7th Quantum Science and Technology Workshop

3rd IKUR Quantum Science and Technology Workshop 2024

Donostia / San Sebastián

October 4, 2024

Program

(last updated: October 1, 2024)

organized by UPV/EHU and DIPC

1 Program

7th Basque Quantum Science and Technology Workshop Oct 4, 2024			
09:20	Welcome		
09:30	I1	Mark	Erbium atoms in tweezer arrays: A new platform for Quantum Simulation
10:00	C1	Gonzalez-Raya	Modelling Frequency Conversion of Quantum Light via Molecular Modulation in Hollow-Core Fibres
10:20	I2	Huang	In-situ subwavelength quantum gas microscopy: control and measurement of dense ensemble
10:50	Coffee break and Posters		
11:20	I3	Toth	Number-phase uncertainty relations and bipartite entanglement detection in spin ensembles
11:50	C2	Bercioux	Spectral Properties of Non-Hermitian Systems Featuring Impurities and Flat Bands
12:10	C3	Barnett	Non-Hermitian Quantum Many-Body Physics
12:30	C4	Patra	Projected Entangled Pair States with flexible geometry
12:50	Lunch and Posters		
15:20	I5	Pistolesi	A nanomechanical Qubit for sensing and computing
15:50	C8	Ortuzar	A tunable Cooper pair diode
16:10	I6	Frederiksen	Electron quantum optics with graphene nanoribbons
16:40	Coffee break and Posters		
17:10	I4	Crespo	Insights in Quantum Information Theory
17:40	C5	Aizpurua	Hacking Cryptographic Protocols with Advanced Variational Quantum Attacks
18:00	C6	Andrade	Real-time evolution of the Schwinger model on IBMQ devices: Gauge invariance as an error-correction tool
18:20	C7	Carreras	Towards Running Quantum Chemistry in Quantum Hardware
18:40	Conclusion & End of Workshop		

2 Venue and Contact Data

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Venue: Cámara de Comercio de Gipuzkoa, Tolosa Hiribidea 75, E-20018 Donostia - San Sebastián

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3 Invited and Contributed Talks and Posters

List of Invited Talks

1. Crespo Bofill, Pedro (Tecnun, Donostia)
   Insights in Quantum Information Theory

2. Frederiksen, Thomas (DIPC & Ikerbasque, Donostia)
   Electron quantum optics with graphene nanoribbons

3. Huang, Ruiyang (Université de Bordeaux)
   In-situ subwavelength quantum gas microscopy: control and measurement of dense ensemble

4. Mark, Manfred (Universität Innsbruck)
   Erbium atoms in tweezer arrays: A new platform for Quantum Simulation

5. Pistolesi, Fabio (Université de Bordeaux)
   A nanomechanical Qubit for sensing and computing

6. Tóth, Géza (UPV/EHU & Ikerbasque, Bilbao)
   Number-phase uncertainty relations and bipartite entanglement detection in spin ensembles

List of Contributed Talks

1. Aizpurua, Borja (Multiverse & Tecnun, Donostia)
   Hacking Cryptographic Protocols with Advanced Variational Quantum Attacks

2. Andrade, Bárbara (ICFO Barcelona & DIPC, Donostia)
   Real-time evolution of the Schwinger model on IBMQ devices: Gauge invariance as an error-correction tool

3. Barnett, Jacob (BCAM, Bilbao)
   Non-Hermitian Quantum Many-Body Physics

4. Bercioux, Dario (DIPC & Ikerbasque, Donostia)
   Spectral Properties of Non-Hermitian Systems Featuring Impurities and Flat Bands

5. Carreras, Abel (Multiverse Computing, Donostia)
   Towards Running Quantum Chemistry in Quantum Hardware

6. González Raya, Tasio (BCAM & UPV/EHU, Bilbao)
   Quantum Hamiltonian model for entanglement-preserving frequency conversion in gas-filled hollow-core fibers

7. Ortuzar, Jon (Nanogune, Donostia)
   A tunable Cooper pair diode

8. Patra, Siddhartha (DIPC & Multiverse Computing, Donostia)
   Projected Entangled Pair States with flexible geometry

List of Posters

1. Agirre, Andoni (DIPC, Donostia)
   tba
2. Alcaine, Jesús Matias (UPV/EHU and BCAM, Bilbao)
   Symmetry-protected gates on superconducting circuits
3. Alvarez, Alatz (BCAM, Bilbao)
   Stability and mitigation of Hamiltonian characterization errors in digital-analog quantum computation
4. Appellaniz, Iagoba (UPV/EHU, Bilbao)
   Gradient magnetometry with atomic ensembles
5. Arcos, Pau (UPV/EHU, Bilbao)
   Dynamic scaling of molecular modulation in hollow anti-resonant fibers
6. Bejarano, Andrés (DIPC & Université de Bordeaux)
   Light emission from current-driven plasmonic nanocavities
7. Boto, Roberto (DIPC, Donostia)
   Addressing electron-spin dynamics in organic molecules
8. Cobos Jiménez, Jesús (UPV/EHU, Bilbao)
   Gaussian statistical phase estimation algorithm for ground states
9. Di Marcantonio, Francesco (UPV/EHU, Donostia)
   Dynamical study of a String through the Roughening Transition on the Lattice
10. Dutkiewicz, Kamil (University of Warsaw and DIPC)
    Energy levels in a 2D spin dependent optical lattice
11. Edalatmanesh, Shayan (DIPC, Donostia)
    Exotic electronic states in borylated graphene nanoribbons on a metallic substrate
12. Er-Riyahi, Oussama (Nanogune, Donostia)
    Quantum Technologies – Modelling of two-dimensional materials heterostructure

13. Frankerl, Moritz (DIPC, Donostia)
Theoretical investigations of light emission from single-molecule junctions

14. García Azorín, Pablo (UPV/EHU, Bilbao)
Robust multi-mode superconducting qubit designed with evolutionary algorithms

15. García Pina, Daniel (DIPC, Donostia)
Topology of functionalized 5-Armchair graphene nanoribbons

16. Gatti, Giancarlo (Mondragon Unibertsitatea)
Contextual Memories: a tool for private and restricted database queries

17. Grass, Tobias (DIPC & Ikerbasque, Donostia)
Lattice bosons with non-local interactions: from Bose metals to supersolids and string-ordered phases of matter

18. Juan Delgado, Adrián (CFM & UPV/EHU, Donostia)
On the different statistics of Zero-Phonon-Line and Stokes-shifted photons emitted from interacting fluorescent quantum emitters

19. Kuzian, Roman (DIPC, Donostia and Institute for Problems of Materials Science NASU, Kiev, Ukraine)
Non-tunneling Hartman effect and negative transit time in electron transmission through graphene multilayers

20. Le, Ngoc Duc (DIPC, Donostia)
Dirac particle collision in a photonic system with synthetic momenta

21. Leumer, Nico (DIPC, Donostia)
Current-based detection scheme for quasi-degenerate singlet/triplet states in open-shell graphene nanoribbons

22. Martinez, Rodrigo (DIPC, Donostia)
Quantum reservoir computing in finite dimensions

23. Martinez Strasser, Carolina (DIPC, Donostia)
Topological properties of a non-Hermitian quasi-1D chain with a flat band

24. McMillan, Stephen (DIPC, Donostia)
Graphene-based Leviton qubits for on-chip spin-center networking

25. Mena, Arturo (UPV/EHU, Bilbao)
Modelling Frequency Conversion of Quantum Light via Molecular Modulation in Hollow-Core Fibres

26. Muguruza, Garazi (QuSoft & University of Amsterdam)
Port-Based State Preparation and Applications

27. Nguyen, Minh (DIPC, Donostia)
Quasi-particle interference in bilayer graphene

28. Pellicer Guridi, Ruben (CFM, Donostia)
Bias-free vector magnetometry with NV centers

29. Peña, Rubén (BCAM, Bilbao)
Benchmarking Quantum Computers: Towards a Standard Performance Evaluation Approach

30. Pouillon, Yann (Nanogune, Donostia)
Interfacing SIESTA with Qiskit

31. Pradhan, Sunny (UPV/EHU, Bilbao)
Oddities in the Shannon Entropy of the XXZ chain

32. Rodríguez, Ángel (CFM, Donostia)
Exploring Discrete Time Crystals: Experimental Probing on latest IBM QPUs

33. Ryu, Jehyeok (DIPC, Donostia)
Ultranarrow Linewidth and Enhanced Photostability in $CsPbBr_3$ Quantum Dots

34. Sajan, Sandra (DIPC, Donostia)
Effectively decoupled unconventional superconducting condensates in a transition metal dichalcogenide

35. Sánchez Hernández, María (Department of Communications Engineering, UPV/EHU, Bilbao)
Stimulated Raman scattering and molecular modulation in gas-filled anti-resonant fibres

36. Trebbia, Jean-Baptiste (Université de Bordeaux)
Sub-nanosecond coherent optical manipulation of a single aromatic molecule at cryogenic temperature

37. Trenyi, Robert (UPV/EHU, Bilbao)
Activation of metrologically useful genuine multipartite entanglement

38. Valentí-Rojas, Gérard (Université de Bordeaux)
Towards "good-enough" qLDPC codes. A physical approach to error correction and Tanner code implementation

39. Vaquero, Nonia (DIPC, Donostia)
Genetic Algorithm-Based Method for Ansatz Updating in ADAPT-VQE

3.1 Book of Abstracts: Talks

Insights in Quantum Information Theory

Pedro Crespo Bofill

Tecnun, Donostia

In this talk we will look at the interplay between Shannon Classical Information Theory and Quantum Information. The concepts of Classical Compression and Channel capacity will be related with their Quantum counterparts.

Electron quantum optics with graphene nanoribbons

Thomas Frederiksen

DIPC & Ikerbasque, Donostia

In this talk I will present theoretical studies on graphene nanoribbon (GNR) junctions as electron beam splitters, enabling coherent wave division with minimal backscattering. Spin-polarized edge states introduce tunable spin-dependent transport, allowing for spin-polarization at the outputs. I will also discuss GNR-based Mach-Zehnder-like circuits, which demonstrate quantum interference and sensitivity to magnetic fields. These findings highlight the potential of GNR devices for quantum sensing, spintronics, and electron quantum optics.

