develop a workflow combining quantum embedding to decompose a molecule into fragments with a heterogeneous quantum-classical (HQC) method to simulate fragments. We sample fragment electronic configurations on two 156-qubit quantum processors (`ibm_cleveland`, `ibm_kobe`), using up to 94 qubits, running 9,200 circuits for over 100 hours, collecting $1.3 \cdot 10^9$ measurement outcomes — the most resource-intensive HQC computation for quantum chemistry to date. We compute fragment wavefunctions via optimized subspace diagonalization on two supercomputers (Fugaku, Miyabi-G), achieving 72.5% parallel efficiency with scalable distributed linear algebra kernels. We simulate two protein-ligand complexes spanning dispersion- and electrostatics-dominated regimes (11,608 and 12,635 atoms), demonstrate $> 40\times$ increase in system size and up to $210\times$ improvement in accuracy over the previous state-of-the-art, with HQC matching coupled-cluster (CCSD) accuracy in fragment energies, and establish a scalable pathway for systematically improvable biomolecular simulations.

Redesigning Trotter Decomposition via Local Symmetry for 2D material

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Quantum dynamics simulations of many-body correlated systems, such as two-dimensional (2D) spin lattices, remain a central and challenging topic in quantum physics. Trotter decomposition is commonly used to approximate the time-evolution operator in digital quantum simulation, and its performance depends critically on how the Hamiltonian is partitioned into tractable blocks. Standard decomposition schemes typically rely on the direct commutativity of Hamiltonian terms in a chosen operator representation, which can lead to large residual errors and deep quantum circuits for complex and practically relevant many-body systems.

We address this fundamental bottleneck by introducing a new decomposition principle that goes beyond commutativity, grouping Hamiltonian terms into local three-site clusters according to the underlying $SU(2)$ symmetry of the local dynamics. We show that the resulting three-site generators fall into at most four $SU(2)$ symmetry classes, each admitting an effective two-qubit $SU(4)$ representation with exact and efficient implementations [1]. By reducing the number of clusters, this decomposition strategy substantially suppresses approximation errors and implementation costs while preserving physical structures that are violated by commutativity-based decompositions. We demonstrate the proposed method on several spin-lattice models, where the reduced cluster structure can even realize a second-order product formula without doubling the circuit depth. In particular, the method can be applied much more efficiently to numerical simulations of two-dimensional frustrated spin systems, such as the Kagome Heisenberg model, reducing both state infidelity and average spin-chirality bias compared with conventional decomposition schemes. These results establish local symmetry as a flexible and practical design principle for product-formula-based quantum simulation, opening a route toward more accurate and hardware-efficient simulations of a broader class of many-body systems.

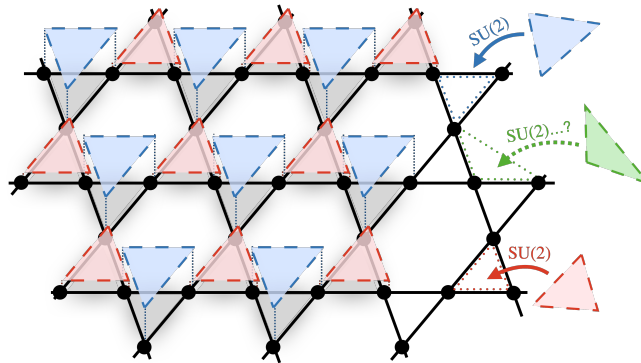


Figure 1: Scheme of an $SU(2)$ -respecting triangular decomposition on a Kagome lattice.

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Complexity-driven ground state estimation of quantum many-body systems

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Understanding which quantum states can be efficiently represented and simulated classically is essential for advancing both fundamental physics and the development of quantum technologies. In this work, we want to leverage knowledge about the complexity of quantum many-body systems to estimate ground states using an efficient balance between quantum and classical resources [1].

We characterize the quantum complexity of ground states through entanglement (e.g., n -tangles), non-stabilizerness (e.g., Stabilizer Rényi entropies, non-local magic), and non-Gaussianity (e.g., fermionic anti-flatness) to illuminate how quantum resources behave throughout the system.

All these measures are not only interesting to improve quantum-classical workflows but can be connected to the phase diagram of the Agassi model that we use as a benchmark. The three different phases (spherical, deformed, and superfluid) make the Agassi model interesting for various areas of physics such as Nuclear and Subnuclear Physics, Condensed Matter Physics and Strongly Correlated Electronic Systems.

Finally, using the techniques developed in [2] we show that (superpositions of) stabilizer ground states describe the ground state of the Agassi model with high fidelity. This allows more efficient simulations of quantum systems by exploiting knowledge about their quantum complexity, and constitutes a step towards exploring more complex systems.

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Quantum Computing and Neural Quantum States in Nuclear Many-Body Theory

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Ab initio nuclear theory has experienced remarkable progress in the last decade, enabling microscopic predictions of nuclear structure and reaction dynamics across the isotopic chart [1]. However, solving the many-nucleon Schrödinger equation remains a fundamental challenge due to both the complexity of the nuclear interaction and the exponential growth of the Hilbert space with particle number. To overcome this wall, novel quantum-centric computational paradigms are being developed with the potential to transform the nuclear many-body landscape.

In this talk, I will present recent advances in integrating quantum computing algorithms and Neural Quantum States (NQS) into the ab initio framework [2]. Variational NQS representations leverage deep neural network architectures to efficiently encode strongly correlated wave functions with favorable scaling [3], providing a promising avenue towards medium-mass isotopes [4].

Concurrently, quantum algorithms offer direct pathways for simulating nuclear structure and dynamics on noisy intermediate-scale quantum and early fault-tolerant devices [5]. I will highlight recent algorithmic advances in this context, ranging from variational quantum eigensolvers [6, 7] to real-time evolution protocols [8]. Finally, I will discuss how combining these quantum-oriented approaches with established many-body techniques, such as Self-Consistent Green's Function (SCGF) theory, unlocks powerful hybrid strategies for evaluating spectral functions, response functions, and open-shell systems [9].

- [1] H. Hergert, *Front. Phys.* 8:379 (2022).
- [2] J. Keeble, A. Rios, *Phys. Lett. B* 809, 135743 (2020).
- [3] A. Lovato, G. Carleo, B. Fore, M. Hjorth-Jensen, J. Kim, A. Rios, N. Rocco, *arxiv:2602.13826*.
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- [5] E. F. Dumitrescu et al., *Phys. Rev. Lett.* 120, 21 (2018).
- [6] A. Pérez-Obiol et al., *Sci. Rep.* 13 12291 (2023).
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Insights into the physics of 2D correlated electrons from Neural Quantum States

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In this talk, I will present an overview of the study of the modulated electron gas in 2 dimensions using Neural Quantum States. The work is based on the Multi-Planewave Message-Passing Neural Quantum State (MP²NQS), an accurate wavefunction ansatz designed for real-space quantum Monte Carlo simulations. MP²NQS integrates a traditional Slater-Jastrow-Backflow wavefunction with a powerful message-passing graph neural network architecture for both Jastrow and Backflow functions, alongside aggressive orbital optimization in a plane-wave basis. This powerful approach achieves ground-state accuracy for the electron gas that rivals, and usually surpasses, state-of-the-art diffusion quantum Monte Carlo (DMC) calculations. By performing orbital optimization in the presence of an accurate description of electron correlation, the approach can successfully locate phase transitions with little human input.

Using this ansatz, we have re-investigated the homogeneous 2D electron gas, achieving consistent improvements over prior DMC results. Notably, we identify the fluid-to-Wigner crystal phase transition at a critical density defined by $r_s \sim 37 \pm 1$, lower than previously reported. More importantly, our results uncover pronounced short-range nematic spin correlations across a wide density range in the fluid phase. I will also discuss recent applications to Moiré continuum Hamiltonians modeling transition metal dichalcogenide (TMD) bilayers. These studies examine the effects of Moiré potential depth, gate screening, hole doping and external magnetic fields on ground-state properties, offering new insights into correlated phases in these systems. Finally, I will present a study of the influence of impurities on the properties of the electron gas, illustrating a strong interplay between disorder and electron localization.

Electron quasicrystal in semiconductor quantum wells: an AI-powered discovery

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The homogeneous electron gas is a cornerstone of quantum condensed matter physics, providing the foundation for developing density functional theory and understanding electronic phases in semiconductors. However, theoretical understanding of strongly-correlated electrons in realistic semiconductor systems remains limited. In this work, we develop a neural network based variational approach to study quantum wells in three dimensional geometry for a variety of electron densities and well thicknesses. Starting from first principles, our unbiased AI-powered method reveals metallic and crystalline phases with both monolayer and bilayer charge distributions. In the emergent bilayer, we discover a new quantum phase of matter: the electron quasicrystal.

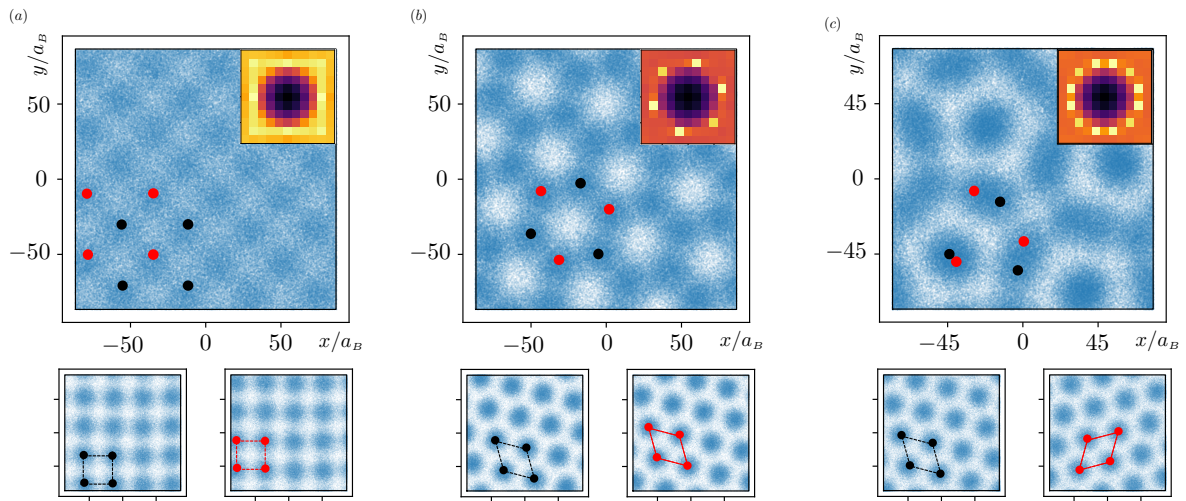


Figure 1: **Bilayer (quasi-)crystal:** Square (a), honeycomb (b) and quasicrystal (c) bilayer. The commensurate stackings (a) and (b) can be understood from minimizing the intra-layer and inter-layer Coulomb repulsion. The electronic quasicrystal, on the other hand, does not have a classical analogue and is stabilized purely by quantum fluctuations, via the zero-point energy contribution of its extensive low-lying excitations. The colored insets show the Bragg peaks of the in-plane structure factor $S(k)$. This highlights the twelve-fold rotational symmetry of the quantum quasicrystal. Bottom panels represent the individual layers.

[1] F. Gaggioli, P.A. Graham, L. Fu, arXiv:2512.10909 (2025).

In search of systematically improvable models for correlated electron materials

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We, among others in the field, have recently developed the capability to variationally optimize strongly correlated wave functions for excited states using an extension of variational Monte Carlo. For many systems, these calculations represent the limit of what is currently possible in finding the many-body eigenstates of the *ab initio* Hamiltonian of explicit electrons and nuclei. What is new is not only that we can compute these states, but that they are accurate enough to serve as a reference against which the standard model-building machinery can be tested. For the first time this lets us ask a question usually left implicit: how faithful are the Hubbard-like models we build for these materials to the *ab initio* physics they are meant to represent? I will address this at 3 levels:

Correlated electron excited states. Using the ensemble variational principle recently developed in our group.[?], we assess the importance of determinant expansions, orbital optimization, and correlation factors, optimizing tens of thousands of parameters for systems of a few hundred electrons. We find that the relative importance varies significantly from system to system; in some systems orbital optimization can be "worth" hundreds or thousands of determinants.

Effective models: evaluation of embedding techniques. With access to many-body ground and excited states, we have investigated the most common way of treating strongly correlated materials: embedding in a mean-field to treat the strongly correlated part separately, in particular density functional theory with constrained RPA (DFT+cRPA) as the standard method. In model systems such as vanadocene[?] and transition metal defects[?], we find that often the underlying density functional theory calculation limits the accuracy in a non-systematic way. In particular the orbitals used to define the correlated subspace heavily affect the accuracy.

Effective models: derivation from many-body states. Time remaining, I will cover the idea of using the many-body states directly as a base to derive models. We have explored a few methods to do this. The most rigorous we call renormalized density matrix downfolding,[?] which attempts to find the best renormalized model of a given class to reproduce the dynamics of the *ab initio* data. We are also currently exploring more efficient but less rigorous methods using accurate wave functions, which may be presented.

- [1] Yueqing Chang, Erik G. C. P. van Loon, Brandon Eskridge, Brian Busemeyer, Miguel A. Morales, Cyrus E. Dreyer, Andrew J. Millis, Shiwei Zhang, Tim O. Wehling, Lucas K. Wagner, and Malte Rösner. Downfolding from *ab initio* to interacting model Hamiltonians: Comprehensive analysis and benchmarking of the DFT+cRPA approach. *npj Computational Materials*, 10(1):1–12, June 2024.
- [2] Kevin G. Kleiner, Sonali Joshi, Woncheol Lee, Alexander Hampel, Malte Rösner, Cyrus E. Dreyer, and Lucas K. Wagner. Quantum Monte Carlo assessment of embedding for a strongly-correlated defect: Interplay between mean-field and interactions, May 2025.
- [3] William A. Wheeler, Kevin G. Kleiner, and Lucas K. Wagner. Ensemble variational Monte Carlo for optimization of correlated excited state wave functions. *Electronic Structure*, 6(2):025001, April 2024.

Role of impurity statistics and constraints on the medium response in polaron-polaron interactions

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We consider the behavior of a small density of mobile impurities (polarons) immersed in a quantum gas, a generic scenario that can be realized in cold atomic gases, liquid helium mixtures and doped semiconductors. We present a unified theoretical framework for understanding polaron quasi-particles beyond the single-impurity limit, and we identify two key factors that control the polaron-polaron interactions: (i) the statistics of the impurities, including whether or not they are degenerate, and (ii) the constraints on the medium response, i.e., whether the medium density or chemical potential is held fixed. By constructing wave functions for two bosonic, fermionic, or distinguishable impurities immersed in a Bose or Fermi gas, we derive rigorous results for the polaron interactions in the limit of weak impurity-medium interactions. We furthermore obtain an exact relationship between the polaron interactions at fixed medium density and at fixed chemical potential, a result which is valid for arbitrary interaction strength. Our work provides an important guide for understanding experiments, and it acts as a starting point for future strong-coupling theories of polaron interactions that capture all of the effects identified in this work.

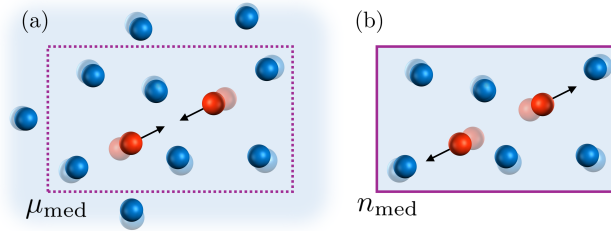


Figure 1: Sketch of the different constraints on the medium (blue particles): either its chemical potential (a) or its density (b) is fixed. These can impact the strength of the interactions between polarons.

[1] J. Levinsen, O. Bleu, M. M. Parish, Phys. Rev. Lett. **135**, 113402 (2025)

[2] J. Levinsen, F. M. Marchetti, O. Bleu, M. M. Parish, arXiv:2512.01413

Quantum droplets in a Bose-Fermi mixture

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We consider the canonical problem of a Fermi gas interacting with a weakly repulsive Bose-Einstein condensate at zero temperature. To explore the quantum phases across the full range of boson-fermion interactions, we construct a versatile variational ansatz that incorporates pair correlations and correctly captures the different polaron limits. Remarkably, we find that self-bound quantum droplets can exist in the strongly interacting regime, pre-empting the formation of boson-fermion dimers, when the Fermi pressure is balanced by the resonant boson-fermion attraction. This scenario can be achieved in experimentally available Bose-Fermi mixtures for a range of boson-fermion mass ratios in the vicinity of equal masses. We furthermore show that a larger fermion density instead yields phase separation between a Bose-Fermi mixture and excess fermions, as well as behavior reminiscent of a liquid-gas critical point. Our results suggest that first-order quantum phase transitions play a crucial role in the phase diagram of Bose-Fermi mixtures.

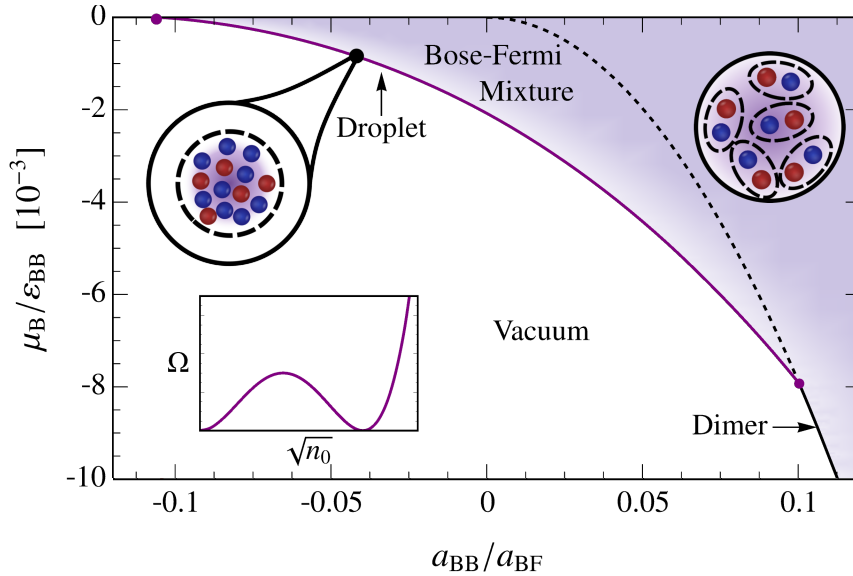


Figure 1: Phase diagram of a Bose-Fermi mixture as a function of boson chemical potential and boson-fermion scattering length. The quantum droplet phase corresponds to coexistence between mixture and vacuum, and occurs in the regime of strong interactions

[1] S. Foster, O. Bleu, J. Levinsen & M. M. Parish, arXiv:2601.12777

Evolution of Kondo Resonance under Generalized Nonequilibrium Bath

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Numerical renormalization group (NRG) is formulated for nonequilibrium steady state by converting finite-lattice many-body eigenstates into scattering states. Extension of the full-density-matrix NRG for a biased Anderson impurity model, simplified by using the original orbital basis of the Hamiltonian, enables detailed studies of the sub-Kondo spectral evolution in the zero-temperature limit, confirming the double-resonance structure emerging at bias V equal to the Kondo energy scale T_K . The distribution shows distinct multiscale spectral features of population inversion at energy ω below the Kondo scale ($\omega \lesssim T_K$) and very strong nonequilibrium excitations at energy beyond the bias ($\omega \gtrsim V$). The strong departure from the Fermi-Dirac distribution leads to the local nonequilibrium temperature T_{loc} scaling as $k_B T_{\text{loc}} \sim V$ for $V \gg T_K$. The current-voltage relation at the low temperatures ($T \ll T_K$) in the strong Kondo regime [1]. We further extend this formulation for an arbitrary non-thermal distribution function by transforming the baths to fully-filled and fully-empty reservoirs, which will pave the way for an NRG-based nonequilibrium dynamical mean-field theory for investigation of nonequilibrium in the lattice limit.

[1] J. E. Han, Phys. Rev. B **113**, 045141 (2026).

Quantum Monte Carlo and uncertainty quantification in nuclear systems

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This talk will address a number of our recent works on first-principles studies of many-nucleon systems (as well as extensions carried out after the present abstract was submitted). One such line of research involves the propagation of theoretical uncertainties from the chiral nuclear interaction all the way to the few- and many-nucleon level, using quantum Monte Carlo and efficient emulators.[1] Another family of works addresses the novel statistical technique known as conformal prediction, which we were the first to apply to nuclear physics [2] and are currently extending to neutron-star equations of state. Finally, time permitting, I will also discuss our ongoing studies of auxiliary-field quantum Monte Carlo for nuclear systems [3] or neural-network wave functions [4].