[1] P. Brandimarte, M. Engelund, N. Papior, A. Garcia-Lekue, T. Frederiksen, and D. Sánchez-Portal, JCP 146, 092318 (2017), arXiv:1611.03337
[2] S. Sanz, P. Brandimarte, G. Giedke, D. Sánchez-Portal, and T. Frederiksen, PRB 102, 035436 (2020), arXiv:2005.11391
[3] S. Sanz, N. Papior, G. Giedke, D. Sánchez-Portal, M. Brandbyge, and T. Frederiksen, PRL 129, 037701 (2022), arXiv:2201.07147
[4] S. Sanz, N. Papior, G. Giedke, D. Sanchez-Portal, M. Brandbyge, and T. Frederiksen, JPCM 35, 374001 (2023), arXiv:2302.04821
[5] S. Sanz, G. Giedke, D. Sánchez-Portal, and T. Frederiksen, arXiv:2408.08787

In-situ subwavelength quantum gas microscopy: control and measurement of dense ensemble

Ruiyang Huang

Université de Bordeaux

Quantum gas microscopy has become a major element for quantum simulations using ultra-cold atoms in optical lattices. They are for example used to observe long-range order such as anti-ferromagnetic correlations in far field optical lattices using density and spin resolved microscopy. Decreasing the period of such lattice offers an interesting perspective to increase atom-atom interaction energies and engineer atom-light coupling that our group tackles via the hybridization of cold atoms and nano-structured surfaces.
In this talk, we will present how such type of sub-wavelength lattice potentials can be generated by trapping atoms in proximity (tens to hundreds of nanometers) of a nano-structured surface. At such atom to surface distance, the attractive Casimir-Polder force can be compensated by a doubly dressed state trapping method that I will discuss. Such method additionally offers solutions to overcome the diffraction limit of conventional imaging that become critical for sub-wavelength lattices. In this work, I will present the experimental characterization of a sub-wavelength resolution absorption imaging applicable to quantum gas detection. Manipulation and resolution of cold atoms at the level of sites can be achieved with a second optical lattice that dresses the atoms' excited level. We show here how the width of atom wavefunction in an individual lattice site changes with respect to the lattice depth and, based on this doubly-dressing method, how we can observe lattice dynamics like tunnelling from one site to its neighbor.

Erbium atoms in tweezer arrays: A new platform for Quantum Simulation

Manfred Mark

Universität Innsbruck

Neutral atoms in optical tweezers are one of the most promising platforms for quantum simulation and computation as they offer the implementation of arbitrary geometries, dynamical reconfiguration, generation of free-defects arrays and controllable long-range coupling via Rydberg-mediated interactions [1,2]. In this context, lanthanide atoms provide a complex electronic structure, which leads to a rich plethora of optical transition for efficient laser cooling and quantum state preparation [3]. Additionally, the presence of the submerged f-shell gives rise to a variety of excitation routes to Rydberg states, which can be exploited for direct optical excitation of large-angular-momentum states yielding the possibility of simulating quantum field theories [4].

We will present our results on the successful loading and detection of single erbium atoms in a linear array of optical tweezers. In our experiment, single atoms detection is accomplished by two complementary techniques: a narrow-linewidth imaging for non-destructive atom detection and a broad-linewidth ultrafast imaging [5]. To achieve single atom occupancies, we characterized the differential light shift for the intercombination line of erbium, and we investigated on the light-assisted collisions (LAC) and heating-induced losses. In addition, in a previous study, we have identified approximately 550 states in the erbium Rydberg series, including a possible state from the g-series to which excitation is only possible due to the incompletely filled erbium f-shell [6]. These results lay the foundations for realising a quantum simulator based on high angular momentum Rydberg states of single erbium atoms in optical tweezers.

References

[1] A. M. Kaufman, and K.-K. Ni, Nature Physics 17, 1324 (2021)

[2] A. Browayes, and T. Lahaye, Nature Physics 16, 132 (2020)

[3] M. Norcia, and F. Ferlaino, Nature Physics 17, 1349 (2021)

[4] A. Kruckenhauser, R. van Bijnen, T. V. Zache, M. Di Liberto, P. Zoller, Quantum Sci. Technol. 8, 015020 (2023)

[5] D. S. Grun, S. J. M. White, A. Ortu, A. Di Carli, H. Edri, M. Lepers, M. J. Mark, F. Ferlaino, arXiv:2406.16146 (2024)

[6] A. Trautmann, M. J. Mark, P. Ilzhöfer, H. Edri, A. El Arrach, J. G. Maloberti, C. H. Greene, F. Robicheaux and F. Ferlaino, Phys. Rev. Research 3, 033165 (2021)

A nanomechanical Qubit for sensing and computing

F. Pistolesi
Université de Bordeaux and CNRS, LOMA UMR5798, F-33400 Talence, France

Mechanical oscillators have been demonstrated with very high-quality factors over a wide range of frequencies. They also couple to a wide variety of fields and forces, making them ideal as sensors. The realization of a mechanically based quantum bit could therefore provide an important new platform for quantum computation and sensing. One of the difficulties is to engineer a sufficiently large anharmonicity that allows to manipulate the first levels of the mechanical qubit, independently of the other levels. In Ref. [1] we have shown that by coupling one of the flexural modes of a suspended carbon nanotube to the charge states of a double quantum dot defined in the nanotube it is possible to induce sufficient anharmonicity in the mechanical oscillator so that the coupled system can be used as a mechanical quantum bit. Remarkably, the dephasing due to the quantum dot is expected to be reduced by orders of magnitude in the coupled system. We outline qubit control, readout protocols, the realization of a CNOT gate by coupling two qubits to a microwave cavity, and how the qubit can be used as a static-force quantum sensor. We will discuss how a similar non-linear behavior is generated when the oscillator is coupled to a single-electron transistor [2] and discuss the theory describing the recent observation of this phenomenon [3].

References

[1] F. Pistolesi, A. Cleland, and A. Bachtold. Proposal for a nanomechanical qubit. *Phys. Rev. X*, 11(3):031027, 2021.
[2] G. Micchi, R. Avriller, and F. Pistolesi. Mechanical signatures of the current blockade instability in suspended carbon nanotubes. *Phys. Rev. Lett.*, 115(20):206802, 2015.
[3] C. Samanta, S. L. De Bonis, C. B. Møller, R. Tormo-Queralt, W. Yang, C. Urgell, B. Stamenic, B. Thibeault, Y. Jin, D. A. Czaplewski, F. Pistolesi, and A. Bachtold. Nonlinear nanomechanical resonators approaching the quantum ground state. *Nature Physics* 1, doi:10.1038/s41567-023-02065-9. 2024.

Number-phase uncertainty relations and bipartite entanglement detection in spin ensembles

Géza Tóth

UPV/EHU & Ikerbasque, Bilbao

We present a method to detect bipartite entanglement based on number-phase-like uncertainty relations in split spin ensembles. First, we derive an uncertainty relation that plays the role of a number-phase uncertainty for spin systems. It is important that the relation is given with well-defined and easily measurable quantities, and that it does not need assuming infinite dimensional systems. Based on this uncertainty relation, we show how to detect bipartite entanglement in an unpolarized Dicke state of many spin-1/2 particles. The particles are split into two subensembles, then collective angular momentum measurements are carried out locally on the two parts. First, we present a bipartite Einstein-Podolsky-Rosen (EPR) steering criterion. Then, we present an entanglement condition that can detect bipartite entanglement in such systems. We demonstrate the utility of the criteria by applying them to a recent experiment given in K. Lange et al. [Science 360, 416 (2018)] realizing a Dicke state in a Bose-Einstein condensate of cold atoms, in which the two subensembles were spatially separated from each other. Our methods also work well if split spin-squeezed states are considered. We show in a comprehensive way how to handle experimental imperfections, such as the nonzero particle number variance including the partition noise, and the fact that, while ideally BECs occupy a single spatial mode, in practice the population of other spatial modes cannot be fully suppressed.

[1] G. Vitagliano, M. Fadel, I. Apellaniz, M. Kleinmann, B. Lücke, C. Klempt, and G. Tóth, Quantum 7, 914 (2023).

Hacking Cryptographic Protocols with Advanced Variational Quantum Attacks

Borja Aizpurua[1,2]

[1]Multiverse Computing, Paseo de Miramón 170, E-20014 San Sebastián, Spain
[2]Department of Basic Sciences, Tecnun - University of Navarra, E-20018 San Sebastián, Spain

In this work [1], we present an enhanced approach to Variational Quantum Attack Algorithms (VQAA) [2] targeting cryptographic protocols, focusing on efficiency and scalability. Our methods demonstrate significant improvements over traditional quantum and brute-force attacks, achieving robust cryptanalysis of well-known algorithms like S-DES [3], S-AES [4], and Blowfish [5]. By leveraging fewer qubits and optimizing circuit design, our approach significantly reduces the number of iterations required to recover secret keys. The introduction of coordinate transformations [6] and the strategic use of non-orthogonal states [7] in our VQAA framework further enhance its performance, offering a promising avenue for future quantum cryptographic research. This advancement is crucial as it opens the door to quantum cryptanalysis on near-term quantum devices, paving the way for practical quantum cybersecurity assessments.

References

[1] B. Aizpurua et al., "Hacking Cryptographic Protocols with Advanced Variational Quantum Attacks," *arXiv e-prints*, 2023, arXiv:2311.

[2] Z. Wang, S. Wei, G. L. Long et al., "Variational quantum attacks threaten advanced encryption standard based symmetric cryptography", *Sci. China Inf. Sci.*, vol. 65, p. 200503, 2022. https://doi.org/10.1007/s11432-022-3511-5.

[3] E. F. Schaefer, "A SIMPLIFIED DATA ENCRYPTION STANDARD ALGORITHM", *Cryptologia*, vol. 20, no. 1, pp. 77–84, 1996. https://doi.org/10.1080/0161-119691884799.

[4] M. A. Musa, E. F. Schaefer, and S. Wedig, "A SIMPLIFIED AES ALGORITHM AND ITS LINEAR AND DIFFERENTIAL CRYPTANALYSES", *Cryptologia*, vol. 27, no. 2, pp. 148–177, 2003. https://doi.org/10.1080/0161-110391891838.

[5] R. Shirey, "Internet Security Glossary, Version 2", FYI 36, RFC 4949, DOI 10.17487/RFC4949, August 2007, https://www.rfc-editor.org/info/rfc4949.

[6] P. Bermejo et al., "Improving Gradient Methods via Coordinate Transformations: Applications to Quantum Machine Learning", *ArXiv*, 2023. https://arxiv.org/abs/2304.06768.

[7] P. Bermejo, R. Orús, "Variational quantum non-orthogonal optimization", *Sci Rep*, vol. 13, p. 9840, 2023. https://doi.org/10.1038/s41598-023-37068-2.

Real-time evolution of the Schwinger model on IBMQ devices: Gauge invariance as an error-correction tool

Bárbara Andrade, Tobias Grass, Maciej Lewenstein

ICFO Barcelona & DIPC, Donostia

The Schwinger model is a theory of quantum electrodynamics on the line and shares interesting features with quantum chromodynamics, such as string breaking. In this work, we use IBMQ devices to perform quantum simulations of a quantum link model description of the Schwinger model, where gauge and matter particles are represented by spin 1/2 operators. We compare the efficiency of simulating different formulations, and use the gauge invariance, in the form of the Gauss' law, as an error-correction tool to remove non-physical configurations and mitigate quantum errors.