- [1] R. Curry, K. Hebeler, S. Gandolfi, A. Gezerlis, A. Schwenk, R. Somasundaram, and I. Tews, arXiv:2510.15860.
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Revisiting the Equation-of-Motion Method: A Universal Framework for Correlated Quantum Systems

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The equation-of-motion (EOM) method is currently experiencing renewed interest across several areas of quantum many-body physics, including quantum chemistry and quantum computing, where recent implementations [1] have demonstrated significant improvements over configuration-interaction-based approaches. In nuclear physics, where the method was originally introduced, EOM techniques have long provided a powerful and versatile framework for the description of excited states, enabling systematic extensions of the random phase approximation (RPA). In its most general formulation, the EOM approach yields the normal modes of a quantum system within a symplectic submanifold of the projective Hilbert space [2].

Despite this formal generality, practical implementations of the EOM method typically depend strongly on the choice of reference ground state, often requiring tailored theoretical developments for each specific many-body framework. This limits its flexibility and complicates its application to modern correlated expansion methods.

In this work, we present a fully general formulation of the EOM method in which the operators entering the secular equation are defined independently of the reference state. Within this framework, the applicability of the method is reduced to the ability to evaluate ground-state expectation values of many-body operators. Building on previous developments that express moments of the strength function in terms of such expectation values [3], we construct a universal approach to the nuclear response that is compatible with arbitrary correlated ground states, going beyond the standard mean-field + RPA paradigm.

We demonstrate the impact of ground-state correlations by comparing response functions obtained at the mean-field level with those computed using in-medium similarity renormalization group (IMSRG) wavefunctions [4] in ab initio nuclear structure calculations based on chiral Hamiltonians. These results highlight the quantitative and qualitative role of correlations in shaping nuclear excitations.

- [1] Ollitrault, Pauline J., et al. "Quantum equation of motion for computing molecular excitation energies on a noisy quantum processor." *Physical Review Research* 2.4 (2020): 043140.
- [2] Rowe, David J., A. Ryman, and G. Rosensteel. "Many-body quantum mechanics as a symplectic dynamical system." *Physical Review A* 22.6 (1980): 2362.
- [3] Porro, Andrea, Achim Schwenk, and Alexander Tichai. "Impact of ground-state correlations on the multipole response of nuclei: Ab initio calculations of moment operators." *Physical Review C* 112.5 (2025): 054303.
- [4] Tsukiyama, Koshiroh, S. K. Bogner, and A. Schwenk. "In-medium similarity renormalization group for nuclei." *Physical Review Letters* 106.22 (2011): 222502.

Ab Initio Study of ${}^7\text{Li}$ with Coupled Mass Partitions

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Lithium plays an important role in nuclear astrophysics, fusion energy generation, and nuclear technology. From a theoretical point of view, the nucleus ${}^7\text{Li}$ presents a remarkable challenge, as its bound states and resonances can be understood as being formed by a ${}^4\text{He}$ and ${}^3\text{H}$ pair, or simultaneously, a single neutron/proton coupled to a ${}^6\text{Li}/{}^6\text{He}$ core. In light of this complexity, a consistent description of ${}^7\text{Li}$ bound-state and continuum properties in a unified model presents a significant advancement towards a predictive theory of nuclear structure and reactions. Towards achieving such a predictive description, we carried out calculations for ${}^7\text{Li}$ within the *ab initio* no-core shell model with continuum (NCSMC), which is capable of describing both bound and scattering states in a unified framework, taking into account the mass/charge partitions ${}^4\text{He} + {}^3\text{H}$, ${}^6\text{Li} + n$, and ${}^6\text{He} + p$ in a single coupled-channels calculation, using chiral nuclear forces as input. These calculations are the first ever application of the NCSMC with three coupled partitions. I will show the effects of the coupling of the partitions on the spectrum of ${}^7\text{Li}$ and present cross sections of charge-exchange and nucleon-transfer reactions, calculation of which is allowed by the coupling.

Tackling the challenge of large model spaces

**Lars Zurek^{1,2}, Pepijn Demol³, Thomas Duguet⁴, Jean-Paul Ebran^{1,2}, Mikael Frosini⁵,
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The ab initio approach to nuclear structure allows us to describe atomic nuclei with controlled and systematically improvable approximations. Applying it to nuclei that are at the same time both heavy and open-shell is largely impossible with current many-body techniques. This is due to the computational cost of handling huge dense tensors. I will show how some surprisingly simple tricks may help us to tackle this hurdle [1]. These tricks are driven by the observation that different contributions to ab initio calculations describe different physics. We leverage this by using adapted model spaces. In addition, we use modern linear algebra methods to develop dimensionality reduction techniques based on the singular value decomposition [2]. By avoiding the construction of large many-body tensors in the first place, we are able to extend the reach of ab initio calculations to nuclei where standard approaches would be too expensive to run.

[1] L. Zurek, P. Demol, U. Vernik, M. Frosini, A. Tichai, T. Duguet, in preparation (2026).

[2] M. Frosini, T. Duguet, P. Tamagno, Eur. Phys. J. A **60**, 183 (2024).

Exotic Superfluid Phases in Spin-Polarized Fermi Gases

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Understanding exotic superfluid phases in imbalanced Fermi systems remains a central challenge in quantum many-body physics, with important implications for ultracold atoms, unconventional superconductivity, and quantum simulation. In this contribution, I will discuss recent advances in both the characterization of exotic pairing states and the development of numerical methods capable of describing them reliably.

Large-scale simulations of two-dimensional spin-polarized Fermi gases in optical lattices provide compelling evidence for the stability of Fulde–Ferrell–Larkin–Ovchinnikov (FFLO) superfluid phases in the regime of high density and small spin imbalance [1]. The analysis of spatial correlation functions reveals nontrivial coexistence of pairing and density modulations, highlighting the rich structure of the underlying broken symmetries.

To address such phases within a controlled computational framework, I will also present an extension of auxiliary-field quantum Monte Carlo based on stochastic evolution in the manifold of Hartree–Fock–Bogoliubov wave functions [2]. By explicitly incorporating pairing correlations at the mean-field level, this approach naturally accommodates finite-momentum pairing and more general pairing mechanisms, enabling the computation of ground-state properties in strongly interacting regimes that are difficult to access with conventional determinant-based methods.

Together, these results illustrate the interplay between emergent exotic order and algorithmic innovation, and open new perspectives for the quantitative study of correlated fermionic matter.

[1] E. Vitali, P. Rosenberg, and S. Zhang, Phys. Rev. Lett. 128, 203201 (2022).

[2] E. Vitali, P. Rosenberg, and S. Zhang, J. Chem. Phys. 161, 134116 (2024).

Kelvin-Helmholtz Instability in Fermionic Superfluids: Numerical Approach

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²*Department of Applied Science and Technology, Politecnico di Torino, Italy*

³*Department of Physics, University of Washington, USA*

The Kelvin–Helmholtz instability (KHI) in superfluid systems with annular geometry has recently attracted significant attention. While numerical studies based on Gross–Pitaevskii and Zaremba–Nikuni–Griffin models have explained some of its dynamics, the inconsistency persists, as evidenced by incorrect predictions of the instability’s growth rates [1, 2]. We employ the SLDA framework [3] to simulate KHI in annular superfluid systems across interaction regimes for temperatures $T/T_c \approx 0.0$ and 0.33 , and compare the resulting dynamics and KHI growth rates with existing theoretical models and experimental observations. We do not observe sensitivity of the instability growth rate to the interaction regime (BCS vs UFG), in contrast to experimental findings. This discrepancy persists even when finite-temperature effects are included. Additionally, systematic deviations from the Point-Vortex Model are identified for modes with $m/\Delta w \in (0.6, 0.8)$, for which no clear mechanism has been established. In the deep BCS regime, the dynamics change qualitatively: vortex proliferation at the inner edge of the ring dominates, operating on shorter timescales than KHI and suppressing its development. Our results indicate a discrepancy between experimentally observed interaction-dependent growth rates and their numerically derived counterparts. Also, we reveal a competing instability mechanism in the BCS regime. These findings highlight unresolved aspects of vortex dynamics in annular superfluids and motivate further theoretical investigation.

[1] D. Hernández-Rajkov, PhD thesis (2024).

[2] D. Hernández-Rajkov, et al: *Connecting shear flow and vortex array instabilities in annular atomic superfluids*, Nat. Phys., 20(6):939-944 (2024).

[3] G. Wlazłowski, P. Magierski, M. M. Forbes, A. Bulgac: *W-SLDA Toolkit: A simulation platform for ultracold Fermi gases* (2026).

Reproducible nucleation and control of stable quantum vortex rings in Bose–Einstein condensates

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We propose and numerically validate an experimentally feasible on-demand protocol for the nucleation and manipulation of stable quantum vortex rings in trapped Bose–Einstein condensates. The method relies on sweeping a laser-sheet barrier that locally constricts the superflow and triggers vortex–ring formation by exceeding the critical relative velocity between the laser sheet and the condensate atoms. By tuning the barrier height and width, and by scanning the barrier velocity, we identify the onset of periodic generation of vortex rings achieve direct, deterministic control over the ring nucleation position, radius, and hence propagation speed. After its formation, ad-hoc optical potentials are applied to reshape the vortex ring, creating clean Kelvin–wave excitations.

Our results provide a foundation for systematic studies of three-dimensional vortices in atomic superfluids and open the door to tailored vortex dynamics and interactions, enabling controlled access to quantum turbulence. Furthermore, recent evidence describes striking similarities between quantum and classical turbulence [1], suggesting that turbulence, independently from its intrinsic nature, may be depicted on the basis of collective and interactive dynamics of thin vortex filaments of fixed circulation [2]: the study of controlled quantum vortex interactions could thus lead to the enhancement of the understanding of the still open issues in classical turbulence. .

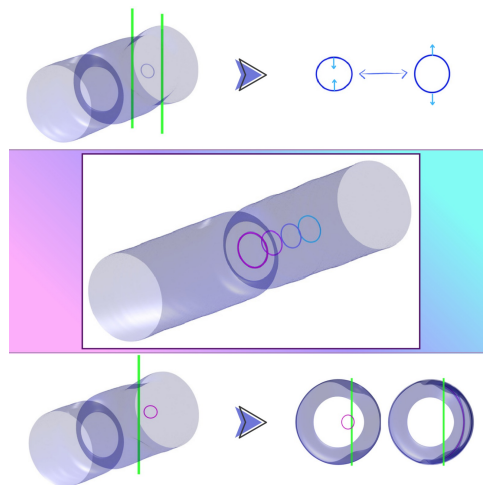


Figure 1: Schematic rendering of generation and manipulation of quantum vortex rings in Bose-Einstein Condensates

[1] L. Galantucci, J. Fluid Mech. **1022**, F1 (2025).

[2] J. I. Polanco, N. P. Muller and G. Krstulovic, Nat. Comms **12**, 7090 (2021).

Quantum dynamics at finite temperature with wavepackets: The thermofield approach

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²*Institute of Physical and Theoretical Chemistry, Goethe University Frankfurt,
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The description of finite-temperature quantum dynamics remains a major challenge in the simulation of dissipative and nonadiabatic processes in molecular and condensed-phase systems. In this talk, I will discuss wavepacket approaches to finite-temperature quantum dynamics based on the thermofield formalism [1], which represents thermal mixed states as pure states in an enlarged Hilbert space. This framework enables finite-temperature simulations using standard wavefunction propagation techniques while retaining a fully quantum-mechanical description of system and environment dynamics.

After introducing the purification of thermal bath states, I will discuss the role of thermal Bogoliubov transformations in obtaining compact and computationally efficient wavefunction representations, together with their implementations based on Multi-Layer Multi-Configuration Time-Dependent Hartree wavepacket methods [2, 3] and their Gaussian-based variants [4, 5]. Applications will be presented for vibrational relaxation, decoherence, excitation-energy transfer, and ultrafast chemical transformations in structured environments, including recent studies of coherent-to-kinetic transitions in donor–acceptor systems [6] (Figure 1) and quantum dynamics at conical intersections in solution [7, 8]. Finally, I will discuss recent extensions of the thermofield framework to anharmonic environments and present simple applications highlighting the role of anharmonicity in the dynamics.

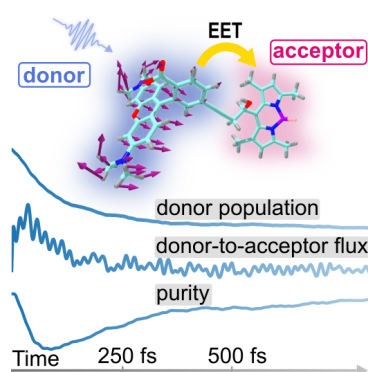


Figure 1: Ultrafast excitation-energy transfer in a non-Förster regime

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- [3] H. Wang, M. Thoss, *J. Chem. Phys.* **119**, (2003) 1289.
- [4] I. Burghardt, H.-D. Meyer, L. S. Cederbaum, *J. Chem. Phys.* **111** (1999), 2927
- [5] S. Römer, M. Ruckebauer, I. Burghardt, *J. Chem. Phys.* **138** (2013) 064106.
- [6] S.L. Choudhury, M. Horz, R. Hegger, R. Martinazzo, I. Burghardt, *J. Phys. Chem. Lett.* **17**, 3117 (2026).
- [7] B Błasiak, D Brey, R Martinazzo, I Burghardt, *J. Chem. Phys.* **163**, 124108 (2025); **163**, 124109 (2025).
- [8] B Błasiak, D Brey, R Martinazzo, I Burghardt, *J. Chem. Phys.* **164**, 044124 (2026).

Wavefunction optimization at the complete basis set limit with Multiwavelets and DMRG

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The Density Matrix Renormalization Group (DMRG) is a powerful numerical technique to solve strongly correlated quantum systems [1]: it deals well with systems which are not dominated by a single configuration and it converges rapidly to the full Configuration Interaction (FCI) limit.

In this work, we develop an algorithm that integrates DMRG within the Multiwavelet-based Multiresolution Analysis (MRA) [2]. Unlike fixed basis sets, Multiwavelets offer an adaptive and hierarchical representation of functions, approaching the complete basis set limit to a specified precision. As a result, this combined technique leverages the multireference capability of DMRG and the complete basis set limit of MRA and Multiwavelets. Specifically, we adopt a pre-existing Lagrangian optimization algorithm for orbitals represented in the MRA domain [3] and improve its computational efficiency by replacing the original CI calculations with DMRG [4].

Additionally, we substitute the reduced density matrices computation with the direct extraction of energy gradients from the DMRG tensors. We apply our method to small systems such H_2 , He, HeH_2 , BeH_2 and N_2 . The results demonstrate that our approach reduces the final energy while keeping the number of orbitals low compared to FCI calculations on an atomic orbital basis set.

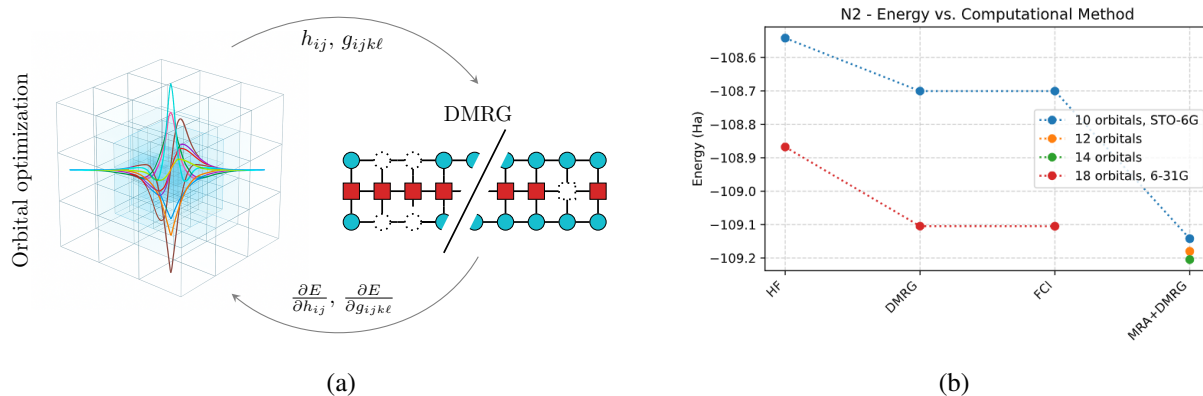


Figure 1: (a) Our algorithm MRA+DMRG performs the orbital optimization via Multiwavelet-based MRA, and optimizes the multireference wavefunction via DMRG. (b) While keeping the number of orbitals fixed, MRA+DMRG reaches significantly lower energies compared to Hartree Fock (HF), DMRG and FCI performed on atomic orbital basis sets.

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Predict, Probe, Reconstruct — Electron Correlation Across Scales: Beams, Bands, and Galactic Chemical Evolution

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In this presentation, we introduce a general theoretical and computational framework that combines *ab initio* and Monte Carlo methods to study the electronic, optical, and transport properties of materials across different time and length scales [1,2]. Photon, electron, and ion beams are used as probes to perturb the system, enabling investigation of its excitation spectrum and direct comparison of simulations with experimental data.

Elastic and inelastic collisions are modelled from first principles by solving the many-body Dirac equation and computing the macroscopic dielectric response using linear-response time-dependent density functional theory. Inelastic processes include single-particle and collective excitations (plasmons), electron–phonon interactions, ionisation, Auger emission, and secondary electron generation.

The resulting scattering cross sections are incorporated into Monte Carlo simulations to track electron cascade trajectories and model charge transport in solids. This approach reproduces experimental Auger electron spectra (AES), reflection electron energy-loss spectra (REELS), secondary electron spectra (SE), and total electron yield (TEY) across a wide range of materials.

Furthermore, I will demonstrate how our approach can be extended to solve the Dirac–Hartree–Fock equation in many nucleon–electron systems for studying Big Bang and stellar nucleosynthesis in astrophysical contexts.

Applications include cosmic radiation charging in the LISA mission [3], material growth [4], dose deposition and DNA damage in hadron therapy [5], advanced imaging techniques such as atom probe tomography with terahertz laser pulses [6], and beta-decay processes relevant to stellar and Big Bang nucleosynthesis [7,8].

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Novel forms of Density Matrix Renormalization Group theory and the discovery of new quantum phases in two dimensional materials

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Two-dimensional materials provide highly tunable platforms for exploring strongly correlated physics, but the sheer number of competing ground states means that uncovering the true physics requires a careful combination of powerful techniques.

In this talk, I will first introduce cylinder Density Matrix Renormalization Group (DMRG), combined with Matrix Product Operator compression, as a versatile method for resolving the strongly correlated ground states of 2D materials. I will highlight how this approach has enabled us to identify novel correlated phases of matter.

I will then focus on the effect of heterostrain in twisted bilayer graphene. Combining Hartree–Fock calculations, DMRG ground-state searches, and an analysis of STM experiments, we find an Incommensurate Kekulé Spiral (IKS) ground state characterized by spatially modulated symmetry-breaking patterns.

Single Impurity in a Luttinger Liquid and Beyond

Charles L. Kane

University of Pennsylvania

A dramatic consequence of electron interactions in one-dimensional conductors is the suppression of transport at low energies due to a single weakly scattering impurity. The ‘single impurity problem’ in a Luttinger liquid, which describes the crossover between the weak-backscattering and weak-tunneling limits, provides a framework for understanding this phenomenon and is a paradigm for a large class of quantum impurity problems described by boundary conformal field theory. It is a problem that I have revisited several times throughout my career. In this talk, I will review our early thinking about this problem, and discuss certain ‘intermediate fixed points’ that arose in the theory of an impurity in a spinful Luttinger liquid. These intermediate fixed points show up in a number of problems of more recent interest, including recent observations of the three-channel Kondo effect in quantum dot devices, as well as theories of a point contact in a quantum spin-Hall insulator and of a multi-channel Luttinger liquid-topological superconductor junction.

Nonlinear Luttinger Liquid

Leonid I. Glazman

Yale University

For many years, Luttinger liquid theory has served as a useful paradigm for describing one-dimensional (1D) quantum fluids in the low-energy limit. This theory is based on a linearization of the dispersion relation of the constituent particles. However, beyond the low-energy limit, the nonlinearity of the dispersion relation becomes essential. Newly developed methods are capable of tackling this nonlinearity, thus extending conventional Luttinger liquid theory. This new nonlinear Luttinger liquid theory combines the phenomenology developed in the context of the single-impurity problem in a conventional Luttinger liquid with perturbative Fermi liquid theory. The new theory made it possible to uncover and fully characterize the threshold singularities of various dynamic correlation functions, including the widely used energy- and momentum-resolved dynamic structure factor and spectral function. It can be applied to a wide variety of 1D quantum fluids, from spin liquids to electrons in quantum wires and cold atoms confined by 1D traps. Moreover, nonlinear Luttinger liquid theory shows how dispersion nonlinearity leads to finite lifetimes of excitations in one dimension. The theory has been successfully applied to explain the results of several experiments with quantum wires and has motivated a number of new experiments. The crossover between the low-temperature regime of a generic nonlinear Luttinger liquid and the high-temperature regime described by the KPZ equation remains an open and conceptually important question.

Edge state transport of Quantum Hall states

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Abstract

In a one-dimensional conductor, interactions between electrons destroy the free-fermion Fermi-liquid description and generally lead to a Luttinger liquid. Observing clean Luttinger-liquid behavior in quantum wires is challenging, however, due to impurity scattering and localization. Remarkably, quantum Hall edge states provide a particularly clean setting: right- and left-moving modes reside on opposite edges of a Hall bar, strongly suppressing backscattering. For Laughlin fractional quantum Hall states at filling $\nu = 1/m$, these edge modes form a chiral Luttinger liquid with a universal Luttinger parameter $g = \nu$. In this talk I will revisit theoretical developments from the 1990's that led to predictions of universal electrical and thermal conductance and noise in quantum Hall edges, including disordered edges with multiple modes and both Abelian and non-Abelian quantum Hall states. I will also discuss how a point contact between opposite edges can reveal the underlying edge structure, most notably through the measurement of fractional charge in shot-noise experiments. I will conclude by briefly discussing experiments and some remaining open questions, particularly concerning the edge structure of non-Abelian quantum Hall states.

Hadron-Hadron Interactions from Lattice QCD

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Abstract

Hadron–hadron interactions provide fundamental input for understanding hadronic and nuclear many-body systems. I will review the current status of their first-principles determination from lattice QCD using the HAL QCD method, which extracts energy-independent and nonlocal interaction potentials from hadronic correlation functions. I will discuss the theoretical foundations of the method and its recent applications to baryon–baryon, baryon–meson, and meson–meson interactions [1, 2].

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Superconducting pairs dynamics in the two-dimensional Hubbard model

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The frequency structure of the superconducting correlations in cuprates provides insights into the pairing mechanism. Here we analyse this problem in the two-dimensional Hubbard model with cellular dynamical mean-field theory. We systematically quantify how the superconducting gap, the frequency scales of d -wave pairing, and their relative contribution to pairing depend on doping δ and interaction strength U . For all model parameters, we find that pair-forming processes are confined to frequencies set by the superexchange interaction and are followed by pair-breaking processes, ruling out both pair-forming and pair-breaking processes on the scale of U . This indicates that at high frequencies, the effect of U is suppressed by the d -wave pairing, whereas at small frequencies, U generates the superexchange interaction, leading to low-frequency pair-forming processes that provide the net contribution to pairing [1].

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Ultradilute quasi-2D Bose-Bose liquid and droplets

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We present the study of ultradilute Bose-Bose bulk mixtures and droplets in an external harmonic potential that confines them in one spatial direction towards the two-dimensional (2D) limit, extending and going beyond our earlier works [1, 2].

We focus on the mixture of two hyperfine states of ^{39}K with attractive interspecies and repulsive intraspecies interactions which we model with potentials that include information on s-wave scattering length a and effective range r_{eff} . Equations of state for several confinements are obtained with Diffusion Monte Carlo method at $T=0$. For several confinements we perform the calculations using two different interaction potential models and determine the range of confinements for which equations of state are universal in terms of a and r_{eff} .

Based on the quantum Monte Carlo (QMC) equation of state we develop a 2D QMC density functional for each confinement strength and use it together with the local density approximation to determine properties of the self-bound drops, and to study the formation of vortices. We compare 2D QMC functional results with the predictions we obtained using previously determined three dimensional (3D) QMC functionals [3] and 2D and 3D Lee–Huang–Yang (LHY) functionals [4, 5]. For moderate squeezing, energies and droplet profiles obtained using 2D QMC functional agree well with the profiles previously obtained using 3D functionals [1], while offering a substantial reduction in computational cost, and a consistent approach in crossover to 2D. Our results approach 2D mean-field + LHY theory predictions only for the most strongly confined systems for which universality in terms of a and r_{eff} is observed, implying very narrow range of confinements for which 2D LHY functionals are applicable. This has important consequences for the study of vortices, which we demonstrate comparing 2D functional results with our previous work [2].

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Learning in the Quantum Universe

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In this talk, I will present our progress in building a rigorous theory to understand how scientists, machines, and future quantum computers could learn models of our quantum universe.

The talk begins with an experimentally feasible procedure for converting a quantum many-body system into a succinct classical description of the system, its classical shadow [1]. Classical shadows can be applied to efficiently predict many properties of interest, including expectation values of local observables and few-body correlation functions.

I will then build on the classical shadow formalism to answer two fundamental questions at the intersection of machine learning and quantum physics: Can classical machines learn to solve challenging problems in quantum physics [2]? And can quantum machines learn exponentially faster and predict more accurately than classical machines [3]? The talk answers both questions positively through mathematical analysis and experimental demonstrations.

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Complexity of the many-body problem - entanglement and beyond

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Synthetic quantum matter is revolutionizing the way we approach the many-body problem - in particular, by demonstrating frameworks where concepts and methods from traditional many-body theory conspire with ideas from quantum information and atomic physics. One particularly interesting direction has been the relation between computational complexity, and many-body properties. In this talk, I will review the historical origin of such a connection, rooted in the context of tensor network states and entanglement, and present a pair of fresh perspectives: sampling complexity and quantum magic. I will discuss their experimental relevance, and discuss in detail recent progress on many-body magic, utilizing examples from critical behavior and topological matter. Finally, I will show how such basic understanding can enable better computational algorithms, where entanglement and magic are incorporated in a single wave function ansatz, illustrating their power utilizing lattice gauge theories.

Observation of real-time string-breaking dynamics in a programmable quantum simulator

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Quantum simulation emerged as a promising pathway to simulating otherwise inaccessible non-perturbative aspects of real-time quantum-field-theory and quantum-many-body dynamics. One of its most important long-term applications is the simulation of particle collisions involving the strong force. Real-time fragmentation of confining strings, in particular, is thought to play a central role in the non-equilibrium quark confinement processes underlying hadronization. In the first part of this talk, I will discuss our recent observation of dynamical string breaking in a programmable trapped-ion quantum simulator. Data revealed an unexpected edge-facilitated string-breaking mechanism, distinct from and faster than the conventional Schwinger mechanism. In the second part of the talk, I will describe a new approach to simulate the multi flavor Schwinger model – a continuum gauge field theory closely related to concrete particle-physics applications – on state-of-the-art neutral-atom arrays. This document is the template for contributed abstracts and provides guidelines for preparing and submitting abstracts to the RPMBT23 International Conference.

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Signature in sound-mode of the exciton bilayer two-dimensional superfluid transition

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Obtaining definitive evidence of exciton superfluidity [1] in electron-hole bilayers in zero magnetic field remains a major longstanding challenge since the condensate is electrically neutral, making its phase coherence difficult to detect directly. We show that the Anderson-Bogoliubov sound velocity provides a dynamical signature of exciton superfluidity. Across the BCS-BEC crossover, the velocity is known to discontinuously drop to zero at the Berezinskii-Kosterlitz-Thouless (BKT) transition. The magnitude of the drop has a strong density dependence. We compute this behavior, with the inclusion of finite-temperature screening, and determine the BKT transition using a renormalization-group approach [2]. We further identify a temperature window which is experimentally accessible, where vortex-antivortex excitations strongly renormalize both the sound velocity and the transition temperature [3].

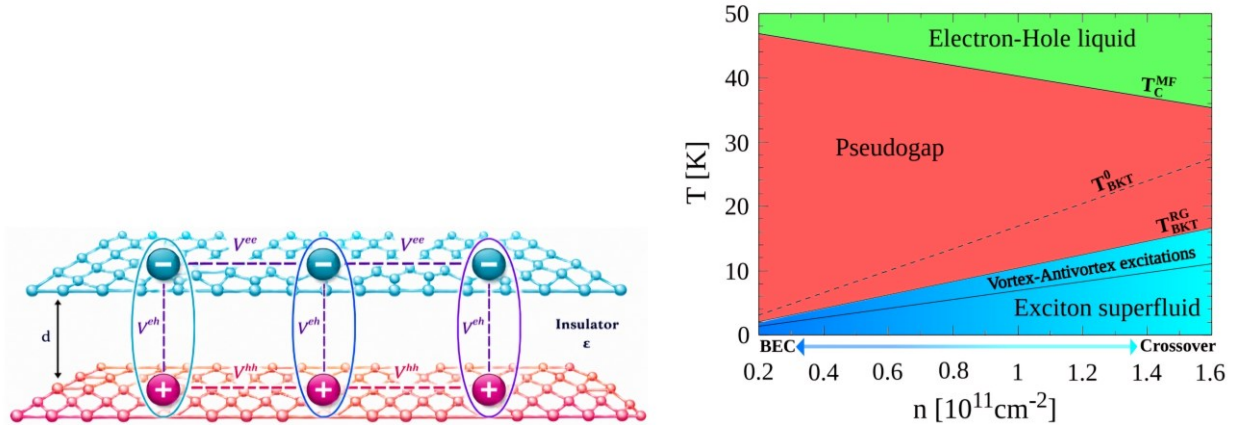


Figure 1: Panel (a), Exciton bilayer system. Panel (b) Temperature-density (T, n) phase-diagram for double bilayer-graphene. T_{MFC} : mean-field critical temperature. T_{BKT}^0 and $T_{\text{BKT}}^{\text{RG}}$: BKT transition temperature without and with Renormalization Group (RG).

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Nonequilibrium exciton dynamics with ab initio real time propagation schemes

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This presentation will review recent theoretical and numerical developments aimed at modeling nonequilibrium dynamics in advanced materials from first-principles. Specifically, I focus on capturing the generation and dynamics of coherent excitons within the Time-Dependent Screened Exchange (TD-HSEX) scheme.

I will discuss recent results obtained in close collaboration with an experimental group at Politecnico di Milano, where pump-probe measurements were performed with attosecond time-resolution in the extreme ultraviolet (XUV) energy range. We analyze the XUV spectra of two systems hosting tightly bound excitons: a monolayer of the 2D material MoS₂ [3], and LiF [4], an insulator featuring the largest known electronic band gap. For LiF, the signature of a high-energy exciton embedded in the continuum will be analyzed (see Fig. 1).

All numerical simulations are based on the lumen project [1] (www.lumen-code.org), a fork of the yambo code [2] developed within the TIMES doctoral network.

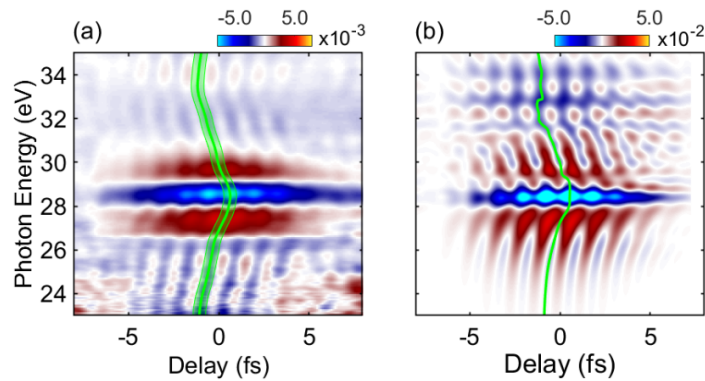


Figure 1: Experimental (left) and theoretical (right) transient absorption signal of LiF.

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Nonequilibrium Dynamical Mean Field Theory for Strongly Correlated Systems: Combining Nonequilibrium Green's Functions and Quantum Master Equations

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The auxiliary master equation approach (AMEA) offers an accurate, controlled framework for investigating strongly correlated systems out of equilibrium [1]. By mapping the physical Dynamical Mean Field Theory impurity problem onto a finite open quantum system, consisting of bath orbitals and a Markovian environment, AMEA yields exponentially accurate fits of the hybridization function. This approach bridges quantum master equations and nonequilibrium Green's functions, granting reliable access to steady-state Keldysh functions and transport observables of strongly-correlated systems.

After an overview of the foundational framework, I will discuss two recent advancements designed to enhance its precision and scale: (i) a functional interpolation expansion that extends the hybridization fit reducing both the required bath size and systematic errors in the self-energy [2], and (ii) a mixed configuration approximation that extends the reach of AMEA to approximately address multi-orbital systems, with an application to SrVO₃ thin films out of equilibrium [3].

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All the ‘Buzz’ about the Nickelates: A Dynamical Mean Field Theory (DMFT) Perspective

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Superconducting nickelates have garnered tremendous interest in hopes of a better understanding of unconventional superconductors. Observation of superconductivity across several platforms under varying conditions, such as, doping, pressure or biaxial strain at ambient pressure have created a distinct ‘buzz’ in the field. Among these are the Ruddlesden-Popper (RP) series, the reduced oxygen RP (infinite layer) systems and hybrid structure compounds. To understand the many-body normal state from which superconductivity emerges, it is important to ascertain the nature and role of correlations in these materials. First-principle many-body approaches, such as, embedded dynamical mean field theory (eDMFT) can be valuable for obtaining the correlated ground and excited states of d- and f-electron systems such as these.

I will first present an overview of the various platforms of nickelates of current interest. Then, I will give a simple picture of what underlies the eDMFT approach. Following this, I will discuss our recent charge self-consistent DFT+ DMFT work on some of the nickelate systems, namely, RP bi-layer [1] and tri-layer nickelates under compressive strain, and time-permitting, undoped [2] and doped infinite-layer nickelates. In bi-layer nickelates, in contrast with DFT+U studies, around the strain where superconductivity has been observed, we find the emergence of an extra Fermi surface sheet associated with a flat Ni-d band, driven by dynamical correlations. This is consistent with recent ARPES results, and may have implications for superconductivity. In doped infinite-layer nickelate, our study, across a range of temperature and doping, suggests possible Ni site-selective behavior.

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Shapiro physics to verify interlayer exciton superfluidity

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Definitive evidence for zero-magnetic-field exciton superfluidity in electron–hole bilayers remains elusive, despite recent experimental indications [1,2]. We propose a direct test based on Shapiro physics in a Dayem-bridge excitonic Josephson junction. A narrow constriction forms an S–S′–S weak link [3], allowing the neutral exciton supercurrent to follow a Josephson-like current–phase relation. Under combined DC and AC driving, the high-frequency Josephson dynamics are converted into measurable DC voltage plateaus, providing a clear phase-coherence signature of the condensate. We calculate the Shapiro response and show that resolvable steps should occur in realistic double-bilayer graphene devices [4], with possible extension to transition-metal dichalcogenide bilayers. By tuning the carrier density, the system can be driven across the BCS–BEC crossover, revealing signatures of the transition from bosonic to fermionic excitations. In particular, we predict Shapiro plateaus in both current–voltage and density–voltage characteristics. Observation of these features would provide direct evidence for a macroscopic exciton superfluid order parameter and open a route toward neutral Josephson devices.

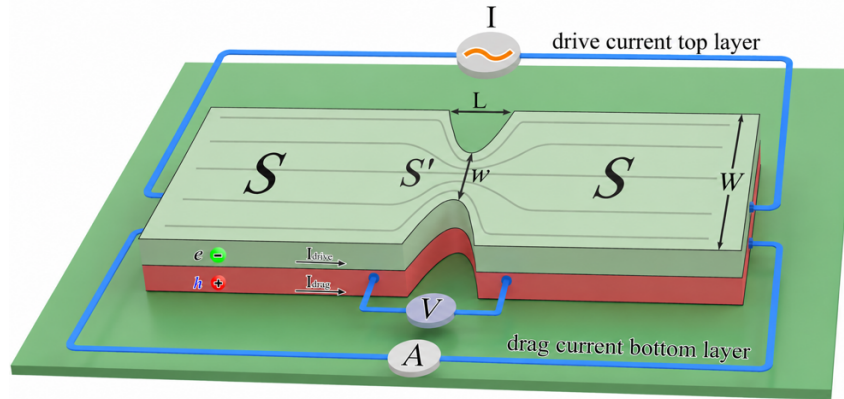


Figure 1. Oblique view of the proposed S–S′–S Dayem-bridge device. The n-doped top layer and p-doped bottom layer are separated by an insulating barrier. The bridge, of width w and length L , connects bulk regions of width W . An AC drive current I_{drive} induces a drag current I_{drag} , while the voltage drop V is measured across the bridge.

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The FFLO transition and non-Fermi-liquid in the 2D spin-imbalanced Fermi gas at zero temperature

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The object of this study is the two-dimensional Fermi gas at zero temperature with attractive contact interaction and spin population imbalance. Beyond the imbalance limit of Chandrasekhar and Clogston homogeneous superfluidity is destroyed but Fulde and Ferrell [1] and, independently, Larkin and Ovchinnikov [2] (FFLO) proposed in the 1960's that it could persist through pairing at a finite centre-of-mass momentum. We provide a comprehensive theoretical characterization of the FFLO transition in a two-dimensional (2D) spin imbalanced Fermi gas going beyond the historical mean-field characterization by adopting a diagrammatic T -matrix approach within two schemes: the non-self-consistent scheme and the partially self-consistent scheme.

The phase-diagram of the critical polarization versus coupling reveals significant differences between the two schemes (see Fig. 1 panel (a)) owing to the crucial role of self-consistency as argued within the Luttinger theorem. A marked effect of dimensionality is also found when compared to the three-dimensional (3D) phase-diagram [3].

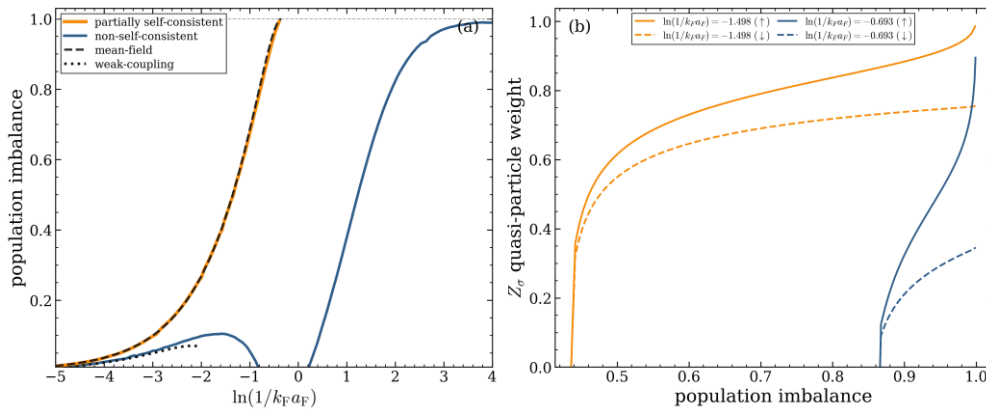


Fig. 1. Left Panel: phase diagram of population imbalance versus coupling strength at zero temperature of a 2D attractive Fermi gas within two computational schemes. Right Panel: quasi-particle weight for two representative coupling strengths as a function of the population imbalance approaching the two respective critical values.

At the critical polarization line, we examine the effect of quantum fluctuations on the quasi-particle scattering rate finding a non-Fermi-liquid behaviour with exponent $2/3$ of the imaginary part of the self-energy on the Fermi surface (rather than the standard value of the Landau theory of 2), akin to that of nematic or charge density wave order in 2D quantum critical metals. However, the exponent is strongly dependent on the fermionic momentum being on the Fermi surface, above or below. This critical behaviour is drastically different to that of the 3D FFLO transition and represents an example of breakdown of the Hertz and Millis theory of quantum phase transitions [4,5].

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Strongly modulated superfluid phases of ^4He on novel adsorption substrates

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Graphite has been the standard substrate for study of adsorbed ^4He on a smooth and geometrically ordered substrate. Experimental and theoretical studies on this system have produced important information on a bosonic strongly interacting many-body system like localization of quantum particles or superfluidity in restricted geometry. We have investigated if other ordered substrates might expand our knowledge on many-body systems in restricted geometry.