Non-Hermitian Quantum Many-Body Physics

Jacob Barnett

BCAM, Bilbao

Non-Hermitian Hamiltonians are a compulsory aspect of the linear dynamical systems that model many physical phenomena, such as those in electrical circuits, open quantum systems, and optics. Additionally, a representation of the quantum theory of closed systems with non-Hermitian observables respecting unbroken PT-symmetry is well-defined.
In this talk, I will second-quantize non-Hermitian quantum theories with paraFermionic statistics. To do this, I will introduce an efficient method to find conserved quantities when the Hamiltonian is free or translationally invariant. Using a specific non-Hermitian perturbation of the Su-Schrieffer- Heeger (SSH) model, a prototypical topological insulator, I examine how PT-symmetry breaking occurs at the topological phase transition. Finally, I show that although finite-dimensional PT-symmetric quantum theories generalize the tensor product model of locality, they never permit Bell inequality violations beyond what is possible in the Hermitian quantum tensor product model.

Spectral Properties of Non-Hermitian Systems Featuring Impurities and Flat Bands

Dario Bercioux

DIPC & Ikerbasque

In this talk, I will present our recent findings on non-Hermitian lattices featuring flat bands and impurities. We investigate the Diamond chain with two distinct non-reciprocal dimerization configurations. Our analysis demonstrates that these configurations are equivalent to the non-Hermitian Su-Schrieffer-Heeger (SSH) model in non-reciprocal and PT-symmetric forms, with an added flat band at zero energy. Additionally, we examine the Hatano-Nelson model in the presence of impurities. Our results reveal that for specific values of the impurity strength relative to the non-reciprocal hopping parameters, the non-Hermitian skin effect associated with the impurity mode can counterbalance the overall skin effect of the Hatano-Nelson model. These insights contribute to a deeper understanding of non-Hermitian systems and their unique properties, potentially paving the way for novel applications in various fields.

[1] C. Martínez-Strasser et al., *Topological properties of a non-Hermitian quasi-one-dimensional chain with a flat band*, Advanced Quantum Technology 7, 2300225 (2023), arXiv:2307.08754.

[2] N. G. Leumer & D. Bercioux, *Impurity-induced counter skin-effect and linear modes in non-Hermitian systems*, arXiv:2408.01265.

Towards Running Quantum Chemistry in Quantum Hardware

Abel Carreras
Multiverse Computing, 20014 Donostia, Euskadi, Spain

Variational Quantum Eigensolver[1] (VQE) based algorithms have emerged as a promising approach for addressing quantum chemistry problems using quantum computers. However, running quantum circuits generated by these algorithms on current quantum hardware is challenging due to the inherent noise present in near-intermediate-scale quantum devices.

To address these challenges, I have focused on developing a series of optimization techniques aimed at improving the efficiency of quantum chemistry calculations on quantum hardware. These techniques target three key areas:

1) Reducing the complexity of the electronic Hamiltonians
2) Improving the classical components of VQE algorithms to better manage noisy energy evaluations
3) Optimizing the quantum circuits to reduce the computational cost and be more resilient to noise

In this presentation, I will showcase a selection of these techniques, discussing their effectiveness in different examples related to quantum chemistry.

[1] Tilly J, Chen H, Cao S, Picozzi D, Setia K, Li Y, et al. The Variational Quantum Eigensolver: A review of methods and best practices. Phys Rep. 2022;986:1–128.

Quantum Hamiltonian model for entanglement-preserving frequency conversion in gas-filled hollow-core fibers

Tasio Gonzalez-Raya [1,2], Arturo Mena[3], Miriam Lazo[4], Luca Leggio [1,3], David Novoa [2,5,6], and Mikel Sanz[1,2,4,6]

1 Basque Center for Applied Mathematics (BCAM), Bilbao, Spain
2 EHU Quantum Center, UPV/EHU, Bilbao
3 Department of Communications Engineering, Engineering School of Bilbao, UPV/EHU, Bilbao
4 Department of Physical Chemistry, UPV/EHU, Bilbao
5 Department of Communications Engineering, Engineering School of Bilbao, UPV/EHU, Bilbao
6 IKERBASQUE, Basque Foundation for Science, Bilbao

Quantum transduction is essential for future hybrid quantum networks, connecting devices across different spectral ranges. In this regard, molecular modulation in hollow-core fibers has proven to be exceptional for efficient frequency conversion. However, insights on this conversion method for quantum light have remained elusive beyond standard semiclassical models. We have therefore introduced a framework to describe the quantum dynamics of both molecules and photons in agreement with recent experiments and capable of unveiling the ability of molecular modulation to preserve entanglement. We do so by means of a Hamiltonian model able to describe both the coherence buildup in a molecular gas through stimulated Raman scattering, as well as the subsequent thresholdless frequency-conversion process at the single-photon level. In particular, considering the experimental scenario reported in [R. Tyumenev, et al., Science 376, 621 (2022)], we are able to characterize the state of the molecules and predict a complete transfer of entanglement between one of the modes of a Bell state and its corresponding frequency-converted counterpart. We expect this general theoretical framework to aid the design, optimization and interpretation of future experiments in light-based quantum technologies using anti-resonant fibers and their subsequent applications.

A tunable Cooper pair diode

Jon Ortuzar

Nanogune, Donostia

The contributed talk will present the current status in our laboratory about observing a diode effect in superconducting Josephson junctions in small lead particles.

Projected Entangled Pair States with flexible geometry

Siddhartha Patra,[1,2] Sukhbinder Singh,[3] and Román Orús[1,2,4]

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[4] *Ikerbasque Foundation for Science, Maria Diaz de Haro 3, E-48013 Bilbao, Spain*

Projected Entangled Pair States (PEPS) are a class of quantum many-body states that generalize Matrix Product States for one-dimensional systems to higher dimensions. In recent years, PEPS have advanced understanding of strongly correlated systems, especially in two dimensions, e.g., quantum spin liquids. Typically described by tensor networks on regular lattices (e.g., square, cubic), PEPS have also been adapted for irregular graphs, however, the computational cost becomes prohibitive for dense graphs with large vertex degrees. In this paper, we present a PEPS algorithm to simulate low-energy states and dynamics defined on arbitrary, fluctuating, and densely connected graphs. We introduce a cut-off, $\kappa \in \mathbb{N}$, to constrain the vertex degree of the PEPS to a set but tunable value, which is enforced in the optimization by applying a simple edge-deletion rule, allowing the geometry of the PEPS to change and adapt dynamically to the system's correlation structure. We benchmark our flexible PEPS algorithm with simulations of classical spin glasses and quantum annealing on densely connected graphs with hundreds of spins, and also study the impact of tuning κ when simulating a uniform quantum spin model on a regular (square) lattice. Our work opens the way to apply tensor network algorithms to arbitrary, even fluctuating, background geometries.

3.2 Book of Abstracts: Posters

tba

Andoni Agirre

DIPC, Donostia

tba

Symmetry-protected gates on superconducting circuits

Jesús Matias Alcaine

UPV/EHU, Leioa, Bilbao

The study of qubit architectures with intrinsic protection against noise has been an ever-growing field of research. The $0-\pi$ qubit is an exciting case, owing to its multimode nature and resilience against noise. Here we deeply study the $0-\pi$ qubit phenomenology and its symmetries for some protected single-qubit gate approaches, including one via adiabatic time evolution.

Some references:
[1] I.L. Eguskiza, A. Íñiguez, E. Rico, et al. Physical Review B 105 (May 2022).
[2] A. Gyenis, A. Di Paolo, J. Koch, et al. PRX Quantum 2 (Sept. 2021).
[3] P. Grozowski, A. Di Paolo, A.L. Grimsmo, et al. New Journal of Physics 20.4 (Apr. 2018).
[4] P. Brooks, A. Kitaev and J. Preskill, Physical Review Letter A 87 (May 2013).

Stability and mitigation of Hamiltonian characterization errors in digital-analog quantum computation

Alatz Alvarez

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Digital-analog is a universal quantum computing paradigm which employs as resources the natural entangling Hamiltonian of the system and single-qubit gates. Here, we study the stability of these protocols against Hamiltonian characterization errors in terms of the deviation from the expected value of an observable and the weak universality condition. We conclude that digital-analog is stable for local Hamiltonians, in the sense that the connectivity of the two-body interactions of both the problem and the system Hamiltonians does not grow with the system size. We further propose a protocol for mitigating calibration errors which resembles dynamical-decoupling techniques. These results open the possibility of scaling digital-analog to intermediate and large scale systems with constant errors.

Gradient magnetometry with atomic ensembles

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We study gradient magnetometry with an ensemble of atoms with arbitrary spin. We calculate precision bounds for estimating the gradient of the magnetic field based on the quantum Fisher information. For quantum states that are invariant under homogeneous magnetic fields, we need to measure a single observable to estimate the gradient. On the other hand, for states that are sensitive to homogeneous fields, a simultaneous measurement is needed, as the homogeneous field must also be estimated. We prove that for the cases studied in this paper, such a measurement is feasible. We present a method to calculate precision bounds for gradient estimation with a chain of atoms or with two spatially separated atomic ensembles. We also consider a single atomic ensemble with an arbitrary density profile, where the atoms cannot be addressed individually, and which is a very relevant case for experiments. Our model can take into account even correlations between particle positions. While in most of the discussion we consider an ensemble of localized particles that are classical with respect to their spatial degree of freedom, we also discuss the case of gradient metrology with a single Bose-Einstein condensate.

Dynamic scaling of molecular modulation in hollow anti-resonant fibers

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Optical systems are scalable under low-intensity illumination since their governing equations are independent of the optical signal strength. Nonetheless, in high-intensity regimes, the behaviour of the optical signal becomes nonlinear, yielding nontrivial outcomes. In spite of this, canonical nonlinear phenomena such as filamentation and high-harmonic generation in free space have recently been demonstrated to be scalable. Here we will discuss the extension of the scale-invariance paradigm to stimulated Raman scattering and molecular modulation in hollow anti-resonant fibres filled with Raman-active gases. We have found that the complex dynamics within the fibre can be accurately reproduced under very different conditions by controlling certain parametric ratios. Such scaling strategy enables access to different nonlinear propagation scenarios without sacrificing performance, opening routes to the design of nonlinear devices operating in exotic frequencies like the ultraviolet or quantum frequency convertors of non-classical states such as biphoton pairs.

Light emission from current-driven plasmonic nanocavities

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In recent years, the scientific community has shown growing interest in the study of light emission in molecules. The Scanning Tunneling Microscope (STM), in particular, stands out for its remarkable ability to inject electrons with atomic precision. This precision enables the probing of various internal molecular transitions, shedding light on the intricate mechanisms behind molecular light emission.

In fact, it has been reported that when the STM tip is positioned close to the molecule, a distinct sharp resonance appears in the emission spectrum. This phenomenon, known as the Purcell effect, arises from the weak interaction between the confined electric field and the molecule, enhancing the emission efficiency [1, 2, 3]. Additionally, several research groups have investigated the statistical behavior of the emitted photons and observed antibunching. This phenomenon indicates that it is unlikely to detect two photons in close temporal proximity, providing further insights into the quantum nature of the light emission process [4, 5, 6].

We propose a microscopic model based on the quantum master equation to accurately describe the emission spectrum and photon statistics. Our model, through different levels of approximation, enables precise predictions of the various lifetimes of the involved excitations. This approach offers insights into the underlying mechanisms of light emission.

[1] B. Doppagne et al., PRL **118**, 127401 (2017)
[2] G. Chen et al., PRL **122**, 177401 (2019)
[3] S. Jiang et al., PRL. **130**, 126202 (2023)
[4] P. Merino et al., Nat. Commun. **6**, 8461 (2015)
[5] L. Zhang et al., Nat. Commun. **8**, 580 (2017)
[6] A. Rosławska, ACS Nano, **14**, 6366 (2020)

Addressing electron-spin dynamics in organic molecules

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Research on materials for storing quantum information has been accelerated by the quick development of quantum technologies.[1] The synthesis of organic molecules able to host spin qubits has attracted significant attention for the development of carbon-based materials with applications in information storage and processing.[2,3] Magnetic states in carbon-based materials have been proposed as a promising framework for developing qubits.[3] The application of such materials for quantum technologies requires precise control of the mechanisms that drive the relaxation of magnetic states, and thus the coherence times.

In this work, we study the dynamics of the magnetic states for some selected boron-doped coronene dimers (BCDs) (Fig. 1a). We combine Redfield equations and first principle calculations of magnetic properties to solve the rate equations of the spin density for the selected molecules, and to compute the relaxation (coherence) time. We address the impact of the position of the dopants on the relaxation time and on the relaxation mechanism for the lowest-energy triplet state of these BCDs. We observe that the selected BCDs exhibit relaxation times in the order of 1 millisecond (Fig. 1c,d). The relaxation process is mainly determined by time fluctuations (induced by molecular vibrations) of the spin-orbit coupling (SOC; Fig. 1c), and the hyperfine interaction (HFI; Fig. 1d). The latter accounts for the interaction between the electron spin density and the nuclear spins of the atoms of boron and hydrogen. The combination of strongly localized spin density (Fig. 1b) and weak SOC offers the perspective of designing attractive organic materials with extended coherence times.

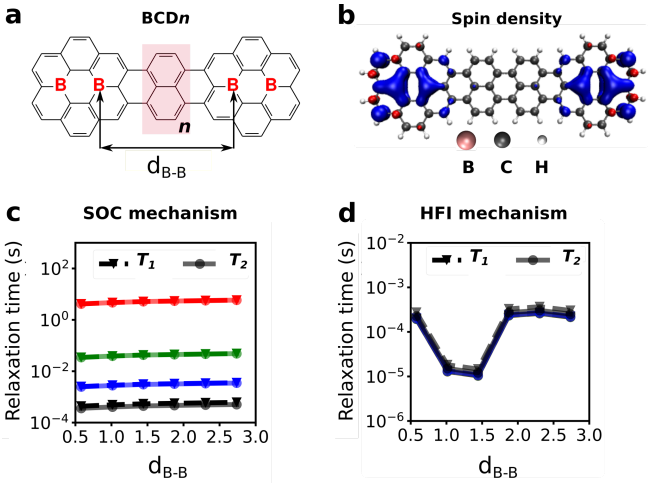

Figure 1: Relaxation times for the selected boron-doped coronene dimers (BCDs). *(a) Schematic representation of the selected boron-doped coronene dimers. (b) 0.02 bohr^{-3} isosurface of the spin density for the triplet ground state of a selected BCD computed within DFT (UB3LYP/6-31g(d,p)). The regions coloured blue and red represent regions of accumulation of spin-up and spin-down electrons, respectively. The spheres coloured pink, grey and white represent the atoms of boron, carbon and hydrogen, respectively. (c, d) Relaxation times T_1 (dashed lines) and T_2 (solid lines) induced by fluctuations of the (c) SOC, and (d) HFI for BCDn (n=0-5) as a function of the boron-boron distances ($d_{B\text{-}B}$; definition in panel a). Magnetic fields of 30 mT (red lines), 330 mT (green lines), 1250 mT (blue line) and 3500 mT (black line) are applied for computing the relaxation times depicted in panels c and d.*

References

[1] A. Gaita-Ariño *et al*, *Molecular spins for quantum computation,* Nature Chemistry. 11, 301 (2019)

[2] F. Lombardi *et al, Quantum units from the topological engineering of molecular graphenoids,* Science. 366, 1107 (2019)

[3] N. Friedrich *et al*, *Addressing electron spins embedded in metallic graphene nanoribbons*, ACS Nano. 16, 14819 (2022)

Poster submission abstract 7th Basque Quantum Science and Technology Workshop

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Gaussian statistical phase estimation algorithm for ground states

The study of ground states is one of the most relevant tasks in quantum simulation. In recent years there has been a lot of activity in the development of statistical phase estimation algorithms, which are intended to solve the Hamiltonian eigenvalue estimation task with considerably fewer resources than the traditional Quantum Phase Estimation algorithm [1-3]. In these algorithms, a quantum simulator is used to measure Loschmidt amplitudes at different times, and a classical postprocessing step is then performed to reconstruct the convolution of some function with the density of states associated with an initial state that is an input of the algorithm. Under this setting, several different algorithms have been proposed, each concerned with which function is convolved, determining at which times the Loschmidt amplitudes are measured, and what strategy to follow to find the desired eigenvalues. We propose a novel algorithm for ground state energy estimation based on the convolution of a Gaussian with the density of states and does not require a lower bound on the gap as input. Our proposal is also formally valid when the ground state does not have a large overlap with the initial state. The result is an algorithm with shorter circuit depth compared to previous approaches without requiring additional a priori information about the ground state.

[1] Lin Lin and Yu Tong. *Heisenberg-Limited Ground-State Energy Estimation for Early Fault-Tolerant Quantum Computers*. PRX Quantum 3, 010318 (2022)

[2] Guoming Wang, Daniel Stilck França, Gumaro Rendon and Peter D. Johnson. *Faster ground state energy estimation on early fault-tolerant quantum computers via rejection sampling*. arXiv:2304.09827 (2023)

[3] Zhiyan Ding, Haoya Li, Lin Lin, HongKang Ni, Lexing Ying and Ruizhe Zhang. *Quantum Multiple Eigenvalue Gaussian filtered Search: an efficient and versatile quantum phase estimation method*. arXiv:2402.01013

Dynamical study of a String through the Roughening Transition on the Lattice

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We study the Z2 lattice gauge model in (2+1) dimensions, focusing on the confined and deconfined phases separated by a quantum phase transition at critical coupling g_c. By analyzing the vacuum structure and string-tension using square and rectangular lattices, we identify g_c and examine the Lüscher term correction near the roughening transition. Dynamically, we simulate the time evolution of the electric string, tracking critical behavior through fidelity susceptibility and Loschmidt echo analysis. Further studies of finite-size effects and quenching dynamics aim to clarify the roughening transition and its connection to the Kibble-Zurek mechanism.

Energy levels in a 2D spin dependent optical lattice

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In this study the energy levels of a ^{87}Rb atom in a 2D spin dependent optical lattice are examined. Four counter-propagating laser beams produce a periodic scalar potential. As shown by Le Kien et al. [1], polarizing the beams by 45° results in an additional, spin dependent vector potential, that can be expressed through a fictitious magnetic field B_{fic}. The spectrum of energy levels is analyzed as a function of the external magnetic field B_{ext}, in lattice cells of various n x m sizes, with either Dirichlet (DBC) or periodic (PBC) boundary conditions. It is found that avoided crossing between multiplets of eigenstates occurs only for cells larger than 1 by 1 with DBC. Szulim et al. [2] also observed level crossing in a 1 by 1 DBC cell of a honeycomb lattice and suggested hexagonal symmetry as the cause. Rectangular cells are studied by varying the angle between the laser beams and it is shown that even with the loss of rotational symmetry, avoided crossing does not occur with PBC or in a 1 by 1 cell with DBC. Furthermore, eigenstates are discovered in DBC cells, with energies lying outside the bands computed for a PBC cell. Analysis of the probability density of their wave functions reveals that they are hinge states. It is further demonstrated how the states localized near the Dirichlet walls tend to have higher energies than corresponding states localized in the center of the cell.

[1] F. Le Kien et al., European Physical Journal D 67 92 (2013).
[2] P. Szulim et al., New Journal of Physics 24, 033041 (2022).

Exotic electronic states in borylated graphene nanoribbons on a metallic substrate

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Graphene nanoribbons (GNRs) have emerged as promising platforms for π-magnetism [1], with recent findings revealing the presence of uncompensated spin-polarized states at ribbon edges or interiors due to non-conventional band topology effects. Additionally, advancements in bottom-up growth techniques have enabled the synthesis of GNRs directly on surfaces [2], further enhancing their potential for applications in spintronics and quantum computing.

Here, we investigate the induction of spin polarization in topologically trivial, densely 2B-doped 7AGNRs [3,4] when detached from a metal support. Utilizing a combination of density functional theory (DFT) [5], mean-field Hubbard calculations and topological band theory, as well as low-temperature scanning tunneling microscopy (STM) transport experiments and simulations [6] on borylated GNRs, we demonstrate and study the presence of a Kondo resonance for specific tip-substrate distances while slowly lifting a 2B-7AGNR from an Au(111) substrate using the tip of an STM.

Additionally, we observe the emergence of a low-energy electronic state (+5mV) at the terminal of an asymmetric 2B-7AGNR, with an additional anthracene unit on one end. Due to asymmetry, a topological classification based on the bulk-boundary correspondence isn't possible for this structure. However, our theoretical analysis of the electronic structure underscores the potential for substrate-mediated charge transfer effects and hopping processes, enabling the emergence of topological edge states. This discovery provides a compelling basis for exploring complex spin physics and exotic quantum phases in low-dimensional organic materials.