We have investigated some of the new layered materials that have been developed in the laboratory and found that two of them, fluorographene [1] and borophane [2], turn out to be of great interest as substrate for ^4He . In the first place we have computed the adsorption potential of He with a suitable *ab initio* density functional theory including dispersion forces. The computations of the properties of the adsorbed ^4He have been performed at finite temperatures with path integral Monte Carlo and in some cases also at $T = 0$ K with variational path integral.

Fluorographene is a sheet of graphene in which each C atom is chemically bound to a F atom. We find that the adsorption potential of a He atom has a very large corrugation and it differs from that on graphite in several respects. For the first adsorbed layer of ^4He we find that the lowest energy state is not an ordered commensurate state like on graphite but it is a disordered and superfluid state. The first layer of ^4He on fluorographene allows to probe superfluidity under special conditions: the system is highly spatially modulated in the basal plane (the ratio of the largest to the smallest density is about 6), the $T=0$ K superfluid fraction is strongly reduced to about 50% and the roton energy has a strong dependence on the direction of the wave vector in the basal plane.

Borophane is a sheet of boron atoms to which hydrogen atoms are chemically bound. Borophane has a number of allotropes and we found of special interest the one called Rect-2H. In fact the adsorption potential of He on Rect-2H borophane is characterized by ridges with modest energy barriers in one direction of the basal plane and a much higher barrier in the orthogonal direction, thus forming channels for motion of the adsorbed atoms. This leads to strong planar

anisotropy not only in the first adsorbed layer but also in additional layers with presence of ordered and disordered regions. In the second, fourth, and fifth layers we find superfluidity on the length scale of the simulated systems. In the second layer, the superfluidity is one-dimensional (1D) along the grooves. In a narrow low-coverage region of the fourth layer we observe an intriguing state with one unidirectional structure across the grooves which supports a tiny superfluid signal. In the fifth layer we find two states with two-dimensional (2D) superfluidity. At low coverage of this layer the superfluidity is strongly anisotropic (the ratio of the superfluid fraction along the grooves or across them is as large as 3) and for coverages near layer completion there is a crossover to isotropic superfluidity.

In conclusion our prediction is that ^4He adsorbed on fluorographene and on Rect-2H borophane offers the possibility of studying strongly modulated superfluid states in 1D and 2D as well as localized states.

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A walk through nuclear Density Functional Theory: achievements and some open questions

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Nuclear Density Functional Theory (DFT) is a widely used theoretical framework that has been developed over several decades and is accurate in describing nuclear ground-state properties such as nuclear masses and radii, as well as excitation spectra, decay properties, reactions, and fission. However, the results often depend on the specific Energy Density Functional (EDF) employed. EDFs that are equally successful for all observables have not yet emerged, and systematic ways to improve them remain unclear.

Nuclear DFT still lags behind electronic DFT in terms of its connection to exact conditions and to more fundamental calculations. I will explain the differences between the nuclear and electronic cases, as well as the current status and future perspectives of nuclear DFT grounded in *ab initio* nuclear theory.

I will then discuss two further topics. The first is how DFT can be made efficient for heavy nuclei and for complex, extended systems such as the crust of neutron stars; algorithmic improvements and the role of orbital-free DFT will be highlighted. The second concerns the relationship between DFT and many-body approaches. I will focus on many-body models of the nuclear response, such as second RPA and particle-vibration coupling, which have counterparts in the electronic case.

Multi-configuration time-dependent Hartree-Fock method towards nuclear reaction

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A many-body tunneling phenomenon has been paid attention to in nuclear physics community, which is essential to describe nuclear fusion procmicroscopically; Nevertheless, it is still a difficult to describe theoretically; for instance, a simple time-dependent Hartree-Fock (TDHF) calculation cannot describe it because of the lack of the correlation and a time-dependent generator coordinate method (TDGCM) was applied to this problem recently [1, 2].

Motivated by this, multi-configuration time-dependent Hartree-Fock (MCTDHF) method is applied for such a calculation. The trial wave function of the MCHF method is the superposition of Slater determinants of the ground and excited states, while that of the GCM is the superposition of the ground-state Slater determinant of different configurations such as shape. The MCTDHF is the time dependent version of the MCHF and was originally developed for multi-electron dynamics [3–6]. The time evolution of both single-particle orbitals and the coefficients of the trial wave function is considered.

In this work, we apply this MCTDHF method for the α - α scattering in one dimension compared with the TDHF [1] and TDGCM [2] results. This will be a starting point for a detailed discussion on many-body tunneling phenomena.

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Covariant density functionals from relativistic Brueckner theory

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Covariant density functional theory provides one of the most successful microscopic frameworks for describing finite nuclei, nuclear matter, and compact-star matter within a unified relativistic formulation. In its density-dependent form, many-body correlations are encoded through effective meson-nucleon vertices that depend on the baryon density. This approach is particularly attractive because it preserves the Lorentz structure of the nuclear self-energy while allowing the functional to incorporate information from microscopic many-body calculations. We have constructed a density-dependent covariant functional based on a Chebyshev expansion and constrained by full-Dirac-space Brueckner single-particle potentials. The scalar and time-like vector components of the microscopic single-particle potentials at the Fermi surface are mapped onto the corresponding Hartree mesonic channels. The resulting parametrization is particularly well suited to Bayesian analyses that combine laboratory and astrophysical constraints, because the Chebyshev representation reduces spurious correlations among the coefficients governing the density dependence of the functional.

POSTER CONTRIBUTIONS

RPMBT23

NuQShell: A New Quantum Nuclear Shell-Model Python Library

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Calculations of nuclear many-body physics are known to be computationally expensive. Quantum computing is arising as a possible solution to this issue, as quantum processors might exploit their quantum nature to simulate quantum systems more efficiently. To potentially exploit this advantage, one needs to find a well suited algorithm for their system of interest.

The field currently features many mature Python libraries for quantum chemistry, but utilities to deal with nuclear systems are notably absent. To address this gap, we present an efficient Python package for the Nuclear Shell Model that enables easy implementation and testing of quantum algorithms. This library handles the operator representation and provides seamless integration with NumPy and quantum simulation frameworks such as Qibo. In this talk, we will show the basics of the package and present some applications, showcasing the ease with which it can reproduce previous results of our group [1]. Ultimately, this tool aims to bridge the gap between quantum computing and nuclear physics, allowing researchers to exploit the inherent structure of nuclear systems in the pursuit of quantum advantage.

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Static string breaking in LSH SU(2) and prospects for quantum simulation

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String breaking is a defining feature of non-Abelian gauge theories, yet first-principles studies remain demanding. We investigate this phenomenon in an SU(2) lattice gauge theory in 1+1 dimensions coupled to dynamical fermions, using the loop-string-hadron (LSH) formulation [2], which is equivalent to the Kogut-Susskind Hamiltonian in the physical sector but carries only gauge-invariant, local degrees of freedom and requires imposing only Abelian Gauss's law constraints.

This work reproduces the static string-breaking results of Gupta et al. [1] as an independent validation and extends them to parameter regimes not covered in the original study. Using density matrix renormalization group on lattices of up to 30 sites, we compute the ground-state energy in the presence of static external charges and extract the static potential as a function of charge separation. We identify the breaking distance at which the potential flattens and map its dependence on the gauge coupling and the fermion mass, quantifying truncation and finite-volume effects throughout.

Because the LSH formulation is built from gauge-invariant degrees of freedom, it is a natural starting point for quantum simulation. We outline a qubit encoding of the LSH Hilbert space and discuss the resources required to prepare and measure these static configurations on digital quantum hardware.

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Symmetry-projected coupled-cluster theory for strongly correlated nuclei

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Atomic nuclei are complex quantum many-body systems characterized by rich emergent collective phenomena. Describing these features from first principles requires advanced theoretical tools capable of capturing both strong single-particle correlations and collective degrees of freedom. In this work, we present an *ab initio* framework based on symmetry-broken and restored coupled-cluster (CC) theory to investigate nuclear deformation using inter-nucleon interactions derived from chiral effective field theory [1].

By employing axially and triaxially deformed reference states, the CC formalism efficiently captures static correlations. Rotational symmetry is subsequently restored via angular-momentum projection, enabling a rigorous microscopic description of laboratory-frame observables, including low-lying spectroscopy and enhanced electromagnetic transitions, as currently applied to *sd*-shell nuclei [2, 3]. While recent advances have demonstrated the feasibility of extending coupled-cluster methods to strongly deformed systems [4], these calculations remain computationally demanding and are often restricted to axial symmetry. To circumvent this bottleneck and unlock unexplored mass regions, we leverage symmetry-adapted tensor networks and GPU acceleration. These developments open the door to a systematic and unified treatment of nuclei with complex intrinsic shapes across the nuclear chart, while establishing strong methodological parallels with neighboring fields like quantum chemistry and condensed matter physics [5].

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Symmetries in zero and finite center-of-mass momenta excitons

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We present a symmetry-based framework[1] for the analysis of excitonic states, incorporating both time-reversal and space-group symmetries. We demonstrate the use of time-reversal and space-group symmetries to obtain exciton eigenstates at symmetry-related center-of-mass momenta in the entire Brillouin zone from eigenstates calculated for center-of-mass momenta in the irreducible Brillouin zone. Furthermore, by explicitly calculating the irreducible representations of the little groups, we classify excitons according to their symmetry properties across the Brillouin zone. Using projection operators, we construct symmetry-adapted linear combinations of electron-hole product states, which block-diagonalize the Bethe-Salpeter Equation (BSE) Hamiltonian at both zero and finite exciton center-of-mass momenta. This enables a transparent organization of excitonic states and provides direct access to their degeneracies, selection rules, and symmetry-protected features. As a demonstration, we apply this formalism to monolayer MoS₂, where the classification of excitonic irreducible representations and the block structure of the BSE Hamiltonian show excellent agreement with compatibility relations derived from group theory. Beyond this material-specific example, the framework offers a general and conceptually rigorous approach to the symmetry classification of excitons, enabling significant reductions in computational cost for optical spectra, exciton-phonon interactions, and excitonic band structure calculations across a wide range of materials.

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Self-Consistent Green's Function Simulations of the Isospin Dependence in Infinite Nuclear Matter

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The equation of state (EOS) of infinite nuclear matter is a cornerstone of nuclear many-body theory and provides the microscopic foundation for describing nuclear systems, from finite nuclei to neutron stars [1, 2]. In particular, the dependence of the EOS on the isospin asymmetry impacts a variety of observables like masses of neutron-rich nuclei, collective excitations like the dipole resonances, heavy-ion collisions and the properties of neutron stars as well as neutron star mergers.

Recent advances [3] in the treatment of pairing correlations have opened the possibility of performing ab initio calculations of infinite nuclear matter at arbitrary isospin asymmetry using self-consistent Green's function (SCGF) methods. By means of a numerical implementation of the SCGF equations, we investigate the properties of infinite nuclear matter across the entire range of isospin asymmetries, from SNM to PNM.

Preliminary results exhibit the expected quadratic dependence of the energy per particle on the isospin symmetry, in agreement with the standard parabolic approximation (see Figure 1).

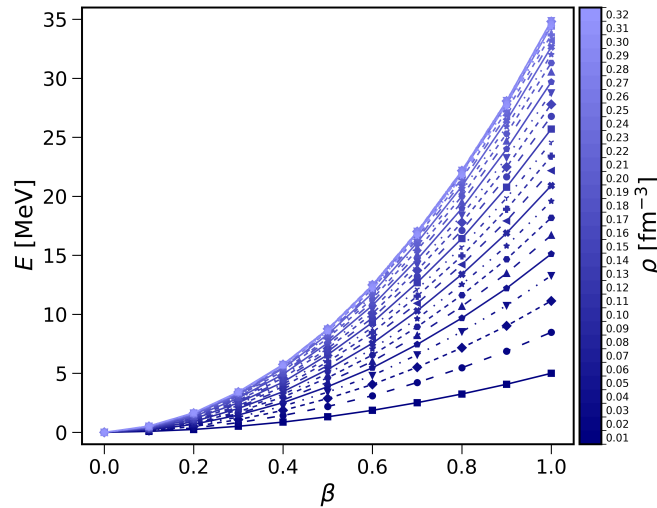


Figure 1: Symmetry energy as a function of the isospin asymmetry parameter β at different densities ρ . The calculations are performed within many-body perturbation theory up to third order, MBPT(3), using the $\text{NNLO}_{\text{sat}}(450)$ nuclear interaction.

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Phonon-induced anyon condensation in open quantum spin liquids

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Dissipative dynamics play a crucial role in the quantum simulation and material realization of exotic states of matter such as quantum spin liquids. In this work, we derive a Lindblad master equation from a phenomenological spin-phonon coupling in Kitaev magnets to study the late-time dynamics of $\mathbb{Z}_2$ and non-Abelian spin liquids coupled to a thermal phonon bath. Using both analytical and numerical techniques, we show that the resulting Lindbladian preserves the static flux excitations of the Kitaev honeycomb model and drives the system toward a nonequilibrium steady state (NESS). Within the representation provided by the Choi–Jamiołkowski isomorphism, we interpret the NESS in terms of anyon condensation associated with the dynamical transition to a steady-state $\mathbb{Z}_2$ spin liquid, and characterize the thermal crossover induced by the phonon-bath temperature. Our work elucidates novel phenomena that can emerge in open quantum spin liquids under realistic dissipative conditions.

Neural Network Quantum States on the Spatial Lattice

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Neural-network quantum states (NQS) have recently emerged as powerful tools for tackling quantum many-body problems by recasting the variational optimization of a many-body wave function as an efficient machine-learning problem [1]. In particular, restricted Boltzmann machines (RBMs) with complex-valued parameters can represent the wave functions of lattice systems in the second-quantization formalism, with each visible node associated with a lattice site. This formulation offers several advantages: fermionic antisymmetry is handled intrinsically, the method is naturally suited to ab initio calculations, and the number of visible nodes is independent of the number of particles, facilitating efficient transfer learning to larger systems. We first tested the expressive power of this approach in few-electron systems by calculating the ground-state energies and spatial configurations of hydrogen, helium, and lithium confined in a box [2]. Our latest work extends the method to nuclear lattice systems [3] through simulations of the deuteron ground state using the Argonne v6' nucleon–nucleon interaction [4]. This proof-of-principle implementation exploits symmetries specific to the two-nucleon system; a natural next step is therefore to generalize the sampling algorithm to many-nucleon systems. Incorporating modern optimization techniques may ultimately provide access to regimes in which traditional methods become computationally prohibitive.

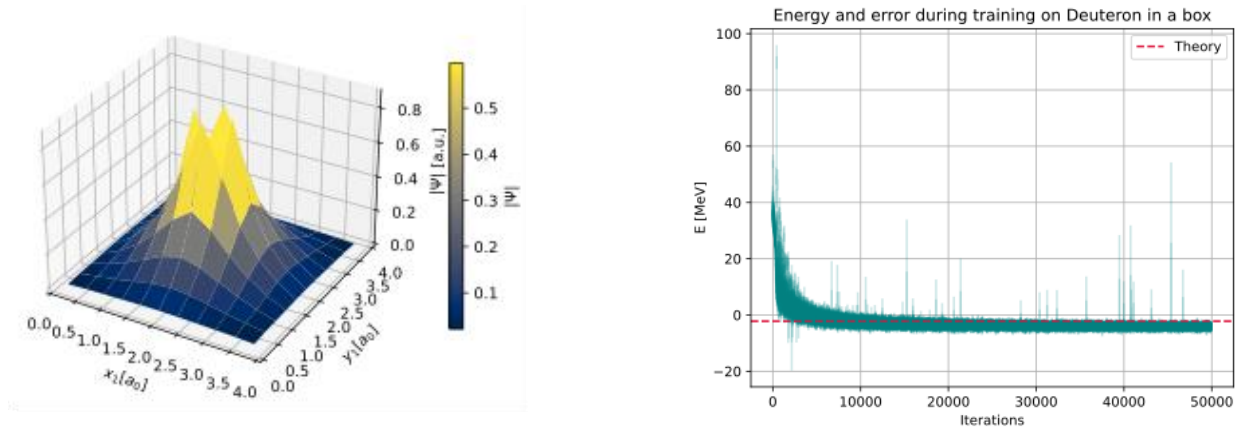


Figure 1: (Left) Motion of two spin-up electrons in the equatorial plane of a Li atom, with the third (spin-down) electron near the atom’s center. (Right) Energy during RBM training for the deuteron.

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Spectral properties of Bose-Fermi mixtures in two dimensions

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Ultracold dilute Bose-Fermi (BF) mixtures are highly tunable and controllable systems, allowing for the investigation of substantially different conditions and quantum effects in matter. In such mixtures with a pairing interaction, one can study the competition between the formation of fermionic composite molecules and the tendency of bosons to condense. One possible application is a recent proposal to obtain a quantum simulator for p -wave superfluidity [1].

In previous work [2], we considered a 2D ultracold Bose-Fermi mixture at $T = 0$. We described the system applying to two dimensions an (imaginary-time) T-matrix many-body approach, which has also been successfully applied to 3D systems [3, 4].

In the present work, we focus on single-particle spectral properties, which could be relevant for future radio-frequency spectroscopy experiments (as done in 3D in [5]). To calculate dynamic quantities, we reformulate our theory for real-time and frequencies. We study the evolution from the (Fermi) polaron regime to the case of a finite concentration of partially condensed bosons. In the literature, the Fermi polaron has been abundantly studied (e.g., in [6]), while the study of a finite bosonic density with arbitrary boson-fermion attraction is almost absent.

In our results, the presence of a finite condensate fraction generates a second dispersion of poles of the T-matrix at negative frequencies (first predicted in 3D mixtures in [7]). The two dispersions show an avoided-crossing behavior and have a hybrid nature between atomic and composite fermion, mediated by the condensate.

In the fermionic spectral weight function, we observe structures at positive frequencies, directly associated with the condensate, and at negative frequencies, associated with the bosonic statistics of the minority species. We also observe the correspondence between the molecular dispersion and the dispersions of poles of the fermionic Green's function (exact for vanishing bosonic density).

For the bosonic spectral weight function, we observe how, at small bosonic concentration, the dispersions of the attractive and repulsive polaronic branches are only slightly modified (but acquire, however, a finite lifetime). Additionally, going from the polaronic case to a finite condensate fraction generates additional structures in the bosonic spectrum, a prediction that could be verified via RF spectroscopy experiments. Finally, considering a finite (weak) BB repulsion, we study how the bosonic Goldstone mode displays a non-trivial dependence on the BF and BB interactions, with a peak in its stiffness at intermediate BF attractions.

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Comparative Many-Body Analysis of Electron Correlation Effects in the Clock Properties of Alkaline-Earth Ions

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We present rigorous first-principles calculations of the clock properties of the singly charged calcium (Ca^+), strontium (Sr^+), and barium (Ba^+) alkaline-earth ions [1]. Using the singles, doubles, and triples approximated relativistic coupled-cluster (RCCSDT) method, we estimate highly accurate scalar and tensor polarizabilities of the ground and metastable $D_{3/2,5/2}$ states of these ions. We also study the correlation effects across various many-body methods, such as the Rayleigh-Schrödinger (RS) and Brillouin-Wigner (BW) many-body perturbation (MP) theories, the random phase approximation (RPA), and the single and double excitation approximated relativistic coupled-cluster method (RCCSD), along with the Dirac-Hartree-Fock (DHF) method (see Figure 1). We further determine the quadrupole moments (Θ) of the metastable states using various many-body methods. Our findings demonstrate that the inclusion of triple excitations is important for achieving high precision in these highly correlated systems. Additionally, we observe a different trend of correlations in the Θ values than an earlier study with respect to orbitals with higher angular momenta [2]. To validate our results, we present energies, lifetimes, and magnetic dipole hyperfine structure constants of the clock states of $^{43}\text{Ca}^+$, $^{87}\text{Sr}^+$, and $^{137}\text{Ba}^+$ ions and compare them with experimental values. Nuclear quadrupole moments of these isotopes are also estimated by combining our calculations with the measured electric quadrupole hyperfine structure constants.