References

[1] D. G. de Oteyza and T. Frederiksen, JPCM **34**, 443001 (2022)
[2] J. Cai, et al. Nature **466**, 470-473 (2010)
[3] E. Carbonell-Sanromà, et al. J. Phys. Chem. **122**,16092–16099 (2018)
[4] N. Friedrich, et al. Phys. Rev. Lett. **125**, 146801 (2020)
[5] J. M Soler, et al. JPCM **14**, 2745 (2002)
[6] O. Krejčí, et al. Phys. Rev. B **95**, 045407 (2017)

Quantum Technologies – Modelling of two-dimensional materials heterostructure

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The 2004 discovery of graphene exfoliation spurred interest in two-dimensional (2D) materials, leading to the creation of materials like hexagonal boron nitride, phosphorene, and others. These materials can be stacked to form van der Waals heterostructures with unique properties. In 2018, researchers found that rotating stacked graphene layers could result in new phenomena, a field now known as twistronics. Twistronics explores how rotational mismatches between 2D layers affect electronic properties, revealing effects like superconductivity and spin polarization. Understanding the relationship between rotation angles and Moiré crystal structures is crucial for designing novel nanodevices. The project focuses on the electronic properties of graphene/PbI_2 heterostructures, aiming to develop models that describe their physics through large-scale first-principle calculations.

Theoretical investigations of light emission from single-molecule junctions

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The scanning tunneling microscope (STM) is a great tool to study molecules on their intrinsic length scales and therefore it can also be used effectively to study light matter interaction on sub-nanometer length scales. Recently, there has been an increasing interest in light emission from single molecules in scanning tunneling microscopy (STM) set-ups. [1,2,3] To study molecular properties the hybridization with the metallic substrate is suppressed by placing thin NaCl films in between.
Focusing on electrofluorescence in these junctions we employ a generalized master equation approach for the reduced density matrix of the central system, i.e. the molecule. We study the interplay between the coupling of the molecule to the electronic leads and to the cavity. Furthermore, we include coupling between the molecule's electronic and phononic degrees of freedom. This enables us to illuminate the effect of electron-phonon coupling on the light emission spectrum.

[1] B. Doppagne, M.C. Chong, H. Bulou, A. Boeglin, F. Scheurer, G. Schull, Science 361, 251-255 (2018)
[2] J. Doležal, S. Canola, P. Hapala, R.C. de Campos Ferreira, P. Merino, M. Švec, Nat. Comm. 13, 6008 (2022)
[3] L. Zhang, YJ. Yu, LG. Chen, Y. Luo, B. Yang, FF. Kong, G. Chen, Y. Zhang, Q. Zhang, Y. Luo, JL. Yang, ZC. Dong, J.G. Hou, Nat. Comm. 8, 580 (2017)

Robust multi-mode superconducting qubit designed with evolutionary algorithms

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Multi-mode superconducting circuits offer a highly promising platform for engineering robust systems for quantum computation. However, as the system's dimensionality increases beyond the usual single-mode, its design and study become exponentially complicated and less intuitive. Previous studies of single-mode devices have demonstrated that superconducting quantum systems can be engineered to be robust against various sources of noise and decoherence [1, 2]. Nevertheless, advancements in single-mode device design have revealed that no device with a single degree of freedom can be engineered to be simultaneously resilient to multiple sources of decoherence, as the necessary protection requirements often conflict [3]. This observation highlights the need to explore systems with a larger number of degrees of freedom, which have proven effective in providing protection against different error sources simultaneously [4, 5]. Unfortunately, this protection typically comes with construction constraints (such as symmetry requirements) and limitations in manipulability.

In this study, we present a novel multi-mode qubit architecture designed using evolutionary algorithms [6] that exhibit desirable qubit characteristics, including restricted transitions, improved relaxation and dephasing times, and resilience against fabrication defects. The additional degrees of freedom offered by the multi-mode structure are utilized to mitigate noise sensitivity. We explore heterogeneous configurations where different parts of the system are suitable for specific operations, such as readout or control. This approach is valuable for identifying configurations that, although lacking the complete protection of symmetry-protected systems, strike a balance between manipulability, construction, and noise protection. Furthermore, we analyze how the generated systems respond to fluctuations in parameter values caused by fabrication errors, which is crucial for practical implementation [7].

[1] J. Koch *et al.*, PRA, 76(4), 042319 (2007).
[2] V.E. Manucharyan *et al.*, Science, 326(5949), 113-116 (2009).
[3] A. Gyenis *et al.*, PRX Quantum, 2(3), 030101 (2021).
[4] Y. Chen *et al.*, PRL 113(22), 220502 (2014).
[5] K. Kalashnikov *et al.*, PRX Quantum, 1(1), 010307 (2020).
[6] F.A. Cárdenas-López *et al.*, arXiv preprint arXiv:2302.01837 (2023).
[7] P. García-Azorín *et al.*, arXiv:2407.18895 (2024).

Topology of functionalized 5-Armchair graphene nanoribbons

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In the last years, on-surface synthesis techniques have granted access to unprecedented atomistic control over the of bottom-up fabrication graphene nanoribbons (GNRs). This highly precise experimental platform has given rise to multiple studies in these systems regarding topological properties [1], chemical substitution [2,3], novel morphological structures [4], etc. In this work, we use Density Functional Theory calculations to gain insights into the electronic structure and topological properties of several functionalized GNRs. The systems considered consist of 5 carbon atoms wide armchair GNRs (5AGNRs) with OH and F groups attached to their edges. We study the effect of these radicals in the physical structure, the wavefunctions and the topology of the system. We find that, while retaining their overall structure, functionalization with chemical groups of different electron affinities, different orientations and at different concentrations can change the topology of the system (Fig. 1). Our results might be of interest for the engineering and development of new experiments regarding the topological and magnetic properties of these materials.

References

[1] J. Li, S. Sanz, N. Merino-Díez *et al.*, *Nat Commun* **12** *(2021)* 5538
[2] N. Friedrich *et al.*, *ACS Nano* **16**, **9**, *(2022)* 14819-14826
[3] N. Friedrich *et al.*, *Phys. Rev. Letters* **125** *(2020)* 146801
[4] S. Sanz, N. Papior, G. Giedke, D. Sanchez-Portal, M. Brandbyge, T. Frederiksen, *Phys. Rev. Letters* ***129*** *(2022)* 037701

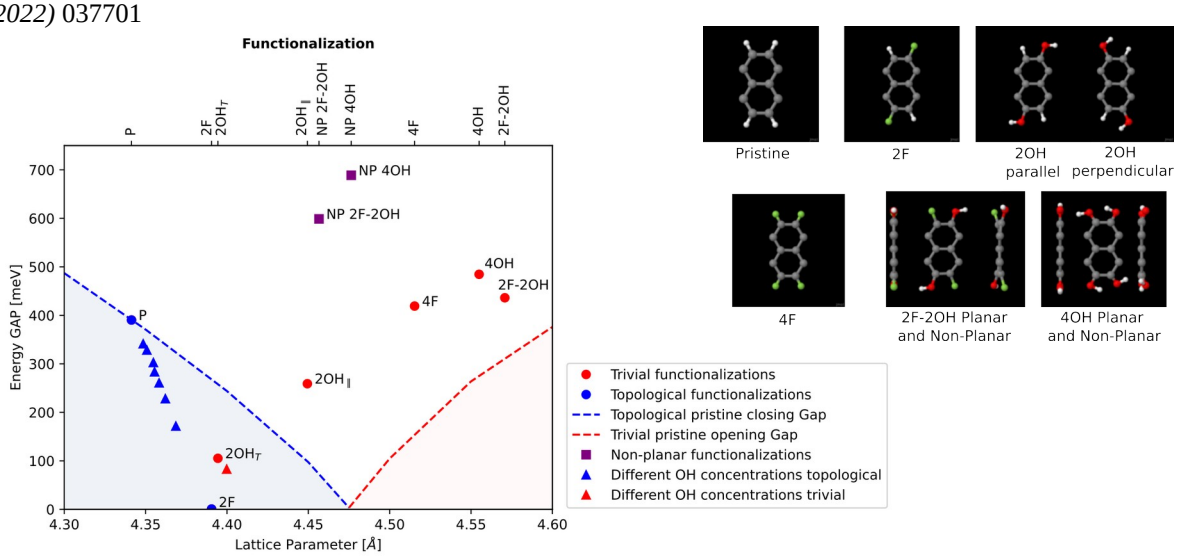

Fig. 1. Left panel: Energy Gap at Gamma point versus lattice parameter for different functionalizations of the 5AGNR. Dots in blue (red) represent topological (trivial) functionalizations. Triangles in blue (red) represent different topological (trivial) concentrations of the OH functionalization, i.e., different number of OH groups per cell. Squares in purple represent non-planar geometries with lower lattice parameter and greater energy Gap. Dashed blue (red) lines represent the closing (opening) of the band gap for the pristine nanoribbon as a function of the lattice parameter.
Right panel: Schemes of the unit cell of different functionalized ribbons..

Contextual Memories: a tool for private and restricted database queries

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Mondragon Unibertsitatea

We employ a class of locally-rotated GHZ states to encode a classical database which can be partially queried in different quantum measurement contexts. Sharing these states between two parties guarantees a restricted and private access to the encoded data, a feature which cannot be reproduced classically without the aid of a trusted third party. This protocol could find application in communication between non-trusting parties and secure data verification.

Lattice bosons with non-local interactions: from Bose metals to supersolids and string-ordered phases of matter

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In a system of bosons, short-range interactions produce a phase transition from a superfluid condensate into an insulating state. The landscape of possible bosonic phases of matter gets significantly enriched through the presence of long- or finite-range interactions: Both condensed and insulating phases may then undergo a symmetry-breaking transition and exhibit crystalline order, giving rise to supersolid or charge-density-wave phases. There is also an intriguing possibility of non-local order: The Haldane phase is characterized by string order, and is known to appear in the insulating regime of bosons interacting in a 1D lattice via finite-range interactions. The co-existence of such string order and superfluidity, however, has remained an open question. The presence of exchange interactions in a 2D lattice (or a ladder) may also produce a transition from a condensed phase into a metal-like bosonic phase. Using DMRG calculations, we have theoretically examined this variety of bosonic phases of matter in chain- or ladder-like lattices in the presence of non-local interaction terms. This provides new insights in the experimental feasibility of exotic bosonic phases and in the existence of string-ordered superfluids. Experimental platforms where these phases can be observed are discussed, specifically the recent experimental case of an extended Bose-Hubbard model with dipolar excitons. We also show that a chain of three-level ions may provide a promising platform to implement the physics related to ring-exchange interactions, giving rise to a kind of Bose-metal behavior.

On the different statistics of Zero-Phonon-Line and Stokes-shifted photons emitted from interacting fluorescent quantum emitters

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Quantum emitters with a very narrow emission line (such as organic molecules and quantum dots at cryogenic temperatures) are powerful single-photon sources [1], which are of great interest for quantum technology applications. Additionally, the interaction between quantum emitters leads to the emergence of superradiant and subradiant states that could find further technological applications [2]. Here, motivated by the interest in characterizing and manipulating the photonic state of the emission from two interacting fluorescent emitters, of large potential in technological applications, we present a detailed analysis of the statistics of light emitted from such a system under different conditions of illumination, emphasizing the importance of the choice of detection schemes.

On the one hand, we analyze the statistics of photons emitted in the Zero-Phonon Line (ZPL), i.e., due to the transition from the pure (0-phonon) electronic excited state to the pure electronic ground state. We show that the statistics of ZPL photons can be tailored over an enormous range of values, from strong antibunching to strong bunching, by tuning the laser frequency and intensity [3]. This rich landscape of light statistics can be of interest to engineer photon sources.

On the other hand, we also analyze the statistics of Stokes-shifted photons, which are lower-energy photons that can be generated due to the decay from the pure electronic excited state to a 1-phonon electronic ground state. This analysis is motivated by available fluorescence experiments where the laser pumps resonantly the pure electronic excited state and light is filtered to ensure that laser photons do not disturb the measurements. This procedure eliminates the ZPL photons so that only the Stokes-shifted ones are detected [2,6]. With the aim to address the statistics of the Stokes-shifted photons, we expand the usual model that treats the emitters as two-level systems [4,5]. We show that our model captures well the experimental measurements of the statistics of Stokes-shifted photons emitted from two interacting organic molecules in Ref. [2] and also a variety of experimental measurements. Additionally, we analyze the statistics of Stokes-shifted photons from two noninteracting emitters and unveil interesting coherence effects in the picosecond timescale (corresponding to the lifetime of the vibrations). Importantly, we find that the statistics of ZPL photons can be drastically different to that of the Stokes-shifted photons, stressing the importance of sophisticating the theoretical description to accurately address each experimental configuration.

[1] B. Lounis, and M. Orrit, Reports on Progress in Physics, 68, 1129 (2005).
[2] J. B. Trebbia, Q. Deplano, P. Tamarat, and B. Lounis, Nat. Comms. 13, 2962 (2022).
[3] A. Juan-Delgado, R. Esteban, Á. Nodar, J. B. Trebbia, B. Lounis, and J. Aizpurua, Phys. Rev. Res., 6, 023207 (2024).
[4] Z. Ficek, R. Tanas, and S. Kielich, Optica acta, 30, 713-731 (1983).
[5] A. Vivas-Viaña and C. Sánchez-Muñoz, Physical Review Research 3, 033136 (2021).
[6] C. M. Lange, E. Daggett, V. Walther, L. Huang, and J. D. Hood, Nature Physics (2024).

Non-tunneling Hartman effect and negative transit time in electron transmission through graphene multilayers

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Attosecond dynamics of electron transmission through graphene multilayers is studied based on the concept of Wigner time delay implemented in an *ab initio* scattering theory. The character of the electron propagation through the multilayers is traced to the band structure of bulk graphite. In the forbidden gaps the wave packet transit time τ_{T} saturates with thickness, which establishes the Hartman effect at classically allowed energies. In the allowed bands τ_{T} oscillates following the transmission resonances. These features are illustrated by an exact solution a one-dimensional (1D) model. In real crystals, the in-plane scattering brings about phenomena missing in 1D models and hitherto unknown: negative transit time is discovered in monolayers of graphene, h-BN, and oxygen, and huge time delay is observed at a point of total reflection from h-BN. Moreover, the Wigner time delay is shown to diverge at the scattering resonances caused by the emergence of the secondary diffracted beams. These unique properties offer a way to manipulate the propagation timing of the electron wave packet without sacrificing the transmitted intensity. The spatial reshaping of the wave packet at the resonances may help elucidate details of the streaking by an inhomogeneous field at the surface.

Dirac particle collision in a photonic system with synthetic momenta

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The method of synthetic momenta recently emerges as a useful way to construct high-dimensional momentum space from structures in lower dimensions. Synthetic momenta naturally break the time-reversal symmetry so structures with synthetic momenta are topologically non-trivial. In this work, we use a 2D photonic crystal slab bilayer to form an effective 2D structure with one genuine momentum and one synthetic momentum. By constructing an effective model, we observe the scattering of two Dirac particles from the genuine momentum axis to the synthetic momentum axis in the hybrid momentum space. The predictions of the analytical model are confirmed by the numerical simulations using the Plane Wave Expansion method. Our work paves the way of exploring the high-dimensional topological phases of matter in photonic crystals.

Current-based detection scheme for quasi-degenerate singlet/triplet states in open-shell graphene nanoribbons

Nico Leumer

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Graphene nanoribbons (GNRs) possess remarkable properties like high carrier mobility, tunable band gaps, mechanical strength, and efficient thermal and electrical conductivity, all controlled by edge functionalities and ribbon geometry. These traits make them ideal for applications as selective gas sensors, supercapacitors, quantum electronics, nanomedicine, transistors, and biosensing. Open-shell GNRs are particularly valuable for their π-magnetism, tunable spin properties, and potential applications in quantum computing. However, they have only recently become experimentally accessible due on-surface synthesis. Fascination for and instability of those GNRs at half-filling stem from the presence of localized, unpaired electrons pinned to the Fermi level (zero energy). This attractive chemical potential to form new, saturated bonds is circumvented by using stabilizing substrates and an ultra-clean vacuum and the local electron's spin is preserved due to the inherently weak spin-orbit/hyperfine interactions of carbon structures. In case of a 7-atom wide armchair graphene nanoribbon (7-AGNR), but not restricted to it, topological zero energy single-particle states at the ribbon's outer left/right termini form quasi-degenerate singlet/triplet states in the interacting case. Since the energy difference depends on effective inter-termini hopping and Coulomb repulsion, it can be tuned experimentally by the ribbon's length causing the energy difference to vanish for long ribbons. Without the use of magnetic fields, the singlet/triplet states are hard to distinguish in current-voltage measurements. However, we propose a current- based detection scheme exploiting that (even degenerate) singlet/triplet states have distinct spatial profiles. Since the latter modifies locally the electron tunneling rate from a reservoir, we envision two movable, metallic (STM) tips, each coupled locally to one GNR atom. An applied bias V between both tips drives a current, whose dynamics is anticipated to distinguish said singlet/triplet states. We give a progress report on a minimal model manifesting the essential physics.

Quantum reservoir computing in finite dimensions

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Quantum reservoir computing (QRC) is a machine learning technique where complex quantum systems are exploited to solve temporal tasks, such as predicting chaotic time series and complex spatiotemporal dynamics. Most existing results in the analysis of QRC systems with classical inputs have been obtained using the density matrix formalism. Our work shows that alternative representations can provide better insights when dealing with design and assessment questions. It has been shown that these vector representations yield state-affine systems (SAS) previously introduced in the classical reservoir computing literature and for which numerous theoretical results have been established. This connection has been used to show that various statements in relation to the fading memory (FMP) and the echo state (ESP) properties are independent of the representation, and also to shed some light on fundamental questions in QRC theory in finite dimensions. Our conclusions can be summarised as: the necessary and sufficient condition that makes a quantum reservoir valuable is strictly contractive dynamics towards input-dependent fixed points.

Topological properties of a non-Hermitian quasi-1D chain with a flat band

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The spectral properties of a non-Hermitian quasi-1D lattice in two of the possible dimerization configurations are investigated. Specifically, it focuses on a non-Hermitian diamond chain that presents a zero-energy flat band. The flat band originates from wave interference and results in eigenstates with a finite contribution only on two sites of the unit cell. To achieve the non-Hermitian characteristics, the system under study presents non-reciprocal hopping terms in the chain. This leads to the accumulation of eigenstates on the boundary of the system, known as the non-Hermitian skin effect. Despite this accumulation of eigenstates, for one of the two considered configurations, it is possible to characterize the presence of non-trivial edge states at zero energy by a real-space topological invariant known as the biorthogonal polarization. This work shows that this invariant, evaluated using the destructive interference method, characterizes the non-trivial phase of the non-Hermitian diamond chain. For the second non-Hermitian configuration, there is a finite quantum metric associated with the flat band. The two non-Hermitian diamond chains can be mapped into two models of the Su-Schrieffer-Heeger chains, either non-Hermitian, or Hermitian, both in the presence of a flat band. This mapping allows to draw valuable insights into the behaviour and properties of these systems. [1]

References

[1] C. Martínez-Strasser, M. A. J. Herrera, A. García-Etxarri, G. Palumbo, F. K. Kunst, D. Bercioux, Topological Properties of a Non-Hermitian Quasi-1D Chain with a Flat Band. Adv Quantum Technol. 2023, 2300225

Figures

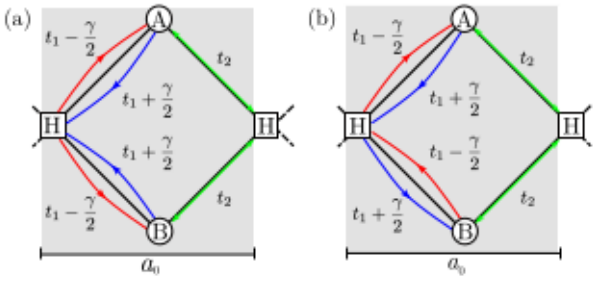

Figure 1: Sketch of the non-Hermitian diamond lattice in the A and B configurations, panel (a) and (b), respectively.

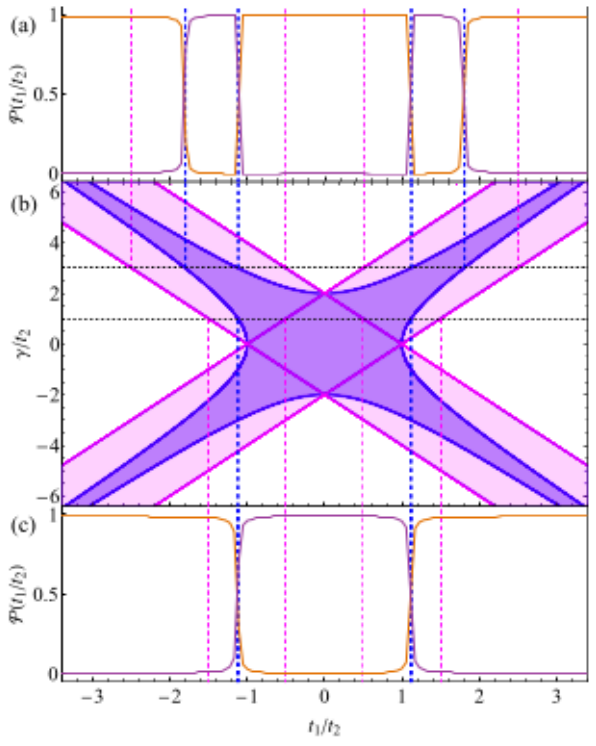

Figure 2: Phase diagram of the DCA model along with the biorthogonal polarization of two cuts in this phase diagram.