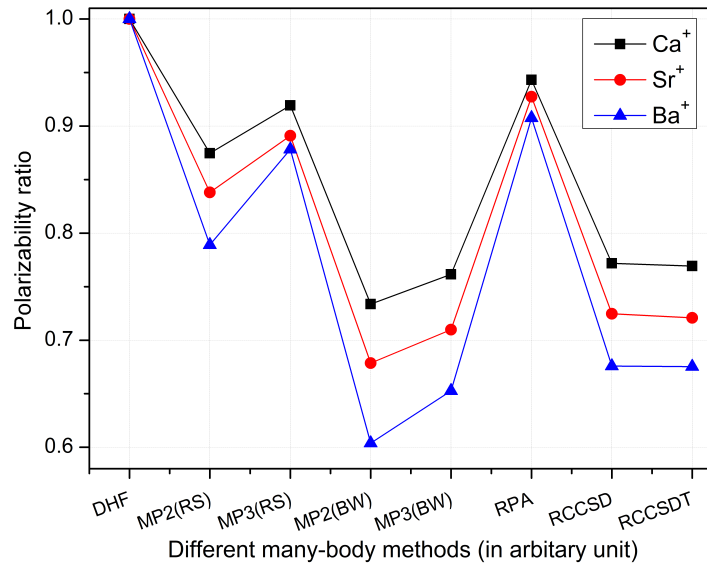


Figure 1: Correlation trend in the electric scalar dipole polarizabilities of the ground states of Ca^+ , Sr^+ , and Ba^+ ions.

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High-precision Estimation of Nuclear and Atomic Properties of $^{229}\text{Th}^{3+}$: A Step Toward Nuclear Chronometers

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We employ the relativistic coupled-cluster (RCC) theory, incorporating singles, doubles, and triples (RCCSDT) excitations, to perform a rigorous assessment of the atomic and nuclear properties of triply ionized Thorium-229 ($^{229}\text{Th}^{3+}$) [1]. The isotope ^{229}Th stands as a sole candidate for nuclear clocks due to its low-lying nuclear isomeric state [2, 3]. Using the RCCSDT method, we report highly accurate values of isotope shift parameters, including field shift and mass shift constants. By combining our theoretical results with experimental data [4], we estimate the differential nuclear charge radii for the $^{232,229}\text{Th}$ and $^{229m,229}\text{Th}$.

We further determine the nuclear magnetic dipole (μ_I) and electric quadrupole moments for both the ground and isomeric states of ^{229}Th and compare them with the available literature (see Figure 1). Additionally, we provide evaluations of electric dipole polarizabilities and hyperfine-induced quadrupole moments, which are critical for characterizing systematic uncertainties and frequency shifts in thorium-based clocks. A significant finding in our analysis is the large contribution from orbitals with higher angular momentum ($l > 6$) and higher-order relativistic effects, which are essential for reaching the accuracy required for next-generation metrology.

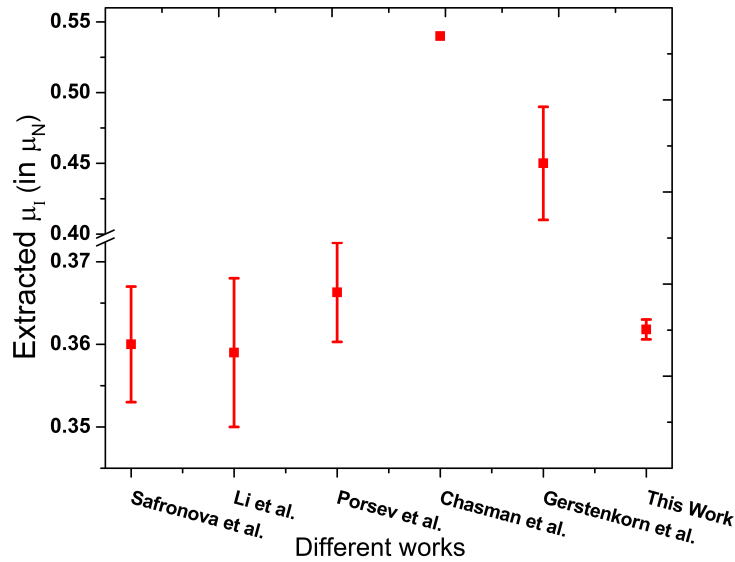


Figure 1: Comparison of μ_I value of the nuclear ground state of ^{229}Th from different works.

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From Hard-Core to Soft-Core Bosons in a Bubble Trap

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A central goal of modern quantum physics is the characterization and understanding of emergent phenomena in many-body systems. This objective is pursued experimentally through several approaches, including ultracold-atom platforms. Among the various strategies available to uncover novel physical behavior, the use of curved trap geometries stands out as particularly powerful, since spatial constraints can deeply alter the collective behavior of many-body systems. A paradigmatic example is provided by a system of identical bosons at low temperature subjected to an external potential mimicking an isotropic bubble trap, which confines the particles to a region of space near a spherical surface. We have employed Path-Integral Monte Carlo (PIMC) simulations and the worm algorithm to investigate the spatial structure, superfluid fraction and exchange-cycle statistics of a system with up to 120 bosons, interacting via the potential $V(r) = c_6/(r_0^6 + r^6)$. In particular, we have explored the crossover from the hard-core to the soft-core regime by varying the core radius r_0 from zero to the radius of the trap. Depending on the number of particles, we observe the system spontaneously organize into 1 to 3 distinct concentric spherical layers. By a proper tuning of the interaction strength c_6 and the quantumness $\lambda = \hbar^2/2m$, we map out the full phase diagram, revealing a rich variety of quantum phases that include bilayer and trilayer insulators and superfluids, as well as cluster crystals and supersolids.

A detailed study on various phases in dissipative anisotropic Dicke model

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We present a comprehensive study of different phases in the Dicke model incorporating both anisotropy and dissipation. We begin with a concise review of the quantum phase transition in this setting, highlighting how these two parameters shift the critical point. We then perform a detailed investigation of the transition from ergodic to nonergodic phases by analyzing the eigenvalue and eigenvector properties of the Liouvillian with the aid of scaling of the Liouvillian gap (Δ) and the average participation ratio. Our results show that the eigenvector properties of the Liouvillian are consistent with its spectral characteristics, leading to a phase diagram that has similarities with the closed counterpart. Furthermore, we demonstrate that the Liouvillian gap exhibits distinct scaling behaviors in these two phases. Finally, we extend our study to the driven case by applying a Thue–Morse quasiperiodic drive. In this case, we find that bosonic dissipation plays a crucial role in stabilizing the prethermal plateau, offering an effective mechanism to halt the heating effect arising from the quasi-periodic drive.

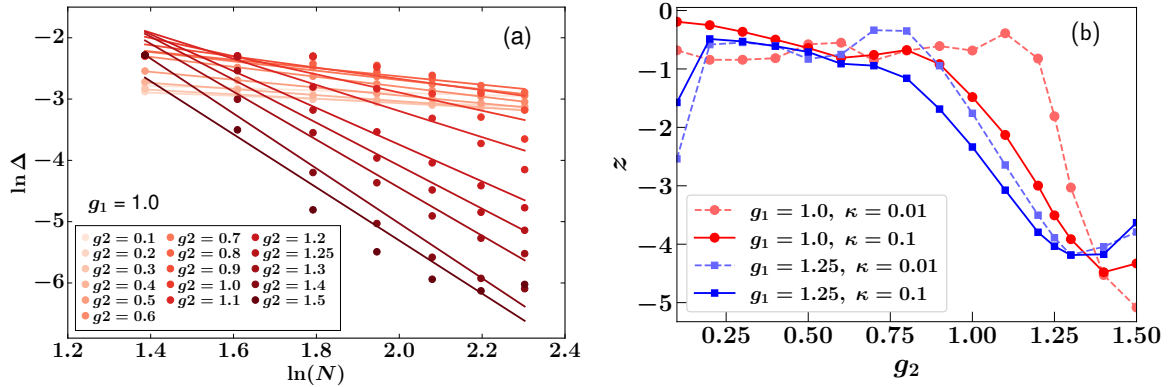


Figure 1: (a) $\ln \Delta$ vs $\ln N$ plot for $g_1 = 1.0$, and $\kappa = 0.1$. (b) The slope z (extracted from the scaling of Liouvillian gap Δ as a function of atom number N) as a function of g_2 for fixed g_1 value, where g_1, g_2 are the anisotropic coupling strengths between spins and bosons. We consider the dissipation strength, $\kappa = 0.1, 0.01$. Here, $n_{\max} = 26$, and the atom number N is changing from 4 – 10. We find that the scaling is different for the ergodic and non-ergodic phases. We also show that for changing κ , the qualitative features of ENET (transition from nonergodic phase to ergodic phase) remain the same.

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Non-stabilizerness and Temporal Entanglement in the Kicked Ising Model

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Quantum many-body systems exhibit rich dynamical phenomena, providing a testbed for exploring new physics and driving the development of theoretical and computational tools. A central challenge is simulating the real-time dynamics of such systems prepared in a non-equilibrium state, a scenario that can be probed in a *quantum quench* [1]. This is generically hard owing to two complementary notions of complexity: entanglement and non-stabilizerness, or magic. Classical methods like tensor networks are limited by the generically linear growth of spatial entanglement with time, making the required computational resources grow exponentially. Transverse contraction methods, such as transverse folding and transverse light-cone contraction, reformulate the problem so that the relevant bottleneck is instead the entanglement of transverse boundary vectors, known as temporal entanglement (TE) [2, 3]. Complementarily, non-stabilizerness quantifies how far a state is from the efficiently classically simulable stabilizer regime, and is therefore relevant to quantum advantage [4]. In this work, we study these notions of computational complexity for the boundary vectors in the kicked Ising model, a minimal Floquet spin chain whose parameter space contains classical limits, integrable regimes, non-integrable dynamics, and a dual-unitary point [5].

Fixing the coupling strength $J = \pi/4$, we scan the parameter space of the longitudinal field h , and the transverse kick strength b . We find that TE is much more structured than the generic volume-law expectation [6, 7]. It is strongly suppressed near the classical limits $b = 0$ and $b = \pi/2$, vanishes exactly at the dual-unitary point $b = \pi/4$ for most product initial states, and is rapidly restored to volume-law growth under infinitesimal detuning from this point. In contrast, changing the longitudinal field h , which controls integrability, mainly modulates the TE scaling rather than changing its qualitative growth. The non-stabilizerness dynamics show a simpler pattern. Across most of the parameter space, it grows approximately linearly in time, with the main qualitative exception again occurring at the dual-unitary point, where it vanishes together with TE. Thus, regimes of low temporal entanglement do not necessarily coincide with regimes of low non-stabilizerness.

Our results identify parameter regimes where transverse contraction remains efficient at long times and show that entanglement-based and magic-based notions of complexity can separate sharply in out-of-equilibrium quantum dynamics.

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Competing orders in many-electron systems: a functional renormalization group perspective

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The renormalization group is an established approach in quantum many-body physics, and this applies especially to one of its modern implementations known as the functional renormalization group (fRG). In particular, the fRG constitutes a flexible and unbiased tool to study competing orders [1, 2]. In this talk, I will outline recent progress in this direction for correlated electron systems. To this end, I will first discuss the competition between antiferromagnetism, charge-density waves and superconductivity in the two-dimensional Hubbard model, thus making a connection with high-temperature superconductors such as cuprates.

A special emphasis will be given to a recent fRG scheme, called the multiloop fRG [3], which has been shown to yield quantitatively accurate results for two-dimensional lattice systems [4, 5]. The special role of a bosonization method, known as the single-boson exchange approach [6], will be highlighted along the way as a means to reduce the numerical cost associated with fRG calculations [5, 7]. I will also show how the fRG can be combined with dynamical mean-field theory to tackle strongly interacting regimes, with a focus on *d*-wave superconductivity [8]. Finally, I will discuss extensions of the multiloop fRG allowing for an efficient treatment of electron-phonon couplings, another relevant development for the description of superconductivity [9].

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Higher-Order Adiabatic Elimination in Atom-Cavity Systems: Its Impact on Spin-Squeezing Generation

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Adiabatic elimination is a model reduction technique that can be applied to bipartite quantum systems whenever the dynamics of the two components have a timescale separation. Since the dimension of the Hilbert space is the product of the dimensions of the two subsystems, the dynamics of the lower-dimensional model describing the slow degrees of freedom after the transient of the fast ones is typically more tractable with both analytical and numerical methods. This is in particular the case for open quantum many-body systems where the main computational challenge is the doubly exponential growth of the dimension of the density operator with the system size. A perturbative expansion in the timescale separation can provide approximate slow-variable models involving induced dissipation at various orders, with higher orders becoming relevant in cases where high-precision quantum control is involved [1].

As a relevant example of such a situation, we consider the generation of spin-squeezed states via dispersive coupling of two-level atoms to an optical cavity. Spin-squeezed states are metrologically useful quantum states where structured entanglement allows for enhanced sensing with respect to the standard quantum limit. Relevant aspects are both the efficient preparation of spin-squeezed states and the scalability of estimation precision with the number N of probes. Recently, it was shown that increasing the atom-cavity coupling can be detrimental to spin-squeezing generation, an effect that is not appreciated in the standard second-order cavity removal approximation [2]. We describe adiabatic elimination techniques to derive an effective Lindblad master equation up to third order for the atomic degrees of freedom. We then show through numerical simulations that the spin-squeezing scalability loss is correctly reproduced by the reduced open system dynamics, pinpointing the relevant role of higher order contributions. Furthermore, we conjecture an extension beyond leading order of the adiabatic elimination technique to the case of conditional dynamics under quantum non-demolition continuous measurement and fast cavity loss, whose reliability is again confirmed by numerical simulation of the dynamics and the corresponding behavior of spin squeezing as a function of N [3].

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Static Response of the Strongly Coupled Electron Gas from Diffusion Monte Carlo

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The static local field factor $G(q)$ of the three-dimensional homogeneous electron gas is a direct measure of exchange-correlation effects, yet accurate ground-state benchmark data have been absent in the strongly coupled regime for three decades. Using diffusion Monte Carlo (DMC), we present calculations of $G(q)$ and the static density-density response function $\chi(q)$ across the liquid phase, up to the vicinity of Wigner crystallization. We find a pronounced nonmonotonic structure in $G(q)$ at intermediate wave vectors, whose amplitude grows with r_s , and identify it as a fingerprint of short-range order in the electron liquid, simultaneously reflected in the static structure factor $S(q)$ and in a pronounced peak of the real-space kernel $f_{xc}(r)$ as the crystallization is approached. Finally, we provide a parametrization of $G(q)$, valid up to $r_s = 100$, which yields a well-defined collective mode that survives inside the particle-hole continuum with a roton-like minimum, and is consistent with the low-energy excitonic mode found in recent Bethe-Salpeter calculations.

Performance and Dynamics of an Ultracold Atomic Superfluid as a Quantum Engine Working Fluid

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Bose-Einstein condensation is a ubiquitous phenomenon, present across a multitude of physical scales, from coherence among some thousands of atoms, to macroscopic superfluidity in liquid helium, up to theorised superfluid-superconducting neutrons and protons responsible for observed glitches in neutron stars. At all of these scales, questions persist around the subject of non-equilibrium dynamics, turbulence, and dissipation, to which the quantum, non-linear nature of superfluidity introduce mechanisms and features intractable by classical approaches. Remarkably, since the inaugural achievement of Bose-Einstein condensation in an ultracold atomic gas in 1995, atomic superfluids have rapidly developed into a highly controllable and flexible platform to probe ever more diverse and complex superfluid phenomena. One system which was fundamental to the study of equilibrium, non-equilibrium, driven-response and dissipative dynamics of fluids in the development of classical thermodynamics, is the engine. Recently, we have seen atomic superfluid experiments demonstrate the feasibility of constructing an engine system in a real laboratory system. Inspired by the work of Simmons et al^[1], in collaboration with experimentalists at Aarhus University we present an investigation of a quantum engine, with a 39K atomic superfluid as the working fluid. We demonstrate efficiency and power performance characteristics subject to variations in compression and interaction strength ratio, as well as finite temperature. We note the rapid convergence of this system to its reversible limit efficiency in finite duration cycles, as well as a novel driving regime which allows simultaneous maximisation of efficiency and power of the cycle.

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Non-perturbative computation of thermal conductivity based on Path Integral Monte Carlo methods

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The calculation of thermal conductivity in insulating solids at temperatures below the Debye temperature is problematic, due to the breakdown of classical and semi-classical approaches. In this work, we present a fully non-perturbative quantum methodology to compute thermal conductivity based on Path Integral Monte Carlo (PIMC) simulations combined with the Green-Kubo linear response theory. The method is applied to rare gas solids modeled by a Lennard-Jones potential, paradigmatic systems where quantum effects strongly affect both thermodynamic and transport properties. From PIMC simulations, we obtain the temperature-dependent phonon frequencies, lifetimes, and specific heat. From the imaginary time correlations of the energy current, we extract the thermal transport coefficients based on a physically motivated prior. We show that the experimentally observed increase of the thermal conductivity of argon and neon at low temperatures cannot be explained within a Peierls-Boltzmann framework using phonon line-widths at equilibrium. In contrast, a distinct transport lifetime emerges from the analysis of heat-current correlations. Our results demonstrate that quantum Monte Carlo methods provide a robust, non-perturbative framework to investigate heat transport in insulating solids, beyond the limits of classical molecular dynamics without relying on perturbative or semi-classical approximations.

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Oscillator–Qubit Compilation for Pre-Born–Oppenheimer Molecular Dynamics via Near-Optimal Trigonometric Gate Synthesis

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Molecular dynamics beyond the Born–Oppenheimer approximation is a coupled electron–nuclear many-body problem, and hybrid oscillator–qubit processors are naturally suited to it: the Ha–MacDonell coupled multi-qubit–boson (cMQB) mapping [1] encodes electrons in qubits and carries nuclei directly in bosonic modes. Gaussian and conditional-Gaussian operations are native, while a time step’s cost concentrates in the non-Gaussian phase gates and their Pauli-controlled rotations; we treat this as a finite-precision channel-formation problem with an explicit cost model.

The core method is a Jacobi–Anger oscillator–qubit generalized quantum signal processing (JA-OQ-GQSP) synthesis [2] of the trigonometric phase gates $\exp[-i\Lambda \cos(\boldsymbol{\mu} \cdot \hat{\mathbf{Q}} + \phi)]$ that appear in the trigonometric-gate-implemented Fourier synthesis (TGIFS) representation of anharmonic potentials [3]; here $\hat{\mathbf{Q}}$ collects the mode position quadratures $\hat{Q} = (\hat{a} + \hat{a}^\dagger)/\sqrt{2}$, $\boldsymbol{\mu}$ is an integer Fourier index, ϕ a phase, and Λ the gate angle, set by the TGIFS Fourier coefficients. A Jacobi–Anger expansion gives an OQ-GQSP query degree $K = O(|\Lambda| + \log(1/\varepsilon)/\log \log(e^e/\varepsilon))$ at target precision ε —the near-optimal QSP scaling—against $O(\Lambda^2/\varepsilon)$ for a first-order small-angle implementation. The same construction handles gates conditioned on an electronic Pauli string at unchanged degree, giving a compilation strategy for the smooth position-dependent cMQB terms. Position encodings with qubits could simulate conditional-Gaussian gates efficiently [4], so any advantage is representational rather than intrinsic to the non-Gaussianity of bosons.

We evaluate the resulting inner-synthesis cost for molecular models that require multi-state, multivariate, anharmonic bosonic phase gates, typically with sparse Fourier structure. At fixed Fourier or ridge support, the construction reduces the number of inner synthesis queries by four to five orders of magnitude relative to a first-order small-angle implementation. These estimates are compared with native oscillator–qubit primitives, position-encoded qubit simulations [4], and classical MCTDH/tensor-network descriptions as separate reference formulations.

The result identifies a concrete regime in which oscillator-native continuous-variable structure changes the compilation cost of molecular many-body dynamics: the Gaussian and conditional-Gaussian parts remain native, while the dominant non-Gaussian trigonometric gates admit near-optimal signal-query synthesis. This provides a resource benchmark for assessing when hybrid oscillator–qubit encodings offer a genuine representational advantage for pre-Born–Oppenheimer quantum dynamics.

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Probability Fluxes and Speed Limit in Thermal and Quantum Annealing

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Simulated annealing provide heuristic solutions to combinatorial optimization problems. In this approach, the cost function of the problem is mapped onto the energy function of a many-body system, with the goal of guiding the system toward its ground state, that is, the optimal solution. During the time evolution of the system, fluctuations are initially set strong and then gradually weakened over time, thereby promoting exploration of the state space while preventing the system from becoming trapped in local energy minima, and ultimately driving the system toward the global energy minimum. Previous studies [1, 2] have extensively debated the differences between thermal and quantum fluctuations in the annealing process. Nevertheless, a fundamental understanding of difference between them has yet to be established, and it remains unclear how and for which problems quantum annealing achieves an advantage over thermal annealing. Here we investigated the many-body dynamics under thermal and quantum annealing across all possible interaction networks of the $\pm J$ model with up to seven Ising spins [3]. As a result, we found that performance differences between thermal and quantum annealing emerge for certain specific interaction network structures. This indicates that thermal and quantum annealing can be distinguished depending on the structure of the energy landscape. Furthermore, examining the behavior of probability fluxes in state space reveals that while thermal and quantum annealing exhibit globally similar behavior, there exist qualitative differences attributable to quantum tunneling. Additionally, investigating the speed limits [4] of magnetization (order parameters) computed from the probability fluxes shows that quantum annealing can surpass the speed limits found in thermal annealing, and that the order parameter evolves at a rate close to the speed limit in almost all cases. With the recent technological advances in cold atom experiments, our results can be experimentally verified in the various platforms [5].

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Toward Engineering Superfluid Dynamics: On-Demand Stable Vortex Rings in BECs

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Understanding vortex dynamics in three-dimensional superfluid systems emerges as a key challenge. While vortex generation and evolution are well studied in two dimensions, the three-dimensional case remains only partially explored. Our work [1] aims to numerically investigate three-dimensional vortex ring dynamics and to develop experimentally reproducible methods for generating, manipulating and characterising vortex rings in harmonically trapped cylindrical Bose–Einstein condensates.

We exploit moving repulsive laser-sheet barriers that locally constrict the superflow to achieve controlled vortex ring nucleation and propagation in the condensate. We then investigate the rings dynamics and assess how it is affected by the barrier parameters. Given the symmetry of the system, we propose and validate the use of cylindrical coordinates to simulate the condensate dynamics: this framework effectively reduces the three-dimensional problem to a two-dimensional problem, leading to significant advantages in computational time while preserving an accurate physical description.

We carry out an energetic analysis throughout the vortex ring generation process and during its propagation in the system to gain insight into the microscopic physics underlying the nucleation mechanism. We also present a preliminary analysis of vortex ring nucleation and dynamics when employing attractive laser-sheet barriers. Moreover, by exploiting additional optical local potentials that break the cylindrical symmetry, we trigger destabilisation of previously formed vortex rings.

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The Caldeira-Leggett model in the NMR context

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In this project, we explore different semiclassical methods, and how they can be applied to study the impact of a surrounding environment on nuclear spin relaxation and various nuclear magnetic resonance (NMR) phenomena. Of particular interest has been the application and adaption of the Caldeira-Leggett formalism [1], in order to simulate line broadening effects in NMR spectra. We do this by utilizing the ideas of Meyer & Miller [2] and others [3], by treating the real and complex parts of the complex coefficients associated with the quantum spin states as classical variables. This makes it easier to rationalize the coupling between the spin degree of freedom and the classical harmonic oscillators of the surrounding environment. On the contrary to how the Caldeira-Leggett formalism or the “Spin-Boson [4] model” is usually used, i.e. to model the impact of the environment on the transition and tunneling between discrete energy states, a large part of our adaptations for simulating line broadening effects instead focus on how it can be used to model dephasing of the coherence associated with an ensemble of spins. Our numerical simulation results, show how the model introduce a line broadening effect in simulated NMR spectra, and how broadening increases with longer correlation times of the surrounding environment, in line with existing relaxation theories of NMR. These are results that show promise, and with some further improvements and details worked out concerning thermodynamical properties of the oscillators of the environment, the methods can be useful alternatives for modeling relaxation within the field of NMR.

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Weighted Hartree-Fock-Bogoliubov method for interacting fermions: An application to ultracold Fermi superfluids

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For several decades it has been known that divergences arise in the ground-state energy and chemical potential of unitary superfluids, where the scattering length diverges, due to particle-hole scattering. Leading textbooks [1, 2] and research articles [3] recognize that there are serious issues but ignore them due to the lack of an approach that can regularize these divergences.

In this presentation, we find a solution to this difficulty by proposing a general method, called the weighted Hartree-Fock-Bogoliubov theory, to handle multiple decomposition channels originating from the same interaction [4]. We distribute the interaction in weighted channels determined by minimization of the action, and we apply this idea to unpolarized Fermi superfluids. Using our method, we solve a long-standing difficulty in the partitioning of the interaction into Hartree, Fock, and Bogoliubov channels for Fermi superfluids, and we obtain a phase diagram at the saddle-point level, which contains multichannel nonperturbative corrections. In particular, we find a previously overlooked superfluid phase for weak interactions, which is dominated by particle-hole processes, in addition to the usual superfluid phase only containing particle-particle physics.

We emphasize that our method is so general, that it can be applied to any fermionic system that can support competing interaction channels. This includes systems from particle and nuclear physics, condensed matter physics, ultracold atoms, and even in astrophysical objects like the crusts of neutron stars [5].

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Search for BSM Boson via Precision Atomic Studies

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Precision isotope shift (IS) spectroscopy is a sensitive probe of physics beyond the Standard Model (BSM), where nonlinearities (NLs) in King's plots can signal new interactions. We present a relativistic many-body analysis of higher-order NL effects in low-lying transitions of Ca^+ , focusing on constraints on a hypothetical electron–neutron interaction mediated by a BSM boson. The corresponding potential is (in atomic units) [1]

$$V_{PS} = (-1)^{s+1} \alpha_{NP} c \frac{e^{-m_\phi r/c}}{r}, \quad (1)$$

with $\alpha_{NP} = (-1)^{s+1} \frac{\gamma_e \gamma_n}{4\pi c}$.

In standard IS theory, an atomic transition is dominated by the mass shift (MS) and field shift (FS), which factorize into isotope- and transition-dependent parts, leading to a linear relation between differential isotope shifts of two transitions known as the King's plot relation. Deviations from this linearity can arise from both BSM boson exchange and SM effects; therefore, unambiguous identification of BSM signals requires precise control of all SM-induced NLs. A generalized form of the King's plot equation that incorporates nonlinear contributions is given by [4, 5]

$$\begin{aligned} \delta \nu_a^{AA'} \simeq & \left[K_{ab} \mu^{AA'} + F_{ab} \delta \nu_b^{AA'} \right] + G_{ab}^{(4)} \delta \langle r^4 \rangle_{AA'} + \left(G_{ab}^{(2)} + F_{ab}^{(2)} \right) \left(\delta \langle r^2 \rangle^2 \right)^{AA'} \\ & + K_{ab}^{(2)} \tilde{\mu}^{AA'} + (A - A') D_{ab} \alpha_{NP}. \end{aligned} \quad (2)$$

Here, $G^{(2)}$, $G^{(4)}$, $F^{(2)}$, and $K^{(2)}$ characterize higher-order SM contributions to the NL, while D represents the BSM contribution. To assess their interplay, we determine bounds on α_{NP} in two cases: Case I, neglecting SM-induced NLs, and Case II, including them explicitly. We find that accounting for SM NLs significantly relaxes the constraint on the electron–neutron coupling, from $\alpha_{NP} < 7.9 \times 10^{-11}$ in Case I to $\alpha_{NP} < 5.9 \times 10^{-10}$ in Case II, underscoring the importance of properly incorporating SM nonlinearities in precision isotope-shift analyses.

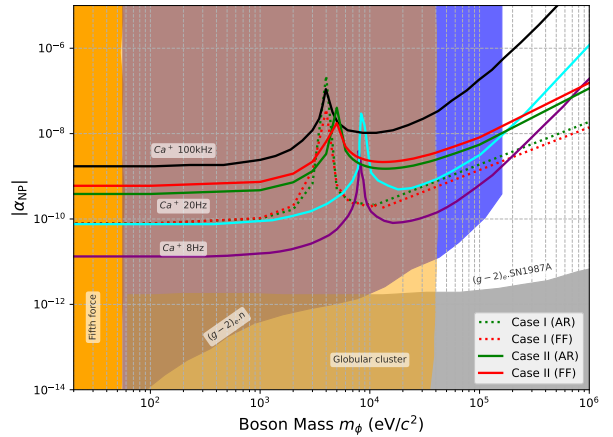


Figure 1: Demonstrating α_{NP} variation with m_ϕ [6].

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Breathing and quadrupole oscillation modes of squeezed ^{39}K Bose-Bose liquid drops

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We investigate the lowest breathing and quadrupole oscillation modes of binary ^{39}K ultradilute droplets confined in one dimension by a strong harmonic potential. The confinement reduces the critical number of particles needed to sustain a self-bound state by reducing a three-dimensional problem to the quasi-two-dimensional regime. [1] Collective excitation modes, such as breathing and quadrupole oscillations, are particularly useful probes of droplet properties since their frequencies are highly sensitive to changes in the energy and geometry of the system. As a consequence, they can provide insight into beyond-LHY physics.

We use the density functional constructed from first-principles quantum Monte Carlo calculations (QMC) [2], which incorporates the effects of the finite interaction range. This system is highly tunable via Feshbach resonances, therefore our analysis is performed for three magnetic field strengths. Increasing the magnetic field weakens the interspecies attraction, leading to significantly lower oscillation frequencies. Additionally, our analysis reveals that stronger confinement significantly lowers both the frequencies and the critical atom number required for a stable droplet. While the quadrupole mode exhibits greater stability in smaller droplets, the breathing mode shows a more pronounced dependence on the confinement strength. The differences between the QMC and MF+LHY results are comparable to those in previously studied unconfined spherical droplets [3], which indicates important beyond-LHY contributions.

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Fault-Tolerant Quantum Computing for Nuclear Physics

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Simulating complex nuclei can be challenging, since the dimension of most nuclear problems grows exponentially with the number of nucleons. One approach to solving the nuclear many-body Schrödinger equation is to use an Effective Field Theory (EFT) as it only focuses on relevant low-energy degrees of freedom. However even then, the Hilbert space can grow large as the order of the EFT is increased, requiring a new approach to solve it.

Quantum computing is an emergent technology that works fundamentally in a different way to normal computers. While quantum computers currently suffer from noise and errors, there is much promise that they will become fault-tolerant. Quantum computers make use of a fundamental unit of information, the qubit. Since the corresponding Hilbert space grows exponentially with the number of qubits growing linearly, using quantum computing to model nuclei can be a naturally advantageous approach.

We demonstrate the pion-less EFT at leading order on a lattice. We explain how the relevant Hamiltonian can be expressed in the language of the quantum computer, using qubits. We solve the nuclear many-body Schrödinger equation on a quantum computer by simulating a selection of fault-tolerant quantum algorithms. Our results show that quantum computing is a hopeful method for simulating complex nuclei.

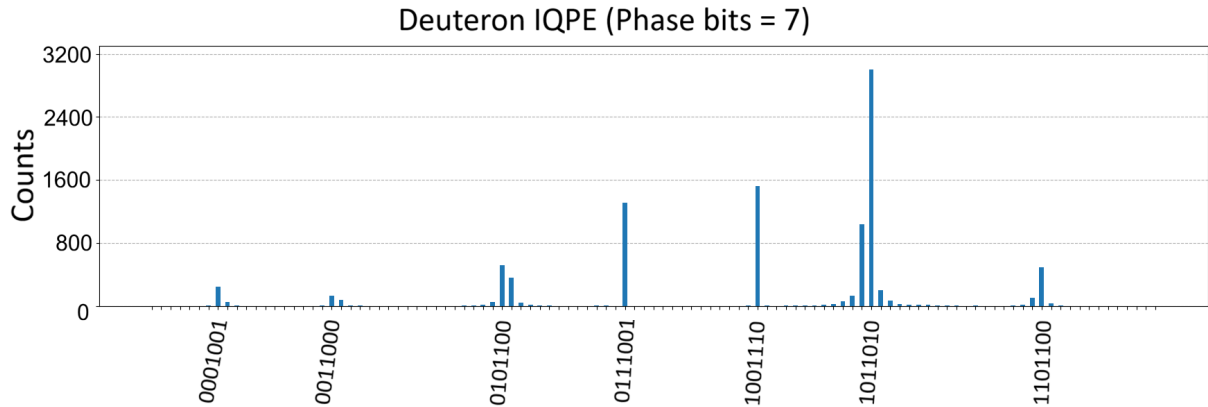


Figure 1: The Iterative Quantum Phase Estimation Algorithm (IQPE) is used to recover the eigenspectra of nuclei by recycling one ancilla qubit.

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Monolayer silicene grown on Ag₂X surface alloys (X=Sn, Ge, Sb, Pb and Bi): A first-principles study

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Silicene is a two-dimensional honeycomb allotrope of silicon, attracting interest for its graphene-like electronic properties and potential as a platform for low-dimensional quantum transport, spin- and valley-dependent phenomena, topological states, and silicon-compatible quantum technologies.¹⁻² Silver (111) is one of the most studied substrates for growing monolayer silicene. Specifically, the formation of various silicene reconstructions (4×4 , $\sqrt{13}\times\sqrt{13}R13.9^\circ$ type I and II, $2\sqrt{3}\times 2\sqrt{3}R30^\circ$, and others) has been observed³⁻⁵, yielding to polycrystalline samples, which in turn introduces scattering centers for charge carriers.

It is instead crucial to synthesize large-scale, misorientation-free single crystals of monolayer silicene. Previous experiments have demonstrated that monolayer silicene of nearly isolated form, with a sample size of the cm² scale, can be successfully grown on Ag₂Sn/Ag(111) via molecular beam epitaxy (MBE)⁶. This process has been well-supported by theoretical calculations⁴, highlighting the potential of a decoupled silicene layer on a single-element-decorated Ag(111) surface.

We extend these studies and explore the feasibility of forming monolayer silicene on Ag₂X surface alloys on Ag(111), where X represents different doping elements (Sn, Ge, Sb, Pb, and Bi). Based on density functional theory (DFT) as implemented in Quantum Espresso software, we examine the equilibrium adsorption structures, silicene buckling, adsorption energies, charge transfer, and electronic properties of silicene on Ag₂X/Ag(111) substrates.

We considered three types of silicene superstructures, namely (4×4 , $\sqrt{13}\times\sqrt{13}$, and $\sqrt{3}\times\sqrt{3}$)¹⁻³, that require different superlattices of Ag(111) ($4\sqrt{3}\times 4\sqrt{3}$, $\sqrt{39}\times\sqrt{39}$, and $2\sqrt{3}\times 2\sqrt{3}$). Our results show that the buckling increases with doping, following the order: Ge, Sb(Sn), Pb, and Bi. Regarding the strength of the Si-substrate interaction, the trend is approximately reversed. These findings suggest that silicene on Bi, Sb, and Pb-doped superlattices is more feasible to form decoupled silicene compared to that on Sn- and Ge-doped superlattices.

Furthermore, charge transfer analysis reveals that for Sn-doped superlattices, minimal charge transfer occurs from silicene to the substrate, while for Ge-doped systems, the charge transfer is considerably larger yet still smaller than on pristine Ag(111). Finally, we investigated the electronic structures of silicene upon adsorption on the Ag₂X/Ag(111) substrates.

Our study offers valuable insights that could guide experimental efforts in the synthesis of high-quality, decoupled silicene monolayers, which are essential for the advancement of future nanoelectronic devices based on this material.

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Generator Coordinate Method with Symmetry-Restored HFB basis: Theoretical Framework and Results

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The Generator Coordinate Method (GCM), utilizing symmetry-restored basis sets, is a crucial technique for performing large-scale realistic shell model calculations. Its effectiveness has been previously demonstrated in works such as Ref. [1, 2], where the Hartree-Fock (HF) basis with angular momentum projection was employed. Although transitioning to the Hartree-Fock-Bogoliubov (HFB) basis with angular momentum projection represents the logical next step, this advancement was initially hindered by a notorious sign-determination problem encountered when evaluating norm overlap using the Ohnishi formula [3, 4]. This issue stemmed from the double-coverness inherent in the HFB transformation and was finally solved with the Pfaffian method by L. M. Robledo [5], leading to subsequent deep theoretical developments [6]. Based upon this foundation, we developed the GCM based on the HFB basis with angular momentum projection [7, 8], making no assumption regarding nuclear shape. In this contribution, we discuss its theoretical framework.

Using this symmetry-restored HFB-GCM, we have successfully investigated several aspects of nuclear structure. In our recent work, we explored the concept of the Quantum Critical Point (QCP) in nuclear structures [9]. This idea was initially introduced using the Interacting Boson Model (IBM) by F. Iachello et al. [10], which described critical-point symmetries such as E(5) and X(5). Since IBM is fundamentally a boson model of collective nuclear motion, investigating this concept within the fermionic framework of the shell model represents an important theoretical extension. For this purpose, the HFB-GCM approach proves highly advantageous because it is rooted in mean-field theory and accurately predicts precise spectroscopic quantities. By using this method, we found a phase diagram—analogue to the extended Casten triangle—derived using two quasi-SU(3) quadrupole coupling parameters. This diagram maps out phase boundaries, revealing energy spectra associated with various symmetries, including the dynamical symmetries U(5), O(6), and SU(3), as well as the critical-point symmetries E(5) and X(5). In this contribution, we explore the phase diagram presented herein, detailing both its underlying physics and the resulting shape phase transitions.

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W and Dicke states engineering using optimal control in neutral atoms qubit arrays

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Motivated by a compelling need for time-efficient and robust schemes for quantum-state engineering in systems of neutral atoms in optical tweezers, we consider a ring-shaped array of qubits with nearest-neighbor Ising-type (zz) coupling and transverse (x and y) global control fields. This system to a large extent mimics – outside of the Rydberg-blockade regime – a circular array of neutral atoms coupled through van-der-Waals type interaction. We investigate the preparation of W and Dicke states in this system starting from the default initial state $|00 \dots 0\rangle$ using two different optimal-control approaches: (i) NMR-like pulse sequence, which consists of instantaneous (delta-shaped) control- and Ising-interaction pulses, and (ii) time-dependent control scheme, which entails shaped control pulses in the presence of always-on Ising interaction between adjacent qubits. By making use of the underlying dihedral symmetry of this system – which allows one to use a symmetry-adapted computational basis with $O(2^N/N)$ states in an N -qubit system – and utilizing suitable global-optimization methods, we find optimal sequences of pulses for realizing W and Dicke states within both approaches. In addition, we demonstrate robustness of these sequences against unavoidable control errors. Finally, using typical values of parameters in realistic Rydberg-atom systems, we show that our control schemes enable the preparation of the desired multiqubit states on time scales much shorter than the relevant coherence times of those systems.

Strong-coupling properties of Fermi superfluidity in the BCS-rashbon BEC crossover

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Since the experimental realization of synthetic Raman-type spin-orbit coupling (SOC) in ultracold atomic gases[1], spin-orbit coupled quantum gases have attracted much attention as a controllable platform for studying unconventional pairing and strong-coupling phenomena. So far, the experimentally realized SOC in cold atoms has mainly been one-dimensional Raman-type SOC. On the other hand, higher-dimensional Rashba-type SOC, whose experimental realization is still an important challenge, has been theoretically predicted to cause more dramatic effects on Fermi superfluidity. In particular, two- and three-dimensional Rashba-type SOC can enhance two-body bound-state formation and drive a crossover from a BCS superfluid to a Bose-Einstein condensate (BEC) of rashbons, even when the bare attraction is weak [2]. A characteristic feature of rashbons is that their effective mass becomes larger than twice the mass of a constituent Fermi atom, which is expected to modify low-energy collective dynamics as well as thermodynamic properties.

In this work, we theoretically investigate the specific heat at constant volume, C_V , of a three-dimensional Fermi superfluid with a tunable Rashba-type SOC. Pairing fluctuations associated with rashbon formation are included within the Nozières-Schmitt-Rink strong-coupling theory [3]. Since the low-temperature specific heat in the superfluid phase is governed by the gapless Goldstone mode in the ordinary BCS-BEC crossover [4], we use C_V as a thermodynamic probe of rashbon collective excitations in the BCS–rashbon BEC crossover.

We show that, in the strong-SOC regime, the collective-mode contribution to C_V is strongly affected by the enhanced rashbon effective mass. The heavier rashbon mass reduces the collective-mode velocity and thereby amplifies the low-temperature specific heat compared with the case of tightly bound molecules with mass $2m$. Furthermore, by analyzing the temperature-dependent power law of C_V , we identify three characteristic temperature regimes. At sufficiently low temperatures, C_V is dominated by linearly dispersing rashbon collective excitations. At higher temperatures, thermally excited collective modes probe the nonlinear part of the rashbon dispersion, leading to an apparent power-law behavior different from that expected from a purely linear mode. In the crossover region closer to the BCS side, fermionic quasiparticle excitations also give a sizable contribution, reflecting the competition between collective and single-particle excitations.