Graphene-based Leviton qubits for on-chip spin-center networking

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This poster outlines our aspiration to develop a theoretical framework for on-chip spin center networks mediated by graphene-based Leviton qubits. Levitons, which are minimal-excitation wave packets in conducting systems, offer unique advantages such as high coherence over micron-scale distances. When realized in graphene, they have potential to serve as flying qubits, facilitating the transmission of quantum information over distances large relative to the spatial extent of a localized spin center's wave function. Coupling these Levitons to bound spin states creates a hybrid system where stationary qubits can interact with flying qubits, opening the potential for quantum state transfer and entanglement generation. Additionally, networking with Levitons provides unique opportunities for exploring interactions between flying qubits that are not present in photonic counterparts. We aim to explore the theoretical foundations, potential experimental setups, and challenges in realizing networks of this type. We emphasize developing an understanding of the conditions in which Levitons form, their stability, and their interactions. These insights will guide our ambition to develop optimization strategies for qubit coherence and gate operations. This framework sets the stage for future research in scalable quantum computing technologies.

Modelling Frequency Conversion of Quantum Light via Molecular Modulation in Hollow-Core Fibres

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The second quantum revolution is enabling the development of technologies with capabilities that extend beyond those of classical systems. Nevertheless, the success of this revolution depends on solving persistent challenges in quantum optics, like the quantum frequency conversion of single photons and entangled pairs, essential for interconnecting the components of hybrid quantum networks operating in different spectral ranges. Most current methods are often inefficient and constrained in their capabilities. In this poster, a theoretical framework is presented to describe a novel solution using hollow anti-resonant fibres filled with molecular gases, which excel in quantum applications due to their ultralow attenuation, high damage threshold, and tunable optical properties. By inducing coherent molecular oscillations through stimulated Raman scattering, efficient quantum frequency conversion is possible while preserving the photonic correlations. With the framework showcased here, we are now capable of, for example, shining light into entanglement dynamics during this conversion process, thereby opening unprecedented pathways for the realization of new fibre-based quantum hardware.

Port-Based State Preparation and Applications

Garazi Muguruza

QuSoft & University of Amsterdam

We introduce Port-Based State Preparation (PBSP), a teleportation task where Alice holds a complete classical description of the target state and Bob's correction operations are restricted to only tracing out registers. We show a protocol that implements PBSP with error decreasing exponentially in the number of ports, in contrast to the polynomial trade-off for the related task of Port-Based Teleportation, and we prove that this is optimal when a maximally entangled resource state is used. As an application, we introduce approximate Universal Programmable Hybrid Processors (UPHP). Here the goal is to encode a unitary as a quantum state, and the UPHP can apply this unitary to a quantum state when knowing its classical description. We give a construction that needs strictly less memory in terms of dimension than the optimal approximate Universal Programmable Quantum Processor achieving the same error. Additionally, we provide lower bounds for the optimal trade-off between memory and error of UPHPs.
arXiv link: [2402.18356] Port-Based State Preparation and Applications (arxiv.org)

Quasi-particle interference in bilayer graphene

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Transport properties of electrons in materials are usually investigated based on the electronic dispersions and their associated topology. However, there may exist hidden mechanisms determining how electrons scatter, such as the conservation of pseudospin in graphene. Quasi-particle interference imaging is a method that provides information on how electrons scatter and is accessible via scanning tunneling microscopy experiments. Employing the kernel polynomial method, we numerically investigate the quasi-particle interference in bilayer graphene systems. The interference spectra exhibit the chiral properties of Dirac electron in graphene-based systems.

Bias-free vector magnetometry with NV centers

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NV centers have been proposed as accurate quantum sensors to measure magnitude and direction of magnetic fields. However, the methods proposed to date do not work when the peaks in the signal used to estimate the fields overlap, such as when measuring in the presence of low static fields. To avoid this overlap, current magnetometry strategies require forcing a known external bias magnetic field to decode the measurement. In this work we present an approach to remove the need of the bias field and sense directly in original environmental conditions. By modifying the polarization of the microwave fields used to drive the electron spins, we are able to selectively switch "on" and "off" the peaks individually, revealing the information needed to estimate the magnetic field. This method opens the door to study systems in their natural condition without perturbations and errors introduced by bias fields.

Benchmarking Quantum Computers: Towards a Standard Performance Evaluation Approach

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The technological development of increasingly larger quantum processors on different quantum platforms raises the problem of how to fairly compare their performance, known as quantum benchmarking of quantum processors. This is a challenge that computer scientists have already faced when comparing classical processors, leading to the development of various mathematical tools to address it, but also to the identification of the limits of this problem. In this work, we briefly review the most important aspects of both classical processor benchmarks and the metrics comprising them, providing precise definitions and analyzing the quality attributes that they should exhibit. Subsequently, we analyze the intrinsic properties that characterize the paradigm of quantum computing and hinder the naive transfer of strategies from classical benchmarking. However, we can still leverage some of the lessons learned such as the quality attributes of a *good* benchmark. Additionally, we review some of the most important metrics and benchmarks for quantum processors proposed in the literature, assessing what quality attributes they fulfill. Finally, we propose general guidelines for quantum benchmarking. These guidelines aim to pave the way for establishing a roadmap towards standardizing the performance evaluation of quantum devices, ultimately leading to the creation of an organization akin to the Standard Performance Evaluation Corporation (SPEC).

Interfacing SIESTA with Qiskit

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The purpose of this project is to enable the high-accuracy first-principles computation of highly-correlated systems through Quantum Computing, using Density Functional Theory embedding (DFT+QC). Such software is of great interest to both research and industry, in particular since a quantum computer is under construction in the campus of Donostia-San Sebastián, Spain. The underlying idea is to consider a highly-correlated subsystem as an active space embedded in a larger system amenable to DFT. DFT embedding is not new: active spaces are already addressed by canonical quantum chemistry techniques such as configuration interaction (CI) or coupled-cluster (CC) methods. But these methods imply efforts that scale exponentially (or polynomially with a high power for good CC) with the number of particles in the system, which has so far limited its usefulness to very small active spaces. Quantum computing and its ability to access CI and CC calculations for much larger systems have opened the possibility of studying a much broader set of correlated systems with high accuracy, allowing at last to address systems of great relevance in, e.g., chemical catalysis, energy materials, batteries, photovoltaics, with systematically improvable accuracy. Therefore, we are implementing a hybrid classical and quantum computing paradigm through DFT embedding in SIESTA, sending the CC or CI calculations to be performed for the active space to the quantum computer by means of calls to Qiskit. It follows the pilot study by the group of Prof. Ivano Tavernelli at IBM Zürich (DOI:10.1063/5.0029536). For SIESTA, the expected results are: (1) make higher-accuracy calculations beyond DFT possible and let the wide community of SIESTA users access quantum computing. (2) reach higher system sizes than current CC and CI calculations via the embedding of quantum computing into DFT. (3) provide sensible use cases for the hybrid quantum-classical paradigm, with both the versatility of classical computers and the power of quantum computation for the relevant parts of a calculation. It will open the way to predictive simulations of condensed matter with high and controllable accuracy yet inaccessible to DFT, expanding its scope and application base significantly, including scientific problems raised by energy, medical, and environmental challenges. At this stage, taking into account the rapid evolution of quantum devices and associated software ecosystems for the years to come, we can consider 4 lines of extensions beyond the current project: enhancing the ground-state workflow, including excited states, accessing vibrational structures, and extending DFT+U+V beyond mean field. On the long run, any company using or wanting to use predictive first-principles calculations in their processes (e.g. the clients of Simune, a spin-off of CIC nanoGUNE) will be able to benefit from quantum computing in a relatively seamless way for simulations previously inaccessible, thereby removing barriers to market.

Oddities in the Shannon Entropy of the XXZ chain

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In this work we study the Shannon-Renyi entropy of the XXZ spin-1/2 chain, in particular in the limit of the Renyi order $n = \infty$, as a method for studying the entanglement of the Quantum Six-Vertex Model on a cylinder.

The Shannon-Renyi entropy for a quantum system is the Renyi entropy of the probability distribution obtained from the amplitudes of the ground state in a chosen basis. The use of these observables is justified by the fact that the Renyi entanglement entropy of a special type of two-dimensional wave-function, called Rohksar-Kivelson, can be reduced to the computation of the Shannon-Renyi entropy of one-dimensional models, reducing the complexity of the task. These wave-functions describe the ground-state of specific class of phases, called conformal quantum critical phases, which are a common occurence for models with local constraints.

In this work we find an extra logarithmic term in the entropy scaling when the system size is odd. This effect is due to the presence of frustration in the spin configurations when periodic boundary conditions are imposed on an odd sized chain.

The presence of the extra term is a deviation from the usual area law of entanglement, and importantly the scaling factor contains important information about the critical field theory that describes the low energy behaviour.

Exploring Discrete Time Crystals: Experimental Probing on latest IBM QPUs

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In periodically driven closed quantum systems, the discrete time translation symmetry can be spontaneously broken, yielding a novel out-of-equilibrium phase of matter called discrete time crystal or Floquet time crystal. These systems manifest rigid long-range order, where the interactions are believed to play a fundamental role, and subharmonic dynamics, which in this case is the response at half the driving frequency. We implement a periodically driven Ising model on the IBM Heron Quantum Processor, a state-of-the- art programmable processor which allows simulating systems with 100+ qubits where the above-mentioned properties are tested.

References:

• V. Khemani, A. Lazarides, R. Moessner, and S. L. Sondhi, Phys. Rev. Lett. 116, 250401 (2016).

• D. V. Else, B. Bauer, C. Nayak, Phys. Rev. Lett. 117, 090402 (2016).

• N. Y. Yao, A. C. Potter, I.-D. Potirniche, and A. Vishwanath, Phys. Rev. Lett. 118, 030401 (2017) and Erratum 118, 269901 (2017).

• J. Zhang, P. W. Hess, A. Kyprianidis, P. Becker, A. Lee, J. Smith, G. Pagano, I.-D. Potirniche, A. C. Potter, A. Vishwanath, N. Y. Yao, and C. Monroe, Nature 543, 217 (2017).

• A. Smith, M. S. Kim, F. Pollmann, and J. Knolle, npj Quantum Inf 5, 106 (2019).