These results demonstrate that the specific heat is not merely a bulk thermodynamic quantity, but a useful diagnostic of the excitation hierarchy in spin-orbit coupled Fermi superfluids. In particular, C_V reveals how the heavy effective mass and nonlinear collective dispersion of rashbons emerge across the BCS–rashbon BEC crossover.

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Critical currents across the UFG-BCS Crossover in ring fermionic superfluids

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Understanding superfluid transport in ring geometries is central to a wide range of systems, from superconducting circuits and quantum technologies to neutron star interiors. In these contexts, persistent currents provide a direct probe of macroscopic phase coherence, and identifying the mechanisms that limit their stability—namely, the critical currents—is of fundamental importance [1]. Ultracold atomic gases offer a highly controllable platform to investigate superfluid transport, particularly in toroidal traps where persistent currents emerge with quantized circulation set by the winding number. Here, using the time-dependent superfluid local density approximation (TDSLDA) [2], we demonstrate that even in the absence of external impurities [3], two distinct critical winding-number (current) thresholds arise. The first corresponds to pair breaking, leading to a mixed superfluid–normal state, while the second marks the complete suppression of superfluid order, leaving only a normal fluid. The latter represents the analogue of the depairing current in superconductors and connects to the physics of gapless superfluids relevant for neutron star matter. We further show how these two critical currents depend on interaction strength across the crossover from the strongly interacting unitary Fermi gas (UFG) to the weak-coupling BCS regime, with the BCS limit exhibiting the lowest critical values. The intermediate mixed phase is dynamically unstable and evolves into an array of quantized vortices, whose number depends on both the interaction regime and the initially imprinted winding number. These results provide a unified picture of current-induced instabilities in fermionic superfluids and clarify the microscopic origin of critical currents across interaction regimes.

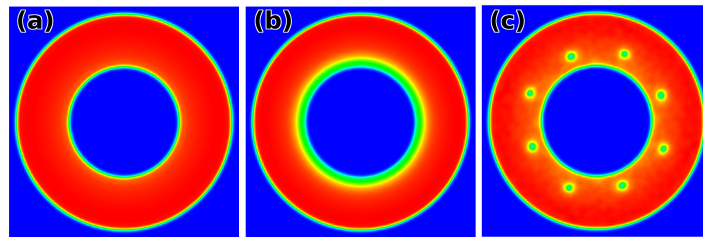


Figure 1: Order parameter amplitude in the strongly interacting unitary Fermi gas limit. (a) Static, homogeneous order parameter amplitude for winding number (persistent current) below the pair-breaking critical current, showing a stable uniform superfluid state. (b) Static order parameter amplitude once the winding number exceeds the pair-breaking critical current, showing the onset of spatial inhomogeneity. (c) Time evolution of the order parameter amplitude for the same parameters as in (b), showing the system relaxing from the unstable mixed superfluid–normal configuration into an array of quantized vortices.

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Dark excitons signature in the infrared transient absorption of MoS₂ monolayer

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Dark excitons constitute a large fraction of the excitonic landscape of two-dimensional transition-metal dichalcogenides, but their optical characterization remains challenging because they cannot be directly coupled to the ground state by conventional linear spectroscopy.[1, 2] Here we present a fully ab initio framework for time-resolved transient absorption based on the *GW* approximation and the Bethe–Salpeter equation. The method extends previous developments by including excitons with finite center-of-mass momentum and treating intraband contributions in a gauge-consistent fashion. We apply it to monolayer MoS₂ and investigate the optical response following exciton relaxation. Our calculations show that the transient absorption spectrum cannot be explained solely by transitions originating from the zero-momentum bright A_{1s} exciton. At finite effective temperatures, dark excitons and finite-momentum states around the Γ , K , M , and Q valleys become thermally populated and jointly shape the spectrum. At 300 K, the calculated response reproduces the main relative structures observed experimentally[3]. A state- and symmetry-resolved decomposition assigns the main peaks to optically allowed transitions from A_{1s}^{*} excitons toward higher A_{2p}^{*}-, A_{3p}^{*}-, and B_{2p}^{*}-like states. These results demonstrate that time-resolved intra-excitonic absorption provides a sensitive optical probe of dark excitons and establish a predictive framework for interpreting their complex nonequilibrium spectra.

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Dynamics of vortices in spatially modulated superfluids

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Superfluids may exhibit spatial density modulations either because of an external potential or because the system is in a supersolid state. This is a topic of current interest, for instance, in the field of cold atoms. We have investigated bosonic systems, studying how the dynamics of a single vortex and of a vortex dipole is modified with respect to their behavior in a uniform superfluid.

We consider ^{87}Rb bosons at $T = 0$ K in a flat geometry under the influence of an external periodic potential, using Gross-Pitaevskii theory [1]. A single vortex excitation has an energy that depends on the position of its core. This energy is lowest where the density is minimal; hence, the equilibrium positions of a vortex coincide with the maxima of the external potential.

In a uniform superfluid, a vortex dipole, namely a pair of vortices with opposite chirality, is a stable excitation that moves with constant velocity. This is no longer true in a modulated superfluid. For a two-dimensional modulation, where the equilibrium positions of the vortices are isolated points, the vortices move mainly by jumping between equilibrium sites and approach each other until they annihilate within a short time. Since our theory includes neither thermal nor stochastic effects, these jumps are manifestations of vortex tunneling between equilibrium sites. This dynamics is very similar to that of a vortex dipole in a supersolid.

In the case of a one-dimensional modulation, where parallel density ridges are present, the equilibrium positions of a vortex are localized in the channels between ridges. The dynamics of the dipole depends on the positions of the two vortices. If they are in the same channel, the vortices approach each other until they annihilate within a short time. If they are in distinct channels, the dipole undergoes translation, with a velocity that depends on the intensity of the external potential and can even change sign with respect to the uniform-superfluid case. Superimposed on this translation, an oscillatory transverse motion is also present. This transverse motion is one-sided, in the sense that the vortex cores never cross the equilibrium positions nearest to their starting positions.

In the presence of a circular trap, an off-center single vortex undergoes uniform circular motion around the trap center. Also in this case, the vortex dynamics is quite different when a one-dimensional modulation is present: the motion is a superposition of translation along a channel and oscillation. This oscillatory motion can be either longitudinal, i.e., along the ridge, or transverse to it, depending on the geometry and on the initial state. In all cases, the transverse oscillatory motion is one-sided.

In conclusion, a vortex dipole can be a short-lived excitation in a spatially modulated superfluid, and a peculiar one-sided oscillatory motion can occur both for a single vortex and for a dipole.

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Bose Hubbard model in a synthetic magnetic field and restricted geometry

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The Bose Hubbard model accurately describes ultracold bosonic atoms in optical lattices, which present themselves as a clean and highly tunable platform for quantum simulation. Despite the apparent simplicity of the Hamiltonian, the Bose Hubbard model is not analytically solvable, and numerical simulations become intractable when including features like non-zero temperatures or the presence of gauge fields, unless the system is too small. The Quantum Rotor Approach (QRA) makes use of a coherent path integral formalism and an approximation consisting of the relaxation of the unimodularity of a complex field into an average unimodularity across the lattice for obtaining closed form expressions for observables and critical lines, while still taking into account the geometry of the system. In this work we make use of the QRA to study the Bose Hubbard model in the presence of a magnetic field and restricted geometry. This allows us to explore possible incompressible states, reminiscent of Fractional Quantum Hall states, that appear around the first Mott lobe at specific fillings in competition with the superfluid, without the limitations of numerical simulations on the size of the system, as well as the possibility of including thermal effects [1].

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Beyond equal time correlations in driven-dissipative many-body systems : a generic cumulant expansion scheme

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The cumulant expansion method is a powerful framework for studying the dynamics of many-body open quantum systems, providing both computational efficiency and physical insight. In this presentation, I will introduce a generalized approach for calculating unequal-time correlation functions that extends the conventional cumulant expansion formalism. A central component of this framework is a novel ansatz that enables the implementation of the quantum regression theorem within the cumulant expansion setting. Building on this idea, I will present a hybrid cumulant scheme that efficiently combines different orders of cumulant expansions for distinct stages of the time evolution.

The method is applied to cascaded optical systems as shown below (Fig. 1). where it is used to compute many-body correlation functions. Results will be compared with exact numerical simulations as well as available experimental observations. Finally, I will discuss the regimes in which the approach provides accurate predictions, highlight its computational advantages, and examine its limitations and potential directions for future development [1].

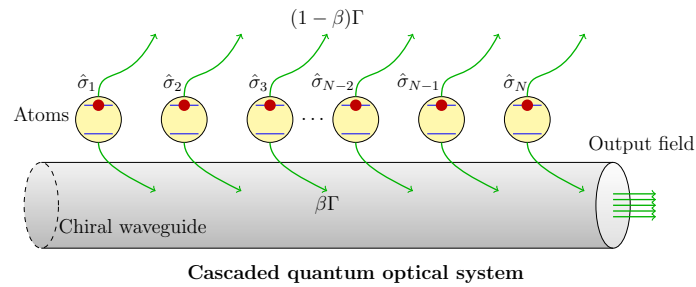


Figure 1: A pictorial depiction of a cascaded quantum system is given here. Non-interacting atoms are trapped in a 1D chiral waveguide and initially prepared in their excited state. Γ is the total emission rate. $\beta\Gamma$ is the emission rate to the wave-guide. Free emission rate is $(1 - \beta)\Gamma$.

- [1] **In preparation:** Unequal time correlations from cumulant expansion scheme in driven-dissipative many-body systems, Saha *et al.*

Efficient solution of nuclear DFT calculations in 3D space

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The solution of the three-dimensional Schrödinger equations for large systems, without any symmetry, requires efficient and robust numerical algorithms due to the large-scale nature of the resulting eigenvalue problem. Conventional methods suffer from slow convergence and require careful tuning depending on the spatial discretization. Conjugate gradient methods have been proposed [1] to accelerate the convergence of symmetry-unrestricted calculations based on the Skyrme energy density functional, widely used in nuclear structure, together with the use of suitable preconditioning of the problem. In this work, we introduce the generalized conjugate gradient method [2] for the self-consistent solution of the Hartree–Fock–Bogoliubov equations. The performance of the proposed algorithm is demonstrated on representative nuclear systems, showing improved convergence speed compared to standard approaches. The method is also successfully applied to study superheavy exotic systems, without spatial symmetry assumptions.

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Adaptive quantum dynamics with the time-dependent variational Monte Carlo method

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Describing the dynamics of quantum many-body systems is a formidable problem in contemporary physics. Understanding these dynamics is crucial for characterizing non-equilibrium phenomena and for the development of quantum technologies. The simulation of such systems with variational methods is a promising yet challenging task, especially in regimes where highly expressive ansätze lead to numerical instabilities. We introduce an extension of the time-dependent variational Monte Carlo (tVMC) method [1] that adaptively controls the expressivity of the variational quantum state during the dynamics. Our adaptive tVMC (atVMC) [2] approach addresses the ill-conditioned equations of motion arising in overparameterized regimes by selectively evolving only the most relevant parameters at each time step. Relevance is quantified through the local-in-time error (LITE), which measures the deviation between variational and exact evolution, using only quantities already available in standard tVMC simulations. We benchmark the method on quantum quenches in the one-dimensional transverse-field Ising model using both spin-Jastrow and restricted Boltzmann machine wave functions. The adaptive scheme significantly improves numerical stability and reduces the need for strong regularization, enabling reliable simulations with highly expressive variational ansätze.

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Two-dimensional system of antidipoles in single and bilayer geometries

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We study a system of particles interacting through an inverted dipolar interaction [1] in a two-dimensional geometry, both in a single as well as a bilayer configuration. We consider zero temperature and employ the Diffusion Monte Carlo method to study the equilibrium properties of this many-body system. The inverted dipolar interaction is achievable in current state of the art experiments by rapidly rotating the magnetic field applied to a system of dipolar atoms [1], like ^{164}Dy , or in experiments of microwave-dressed polar molecules [2]. For a single layer geometry, we characterize the equation of state of the infinite, two-dimensional system for different interaction parameters. At low densities, the system shows liquid properties, while at higher densities it transitions to a crystal phase through a first order phase transition. Remarkably, it does so at a considerably lower density than its dipolar counterpart. In the bilayer geometry, we focus on the liquid phase and characterize the effect of one layer in the equilibrium properties of the other (energy per particle, superfluidity and condensate fraction). We observe inter-layer influence in all these properties.

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Effect of Methylation on Positron Binding in Pyridine and Benzene Related Molecules

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Low-energy positron interactions with atoms and molecules are characterised by strong many-body correlations, including target polarisation (in which molecular electrons are excited above the molecular ground state), virtual positronium formation (in which an excited molecular electron tunnels to the positron), and repulsive positron-hole interactions. They have an overwhelming effect, modifying scattering properties, enhancing annihilation rates, and enabling and enhancing positron binding [1].

A powerful theoretical approach that enables the ab initio description of positron binding in molecules is many-body theory. It was recently developed in our group and implemented in our Gaussian-basis code EXCITON+ [1]. It gave the first ab initio calculations of positron binding in molecules (including non-polar molecules) in agreement with pioneering experiments by the UCSD experimental (Surko) group [2]. It has provided fundamental insight, including on the role of pi bonds [1] and their competition with dipole moments [2], effects of halogenation of hydrocarbons [3], and predictions of positronic bonding in new classes of anions [4]. We have also developed the approach to calculate the continuum processes of positron scattering and annihilation [5], including the Doppler broadened gamma ray spectra [6].

Here, in joint theoretical-experimental work, we present measured (via the Surko buffer gas trap) and many-body theory calculated positron binding energies in three classes of molecules: methylated pyridines (picolines), dimethylated pyridines (lutidines) and dimethylated benzenes (xylenes). Very good agreement is obtained between experiment and theory, and insight on e.g., the effect of methylation provided. For example, we observe that a single methyl substitution increases the binding energy by 30-50 meV relative to the parent molecule. In xylenes, variation in positron binding among positional isomers is insignificant. However, for methylated pyridines containing nitrogen, positron binding increases the farther methyl groups are positioned from the nitrogen.

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Combining Matrix Product States and Mean-Field theory to Capture Magnetic Order in Quasi-1D Strongly Correlated Materials

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Strongly correlated materials remain challenging for conventional electronic structure methods. While density functional theory (DFT) often fails to capture the correct many-body physics, accurate post-Hartree-Fock methods become prohibitively expensive for realistic solids. We combine density functional theory (DFT), constrained random phase approximation (cRPA), and tensor-network (TN) methods to investigate quasi-one-dimensional cuprate chains. Starting from DFT, maximally localized Wannier functions and cRPA are used to construct effective one-band Hubbard models, which are then solved using matrix product states (MPS) [1, 2].

We apply this approach to the quasi-1D cuprates Ca_2CuO_3 , Sr_2CuO_3 , SrBaCuO_3 , and Ba_2CuO_3 . A purely one-dimensional (1D) treatment gives only very weak staggered magnetization (M_s), reflecting the strong quantum fluctuations in one dimension [2]. To include the residual three-dimensional coupling present in real materials, we treat the interchain interactions self-consistently at the mean-field (MF) level while keeping the intrachain physics described by MPS [2]. This MPS + MF framework stabilizes larger finite staggered magnetizations and reproduces the experimentally observed magnetic order [2]. By comparing different cuprate compounds, we find that the magnitude of the ordered moment is determined by both the interchain exchange coupling and the underlying intrachain Hubbard parameters.

These results establish a direct connection between *ab initio* Hubbard parameters and measurable magnetic order in quasi-one-dimensional cuprates, demonstrating how downfolding, TN, and MF theory can be combined to study realistic strongly correlated materials [2]. In future work, this MPS + MF description can be directly compared with fully two-dimensional TN approaches such as infinite projected entangled-pair states (iPEPS).

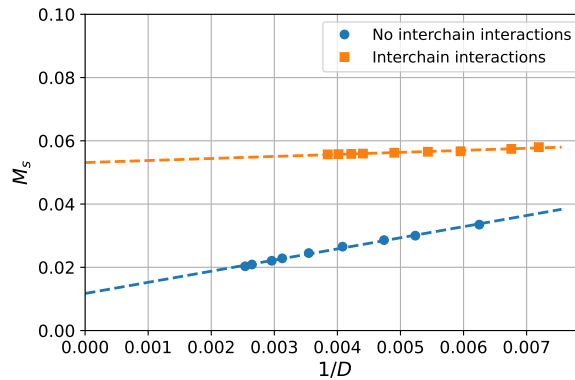


Figure 1: The staggered magnetization M_s as a function of the inverse bond dimension $1/D$ for Sr_2CuO_3 , shown with and without interchain interactions.

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Ab Initio Study of Three-Component Bose Mixtures

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We investigate the effects of adding few impurity atoms to an ultracold self-bound heterogeneous Bose mixture composed of ^{41}K and ^{87}Rb , a realization of a three-component Bose mixture. The impurity atoms of ^{41}K in a different hyperfine state are immersed in a self-bound ^{41}K - ^{87}Rb Bose mixture. We construct interaction potential models that match chosen scattering lengths and effective ranges [1, 2]. Using an ab initio diffusion Monte Carlo (DMC) simulations with pure estimators, we study the microscopic properties of the impurities across different interaction regimes, focusing on the interplay between impurity localization and droplet stability.

The heteronuclear K-Rb platform is particularly appealing because of the mass imbalance and experimentally accessible Feshbach resonances, which enable a fine tuning of interactions. Self-bound states of the bosonic mixture ^{41}K - ^{87}Rb have been observed [3], both in free space and in an optical waveguide. Previous studies investigated one impurity in heteronuclear K-Rb mixtures using Bogoliubov and eGPE/LHY approaches, predicting center- and surface-localized impurity states [2], while independent diffusion Monte Carlo studies of pure K-Rb droplets revealed significant beyond-LHY and finite-range effects [1].

Building on these results, we perform a fully microscopic DMC study of hyperfine-state impurities embedded in a self-bound K-Rb quantum droplet, focusing on impurity localization, binding, and correlation effects beyond mean-field and perturbative descriptions.

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Dimensionality of a strongly interacting 2D-3D mixed-dimensional Fermi gas

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We theoretically investigate the BCS-type superfluid transition in a mixed dimensional Fermi gas with a tunable s -wave pairing interaction, ranging from the 3D-3D case to the 2D-3D limit. Including strong pairing fluctuations within the framework of the self-consistent T -matrix approximation (SCTMA), we numerically determine the superfluid phase transition temperature T_c as a function of the interaction strength and the dimensional imbalance (a solid line in Fig.1)[1]. We show that T_c always vanishes in the 2D-3D limit, irrespective of the interaction strength: In the weak-coupling regime, the vanishing T_c is simply due to the mismatch of the 2D and 3D Fermi surfaces. In the strong-coupling regime where the mean field approximation (MFA) gives non-zero T_c (a dashed line in Fig. 1)[2], on the other hand, the suppression of T_c is found to reflect the 2D character of 2D-3D mixed dimensional pairing fluctuations: In spite of the existence of 3D component, the essence of this vanishing T_c in this regime is found to be the same as the Hohenberg-Mermin-Wagner theorem[3] discussed in low-dimensional Fermi superfluids.

In our poster presentation, we explain the reason why the 3D component in a 2D-3D mixture cannot stabilize the superfluid long-range order at all, in contrast to the ordinary 3D-3D Fermi superfluids. We also show that 3D character of a 2D-3D mixture appears in the pseudogap phenomenon.

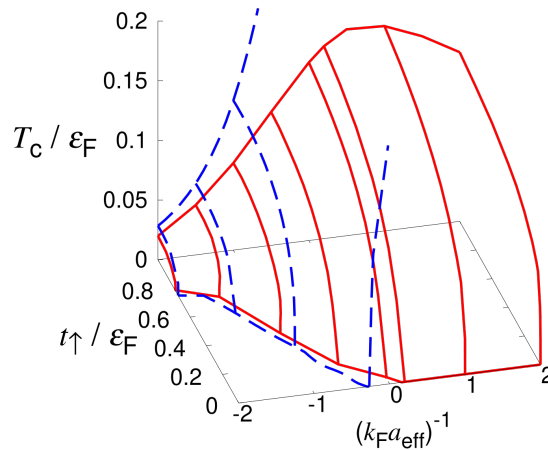


Fig.1. SCTMA result for T_c in a mixed-dimensional Fermi gas (a solid line)[1] and MFA result for comparison (a dashed line). The interaction strength is measured in terms of the inverse scattering $(k_F a_{\text{eff}})^{-1}$, being normalized by the Fermi wavelength. $t_{\uparrow} / \epsilon_F$ is a hopping parameter normalized by the Fermi energy, which tunes the system from a 3D-3D mixture ($t_{\uparrow} / \epsilon_F = 1$) to the 2D-3D limit ($t_{\uparrow} / \epsilon_F = 0$).

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Hybrid-order topology and $\mathbb{Z}_2$ -like bipolar localization in a periodically driven higher-order insulator

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The interplay between periodic driving and crystalline symmetry offers a powerful route to engineer topological phases inaccessible in static systems. We demonstrate this in the context of the Benalcazar-Bernevig-Hughes (BBH) model [1], a prototypical higher-order insulator that hosts zero-dimensional corner modes protected by a $\mathbb{Z}_2$ gauge structure and a projective $\mathcal{PT}$ symmetry. We show that a suitable Floquet protocol fundamentally reshapes the symmetry classification of this model: the drive effectively transmutes the spinless BBH model into one with spinful-like properties, dynamically inducing first-order edge topology while preserving the higher-order corner mode structure. The result is a hybrid-order topological phase in which the dispersive edge states and the localized corner modes coexist at distinct quasi-energies, a phase unfamiliar in the static counterpart. Extending the framework to the non-Hermitian regime via non-reciprocal hopping, we find that this drive-induced spinful character manifests as a $\mathbb{Z}_2$ -like skin effect, characterized by a unipolar-to-bipolar localization transition of eigenstates. Further, to restore the bulk-boundary correspondence in this driven non-Hermitian scenario, we construct a seemingly challenging generalized Brillouin zone theory via a symmetry-reduced mapping to an effective one-dimensional problem, from which non-Bloch topological invariants correctly capture both higher-order topology and localization transitions. Our results establish periodic driving as a versatile and controllable handle for engineering a rare confluence of higher-order topology, symmetry transmutation, and non-Hermitian skin physics beyond the equilibrium setting.

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Optimizing Energy in Tensor Network Simulations with Clifford Transformations

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Tensor network methods like density matrix renormalization group (DMRG) struggle in highly entangled regimes, such as systems with periodic boundary conditions (PBC), long-range interactions, or higher dimensions, where the required bond dimension quickly becomes computationally unfeasible. To overcome this limitation, we introduce an approach that integrates the stabilizer formalism directly into the DMRG algorithm. While previous methods have used Clifford unitaries to minimize ground-state entanglement, our framework optimizes Clifford transformations of the Hamiltonian to directly minimize the state's energy. We benchmark our method against standard DMRG at fixed bond dimensions on three challenging systems: the one- and two-dimensional transverse-field Ising models with PBC at the critical point and the one-dimensional long-range Ising model.

Neural Network Quantum States for Fractional Quantum Hall Physics in the High-Flux Regime of the Bose–Hofstadter Model

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In this project, we study the phase diagram of the paradigmatic Hofstadter model [1]. We focus on interacting bosons on a square lattice, with periodic boundary conditions, in the presence of a uniform perpendicular magnetic field.

In the low magnetic flux regime, energy bands are nearly dispersionless, mimicking continuum Landau levels. In this regime, the continuum Laughlin wave function on the torus [2] provides an accurate approximation even for the lattice ground state [3].

As the magnetic flux increases, lattice effects become prominent, causing bands to acquire significant dispersion and rendering continuum-based models unreliable. This high-flux regime remains relatively unexplored and may host interesting physics, as non-flat topological bands have a characteristic energy scale that competes with the interaction scale.

To address both regimes, we employ Neural Network Quantum States (NNQS) [4]. We demonstrate that continuum Laughlin states on the torus admit an exact mapping to a simple neural-network wave function. Despite this exact representability, we find that optimization remains challenging, consistent with other recent studies [5, 6]. We attribute these difficulties to the limited ability of standard neural-network architectures to capture magnetic representations of lattice symmetry transformations. To overcome this issue, we explicitly restore magnetic translational symmetries via quantum-number projection.

We then optimize the neural-network wave function and benchmark its accuracy against exact diagonalization results, finding reliable performance across both low- and high-flux regimes. Furthermore, the use of quantum-number projectors enables access to excited states and thus to the momentum-resolved excitation spectrum. Using these tools, we investigate the possible emergence of phase transitions from Laughlin-type topological states to charge-density-wave phases, as the interaction strength is varied.

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Combining Downfolding Techniques and Tensor Networks for Strongly Correlated Materials

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Strongly correlated materials challenge standard electronic structure methods such as DFT and Hartree-Fock, which often fail to capture essential many-body physics. We present a framework that combines downfolding techniques with tensor network methods to achieve accurate, first-principles descriptions of such materials [1]. Starting from a DFT calculation, maximally localized Wannier functions define a low-energy target space, and the constrained random phase approximation (cRPA) yields screened Coulomb interaction parameters, producing an effective multiband Hubbard model (Fig. 1). This model is solved with tensor networks, giving systematic control over accuracy through the bond dimension. We benchmark the approach on *trans*-polyacetylene, polythiophene, and the quasi-1D charge-transfer insulator Sr_2CuO_3 , finding band gaps in quantitative agreement with GW, EOM-CCSD, and experiment [1]. We further study three-body interactions on top of the Hubbard model and find that in certain parameter regimes they contribute significantly to the electronic structure. Ongoing work focuses on extracting these terms for real materials via a novel Schrieffer–Wolff-based downfolding procedure.

Since purely 1D systems cannot sustain long-range magnetic order, we developed an extended chain mean-field theory (CMFT) in which frustrating interchain couplings are treated at the mean-field level while intrachain physics is solved exactly with matrix product states [2, 3]. This yields a rich phase diagram of different magnetic phases, and correctly reproduces the magnetic order of the cuprate Li_2CuO_2 . Looking ahead, we are extending the framework to quasi-1D metal–organic frameworks (Fe-MOF-74, MIL-53(V)) and to two-dimensional systems using infinite projected entangled-pair states (iPEPS).

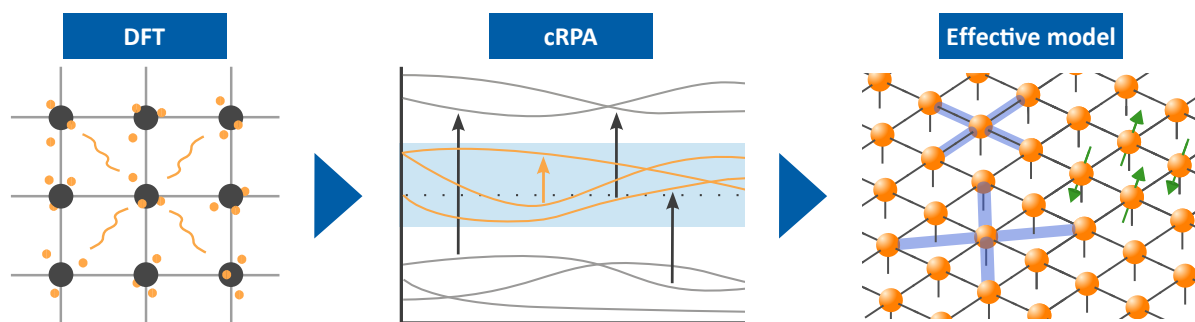


Figure 1: The downfolding procedure (left to right): initial DFT band structure, cRPA screening of the low-energy subspace, effective Hubbard model solved with tensor networks.

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COMPASS: An Adaptive Biorthogonal Neural Quantum State Framework to Non-Hermitian Many-Body Systems

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Non-Hermitian (NH) quantum systems have emerged as a powerful framework for describing open quantum systems, non-equilibrium dynamics, and engineered quantum optical materials. However, solving the ground-state properties of NH systems is challenging due to the exponential scaling of the Hilbert space, and exotic phenomena such as the emergence of exceptional points. Another challenge arises from the limitations of traditional methods like exact diagonalization (ED). For the past decade, neural networks (NN) have shown promise in approximating many-body wavefunctions, yet their application to NH systems remains largely unexplored. In our previous work [1] we showed that this class of systems especially parity-time (PT)-symmetric ones where also solvable via NN. In this work, we introduce a complementary optimization framework for progressive adaptive state search (COMPASS) based on biorthogonal adaptive recurrent neural quantum states. Our approach combines an adaptive autoregressive architecture with a biorthogonal variational Monte Carlo scheme as well as a complementary optimization scheme that alternates adiabatically between energy and variance minimization. This enables the stable convergence to ground-state eigenpairs with high fidelity, while avoiding Markov chain sampling through exact autoregressive generation. We demonstrate that for PT -symmetric Hamiltonians, unconstrained complex ansätze can spontaneously break PT symmetry during optimization—even in the unbroken phase—leading to spurious imaginary energies. Real-valued ansätze in an appropriate basis, on the other hand, naturally constrain the optimization to the correct physical manifold. Conversely, for generic non-Hermitian (NH) Hamiltonians without symmetry protection and complex spectra, complex ansätze are essential for accurately capturing complex ground-state properties. Our results establish that physically-informed ansatz selection is crucial for reliable NH simulations. By combining adaptive architectures, biorthogonal optimization, and symmetry-aware modeling, this framework enables a direct study of 1D and 2D NH many-body systems without Hermitian embeddings or adiabatic continuation.

[1] L. Wah, R. Zen, & F. K. Kunst, *Physical Review Research*, 7(4), 043291 (2025).

Impurity Tuning of Superflow Dissipation in Inhomogeneous Fermionic Rings

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Understanding superflow dissipation in inhomogeneous superfluids underlies key phenomena in superconductors, neutron star crusts, and superfluid helium. Ring-trapped ultracold fermionic gases provide an ideal platform to probe quantized persistent currents set by the winding number.

Using time-dependent density functional theory[1], we show how impurity density and size tune the balance between pair breaking and vortex dynamics [2], the primary dissipation channels of persistent currents in fermionic rings [3]. Below the vortex-emission critical winding w_c , denser or larger impurities enhance pair breaking, dissipating flow energy without changing the winding number, in contrast to clean rings. Above w_c , vortex–impurity interactions--set by impurity spacing, size, coherence length, and flow velocity--produce distinct mobility regimes [Fig. 1]: deflected trajectories, individual or collective pinning, and inter-site tunneling. These regimes shift the dominant dissipation mechanism from pair breaking plus mobile vortices at low impurity densities to mainly pair breaking at higher densities. Impurity size further governs the dependence of w_c on impurity density: small impurities render w_c density-independent, while large ones increase it toward the clean-ring pair-breaking limit. This impurity engineering enables precise control of superfluid transport, informs the design of atomtronic devices and superconducting systems, and offers insight into vortex dynamics in neutron star crusts relevant to pulsar glitches.

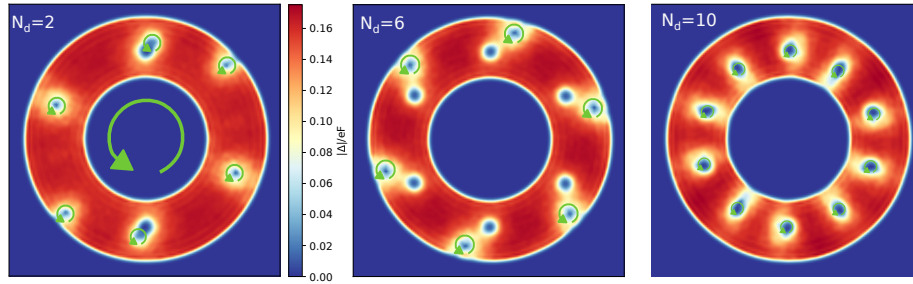


Figure 1: Magnitude of the pairing field $|\Delta(x, y)|$ ($w_0 = 7$, different impurity number N_d) showing the distinct vortex mobility regimes: individual pinning, deflected trajectories and collective vortex pinning. Swirling arrows: imposed flow and vortices positions.

[1] Aurel Bulgac et al., “The Unitary Fermi Gas: From Monte Carlo to Density Functionals,” in *The BCS-BEC Crossover and the Unitary Fermi Gas*, Lecture Notes in Physics, edited by Wilhelm Zwerger (Springer, Berlin, Heidelberg, 2012) pp. 305–373

[2] B. Tüzemen, et al, arXiv:2510.24309 (2025).

[3] K. Xhani et al., Phys. Rev. Research 7, 013225 (2025)

Density functional theory based on functional renormalization group

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The functional renormalization group (FRG) is a theoretical framework for analyzing strongly coupled and strongly correlated many-body systems, and it has been applied across a wide range of fields, from condensed-matter physics to statistical physics and high-energy physics. In FRG, the renormalization-group flow of a system is expressed in terms of exact and closed functional differential equations (FDEs), based on which nonperturbative approximations are constructed.

The idea of applying FRG to density functional theory (DFT) to determine the energy density functional (EDF)—the quantity that ultimately determines the accuracy of DFT calculations—was proposed by Polonyi, Sailer, and Schwenk [1,2]. Within this framework, an FDE for determining the EDF is derived, and in principle, the EDF can be obtained by solving this equation. However, methods for solving the FDE have not yet been established, and ongoing research explores how far FRG can be practically used to determine the EDF. To date, we have implemented calculations based on vertex-function expansions, namely Taylor expansions around a target density. In particular, we have achieved the numerical construction of EDFs within the local density approximation for electronic systems [3–5], as well as applications to classical liquids, including three-dimensional Lennard–Jones liquids [6,7].

In this talk, we explain the FRG and its application to DFT, and present case studies of this approach, including applications to electronic systems.

- [1] J. Polonyi and K. Sailer, *Phys. Rev. B* **66**, 155113 (2002).
- [2] A. Schwenk and J. Polonyi, arXiv:nucl-th/0403011 (2004).
- [3] T. Yokota and T. Naito, *Phys. Rev. B* **99**, 115106 (2019).
- [4] T. Yokota and T. Naito, *Phys. Rev. Research* **3**, L012015 (2021).
- [5] T. Yokota and T. Naito, *Phys. Rev. B* **105**, 035105 (2022).
- [6] T. Yokota, J. Haruyama, and O. Sugino, *Phys. Rev. E* **104**, 014124 (2021).
- [7] T. Yokota, J. Haruyama, and O. Sugino, *Phys. Rev. E* **113**, 014124 (2026).

Quantum and classical correlations in the multi-orbital Hubbard model

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While the single-band Fermi-Hubbard model captures paradigmatic strongly correlated phenomena, from superconductivity and magnetism to the Mott transition, multi-band extensions are required whenever orbital degrees of freedom and Hund's couplings become relevant, as in correlated materials and multi-flavor cold-atom settings. In this context, "orbital" refers to electronic orbitals residing on the same site, while "flavors" indicates distinct fermionic species residing either on the same orbital or on different ones.

In this regard, recent advances have shown that in the single-band Hubbard model, as well as in its $SU(N)$ generalization with N flavors per site, quantum entanglement between fermionic flavors on the same site must be absent, due to symmetry constraints on the single-site reduced density matrix[1, 2]. Consequently, all local inter-flavor correlations are necessarily classical, and are quantified by *non-Gaussianity*, namely the distance from the closest uncorrelated (Gaussian) state.

In this talk, I will show how this remarkable feature persists in the multi-orbital Hubbard-Kanamori model, thereby excluding local inter-flavor entanglement in a broad class of materials and cold atom platforms. Using non-local extensions of Dynamical Mean Field Theory (DMFT), I will further show how quantum correlations between fermionic orbitals can emerge both locally and non-locally in the form of entanglement and non-Gaussianity. Our findings further imply the absence of local *non-stabilizerness*[3], ruling out local "quantumness" in Hubbard-like models, and provide a general framework for the characterization of quantum resources in interacting fermionic systems.

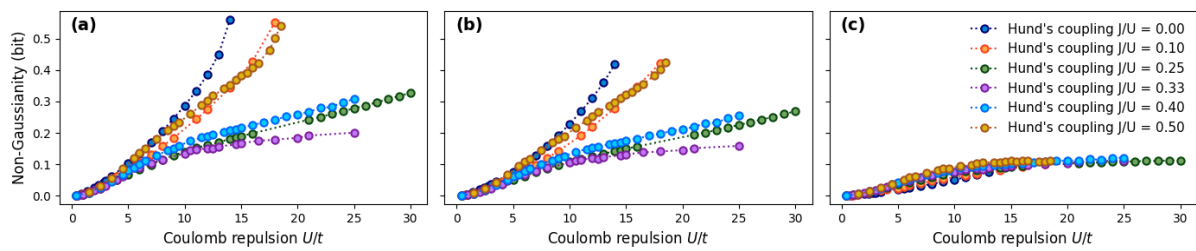


Figure 1: (a) Inter-site, (b) inter-orbital, and (c) inter-flavor non-Gaussianity in the two-bands Hubbard-Kanamori model, solved with cluster DMFT.

[1] G. Bellomia *et al.*, Physical Review B 113 (15), 155158 (2026).

[2] E. Zavatti *et al.*, arXiv preprint 2512.03689 (2025).

[3] E. Zavatti *et al.*, arXiv preprint 2605.18494 (2026).

Dynamics of magic and entanglement in the quantum Ising model: a variational Monte Carlo study

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The dynamics of quantum resources in strongly correlated many-body systems provide valuable insights into the emergence and propagation of quantum correlations. While entanglement, which characterizes nonclassical correlations between subsystems, has been extensively studied in this context, much less is known about the dynamical evolution of *magic*, or nonstabilizerness. Magic quantifies a distinct form of quantum complexity and is closely connected to the classical simulability of quantum states [1].

In this work, we investigate the dynamics of magic and entanglement in the transverse field Ising model, in one and two spatial dimensions. We focus on *open subsystems* embedded in the lattice, and characterize the resulting mixed states with the robustness of magic [1] and the entanglement negativity [2]. This allows us to study the emergence and spreading of these quantities across different spatial scales.

Using time-dependent variational Monte Carlo [3], we access the dynamics of quantum resources in higher-dimensional systems. We characterize their emergence following quenches in the transverse field, and establish the notion of *mutual magic* [4] as a crucial quantity for assessing the spatial distribution of nonstabilizerness. Comparing it with entanglement between subsystems, we find that the latter retains a predominantly short-range character, while magic exhibits a richer and more extended spreading during the time evolution.

[1] M. Howard and E. T. Campbell, "Application of a resource theory for magic states to fault-tolerant quantum computing", Phys. Rev. Lett. **118**, 090501 (2017).

[2] G. Vidal and R. F. Werner, "Computable measure of entanglement", Phys. Rev. A **65**, 032314 (2002).

[3] G. Carleo, F. Becca, M. Schiró, and M. Fabrizio, Sci. Rep. **2**, 243 (2012).

[4] H. Timsina *et al.*, "Robustness of nonstabilizerness in the quantum Ising chain via quantum Monte Carlo tomography", Phys. Rev. B, **112**, 165135 (2025).

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Non-Additivity of Microwave-Shielded Interactions between Dipolar Molecules

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Recent experimental progress in Bose condensation of dipolar molecules [1] has motivated theoretical studies that predict interesting layered quantum liquid and crystal phases due to the peculiarity of the effective interaction between these microwave shielded dipolar molecules [2, 3]. The theoretical models of the effective interactions between microwave-shielded polar molecules typically rely on the assumption of pairwise additivity. In this work, we test the validity of this pairwise approximation by evaluating the full many-body potential energy for configurations of three and four molecules. We demonstrate that the pair-wise approximation fails for molecule configurations in the plane of the circularly polarized microwave field. In these planar geometries, many-body effects significantly increase the depth of the attractive potential well and shift the position of the repulsive barrier; the strength of attraction is crucial for the self-binding into quantum liquid planar cluster. Out-of-plane interactions in three-dimensional arrangements weaken this non-additivity somewhat, but overall the effective interactions between microwave-shielded dipoles cannot be taken as a sum of pair interactions. Our conclusion is that the correct quantitative description of the interactions between microwave shielded molecules requires a full many-body potential energy surface.[4]

[1] N. Bigagli et al. Nature 631, 289 (2024).

[2] T. Langen et al., Phys. Rev. Lett. 134, 053001 (2025).

[3] M. Ciardi et al., Phys. Rev. Lett. 135, 153401 (2025).

[4] F. Prieschl et al, arxiv:2609.01940 (2026).