• M. Ippoliti, K. Kechedzhi, R. Moessner, S. L. Sondhi, and V. Khemani, PRX Quantum 2, 030346 (2021).

• X. Mi, M. Ippoliti, C. Quintana, et al., Nature 601, 531–536 (2022).

Ultranarrow Linewidth and Enhanced Photostability in $CsPbBr_3$ Quantum Dots

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Abstract
Perovskite nanocrystals have emerged as a promising candidate for next-generation quantum dots (QDs) in quantum light sources, owing to their high quantum yield, narrower linewidth, and shorter lifetime. However, despite these excellent optical properties, the stability of perovskite QDs remains a significant challenge for practical applications. In this study, we have enhanced the stability of perovskite QDs both in solution over time and at the single QD level under illumination by employing a simple post-synthetic treatment with additional oleylamine. Furthermore, this treatment results in ultra-narrow emission linewidths, making these QDs highly promising for quantum light source applications.

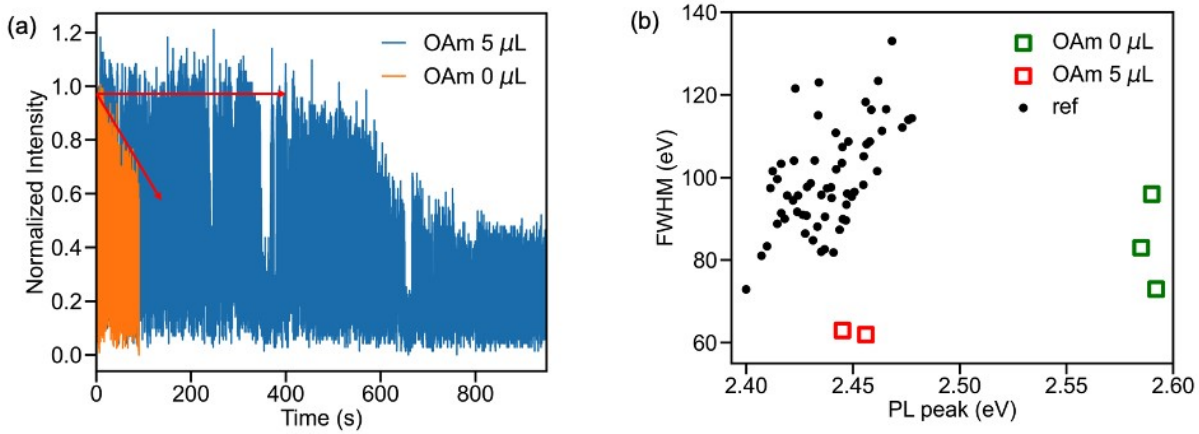

Figure 1. (a) Enhanced photostability of $CsPbBr_3$ QD with additional surface treatment of oleylamine. (b) Ultra-narrow emission linewidth of additional oleylamine treated $CsPbBr_3$ QDs.

Effectively decoupled unconventional superconducting condensates in a transition metal dichalcogenide

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A multicomponent superconducting phase diagram within a single material is quite unusual in nature and has been observed in only a few cases. In this study, we present evidence of the coexistence of two effectively decoupled superconducting phases in a van der Waals-stacked material, specifically the $4H_b$ polymorph of the isovalent alloy TaSSe. This material consists of alternating layers of 1T-TaSSe and 1H-TaSSe. Our findings are based on a detailed comparative analysis of the microscopic superconducting properties of both surface terminations, conducted using high-resolution scanning tunneling microscopy/spectroscopy (STM/STS) at 340mK. We investigated the properties of the superconducting state on both 1T and 1H surface terminations through quasiparticle tunneling and point-contact (Andreev reflection) spectroscopy. Our results reveal significant differences in the size and shape of the superconducting gap of the 1T and 1H phases. Furthermore, our data suggest unconventional pairing symmetry in the superconducting order parameter for both layers. This is further supported by temperature and magnetic field dependence STS measurements, which show disparate critical temperatures and upper critical magnetic fields for the superconducting states of the 1T and 1H surfaces, indicating a decoupled behavior in each termination. Our experimental results are complemented by theoretical calculations, where we solve the superconducting gap equation for a toy model based on a DFT band structure to identify the pairing states compatible with the experimental data. Our observations collectively point to the unique and complex nature of superconductivity in transition metal dichalcogenides.

Stimulated Raman scattering and molecular modulation in gas-filled anti-resonant fibres

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Over the last decade, anti-resonant hollow-core photonic crystal fibres emerged as a disruptive platform in nonlinear optics owing to their unique properties. If filled with gas, these fibres offer additional control over strong light-matter interactions due to their pressure-tunable dispersion landscape. Furthermore, when the filling gas is composed of molecules, stimulated Raman scattering can trigger the generation of coherence waves of synchronous molecular motion in the gaseous core, which can then be subsequently used for different applications. Here we revisit the state-of-the-art applications of in-fibre stimulated Raman scattering and molecular modulation, including the development of e.g. compact gas-based fibre lasers or nonlinear multidimensional convertors, as well as novel quantum technological solutions for single-photon delivery and efficient quantum frequency conversion, among others. We will outline what the current and future trends in the field are, along with an optimistic perspective to what lies ahead.

Sub-nanosecond coherent optical manipulation of a single aromatic molecule at cryogenic temperature

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The second quantum revolution presents challenges in manipulating and controlling quantum systems coherently. In solid-state physics, single emitters like molecules, quantum dots, and defects in diamond (NV centers) are promising for optical qubits or quantum networks due to their controllability with light and compatibility with nano-devices.

Single molecules trapped in the solid state at liquid helium temperatures are promising quantum emitters for the development of quantum technologies owing to their remarkable photostability and their lifetime-limited optical coherence time of the order of 10 ns. The coherent preparation of their electronic state requires resonant excitation with a Rabi period much shorter than their optical coherence time. Sculpting the optical excitation with sharp edges and a high on-off intensity ratio ($\sim 3\times10^5$) from a single-frequency laser beam, we demonstrate sub-nanosecond drive of a single dibenzanthanthrene molecule embedded in a naphthalene matrix at 3.2 K, over more than 17 Rabi periods, which to our knowledge constitutes the largest number of optical Rabi oscillations observed to date with a single solid-state emitter.

Coherent manipulation of the molecular electronic state, such as population inversion or superposition of the ground and excited states with maximal coherence, requires controlled pulse areas. With pulses tailored for a half-Rabi period, the electronic excited state is prepared with fidelity as high as 0.97. In order to characterize the robustness of the molecular transition dipole against decoherence induced by electron-phonon interaction, we have investigated the temperature dependence of the dephasing rate using single-emitter Ramsey spectroscopy. Using single-molecule Ramsey spectroscopy, we prove up to 5 K that the optical coherence lifetime remains at its fundamental upper limit set by twice the excited-state lifetime, making single molecules suitable for quantum bit manipulations under standard cryogen-free cooling technologies.

Reference :

Quentin Deplano, Philippe Tamarat, Brahim Lounis, Jean-Baptiste Trebbia; Sub-nanosecond coherent optical manipulation of a single aromatic molecule at cryogenic temperature. *AVS Quantum Sci.* 1 December 2023; 5 (4): 041402. https://doi.org/10.1116/5.0180689

Activation of metrologically useful genuine multipartite entanglement

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The metrological usefulness of a quantum state can be measured by the amount it outperforms the most useful fully separable state. It is known that maximal metrological usefulness necessitates genuine multipartite entanglement (GME). In contrast, however, not all GME states exhibit utility for metrology. In this work [1], to make non-useful entangled states useful we consider an activation scheme by employing multiple copies of the state. With this scheme, we identify a broad class of practically important GME states that can attain the maximal metrological performance in the limit of many copies, even though in the single copy case these states can be non-useful. Thus, we essentially activate quantum metrologically useful GME. Moreover, this maximal usefulness is reached exponentially fast with the number of copies and the necessary measurements are simple correlation observables. We also provide examples of states not living in the above mentioned class that improve their usefulness. Our scheme can also be used to protect certain quantum states against certain types of errors without the use of full-fledged quantum error correction techniques.

[1] R Trényi, Á Lukács, P Horodecki, R Horodecki, T Vértesi, G Tóth, New J. Phys. 26 023034 (2024).

Towards 'Good-Enough' qLDPC Codes.
A physical approach to error correction and Tanner code implementation

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The accumulation of errors in quantum computers obstructs the execution of powerful algorithms. Hence, current quantum computers require Quantum Error Correction (QEC) in order to be functional and reliable even in the presence of such errors, something known as Fault-Tolerant Quantum Computation (FTQC). Conventional strategies for protecting and correcting against qubit errors, such as *Surface Codes*, suffer from large overheads in the number of physical qubits that are used to encode logical information. In other words, practical implementation of quantum error-correcting codes requires a better ratio between the number of *logical* and *physical* qubits, something known as a high encoding rate. Quantum Tanner Codes have been shown to be optimal in the asymptotic limit due to their rich structure, providing a potential solution this conundrum. However, "good-enough" finite explicit constructions have not been found so far. In this work, we reformulate Tanner codes as unconventional lattice gauge theories describing spin many-body systems. Preliminary results indicate the potential for an unusually robust relative of topologically ordered matter as a key element for the outstanding capabilities of this family of codes.

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Genetic Algorithm-Based Method for Ansatz Updating in ADAPT-VQE

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ADAPT-VQE[1] is an algorithm within the VQE family used to calculate the ground state of a given Hamiltonian by optimizing an ansatz. This ansatz is built iteratively by adding at each iteration the excitation operator with the largest energy gradient. We detected two weaknesses in this method: (1) In the optimized ansatz, some operators have a very small contribution. This suggests that while they may have been important when added, as the ansatz grew they became irrelevant. (2) The operator with the largest gradient is not always the one with the major contribution to the energy[2] .

Genetic algorithm-based methods offer a potential solution to these issues as they allow more flexibility during the ansatz update. Here we analyse two possible mutations within this algorithm: (1) Deleting operators of the ansatz that can be removed without a substantial energy penalty. (2) Adding operators that are not the ones with the largest gradient, but may have a greater impact on the energy.

We believe that this approach can lead to a more efficient and accurate construction of the ansatz, ultimately improving the performance of VQE algorithms by reducing the circuit depth.

References

[1] Grimsley, H. R., Economou, S. E., Barnes, E., & Mayhall, N. J. (2019b). An adaptive variational algorithm for exact molecular simulations on a quantum computer. *Nature Communications*, *10*(1). https://doi.org/10.1038/s41467- 019-10988-2

[2] Ramôa, M. (2022, December 6). *Ansätze for Noisy Variational Quantum Eigensolvers*. arXiv.org. https://arxiv.org/abs/2212.04323

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