Research Highlights and Spotlights

February & March 2024

Pairing-based Graph Neural Network for Simulating Quantum Materials

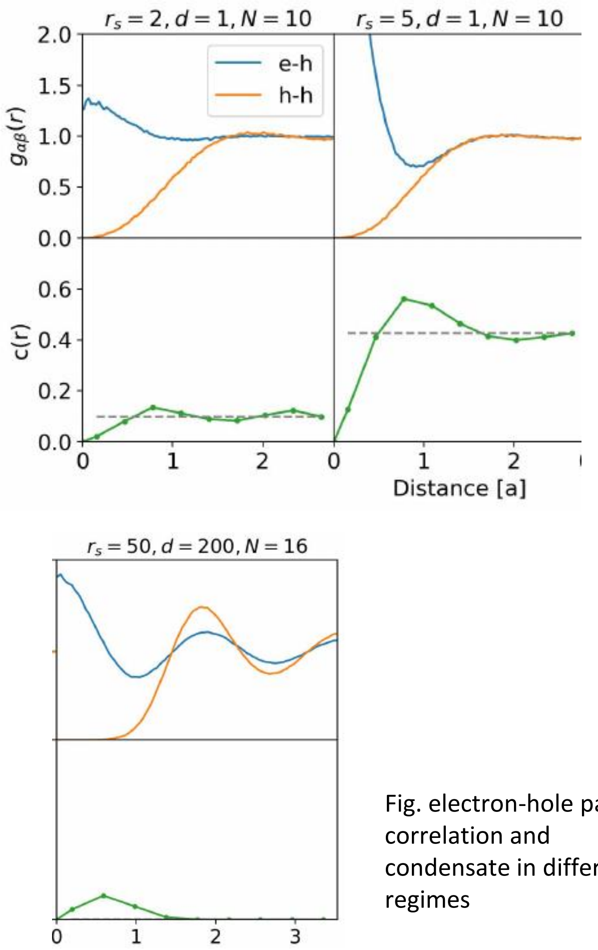

Fig. electron-hole pair correlation and condensate in different regimes

Scientific Achievement

We develop a pairing-based graph neural network for simulating quantum many-body systems.

Significance and Impact

We apply this method to two-dimensional semiconductor electron-hole bilayers and obtain highly accurate results on a variety of interaction-induced phases, including the exciton Bose-Einstein condensate, electron-hole superconductor, and bilayer Wigner crystal.

Research Details

– We construct a Geminal neural wavefunction using physics intuition by starting with a Bogoliubov de Gennes mean-field wavefunction and augmenting it with a generalized pair amplitude by a graph neural network.

– We test the method on the semiconductor electron-hole bilayer and find that it accurately captures various phases, including the Bose-Einstein condensate, electron-hole superconductor, and bilayer Wigner crystal, yielding both the expected correlation functions and ground state energies significantly lower than the mean-field results.

– Our analysis of the correlation functions demonstrates the capability of using one unified neural network ansartz to discover distinct phases of a quantum many-body system with remarkably high accuracy, in contrast to the traditional method of using separate ansatzes for each phase and comparing which ansatz has the lowest energy.

We acknowledge the MIT SuperCloud for providing the computing resources used in this paper. LF acknowledges the support from National Science Foundation (NSF) Convergence Accelerator Award No.2235945. DL acknowledges support from the NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI) and the U.S. Department of Energy, Office of Science, National Quantum Information Science Research Centers, Co-design Center for Quantum Advantage (C2QA) under contract number DE-SC0012704.DDD was supported by the Undergraduate Research Opportunities Program at MIT.

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Di Luo, David D. Dai, Liang Fu
https://arxiv.org/pdf/2311.02143.pdf

C2QA Co-design Center for Quantum Advantage

Relative Contributions

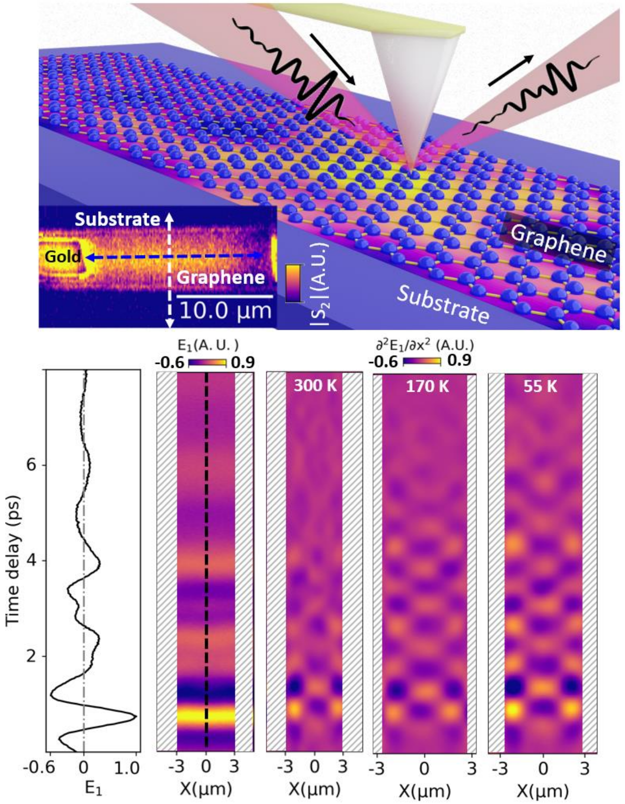
This work was supported, in part, by the U.S. Department of Energy (DOE) Office of Science, National Quantum Information Science Research Center, Co-design Center for Quantum Advantage (C^2QA) under contract no. DE-SC0012704.

- **D.L. supported by C^2QA and IAIFI performed work to:**
  - Design the project
  - Design the neural network algorithm
  - Perform theoretical analysis and numerical simulations
- **D.D. supported by Undergraduate Research Opportunities Program at MIT performed work to:**
  - Design algorithms for HFB calculation
  - Perform theoretical analysis and numerical simulations
- **L.F. supported by NSF Convergence Accelerator Award No.2235945 performed work to:**
  - Design the project
  - Design the experimental connection
  - Perform theoretical and numerical analysis

What We Did

- We develop a pairing-based graph neural network for simulating quantum phases of matter. We construct a Geminal neural wavefunction using physics intuition by starting with a Bogoliubov de Gennes mean-field wavefunction and augmenting it with a generalized pair amplitude by a graph neural network.
- Our architecture is both highly accurate and is scalable to large systems through transfer learning. As a test, we apply the method to the electron-hole bilayer with balanced electron and hole densities, and we perform Hartree-Fock-Bogoliubov calculations for reference.
- We find that our Geminal neural wavefunction is quantitatively accurate across the whole parameter space, including the BEC, BCS, and Wigner crystal regimes.
- Our analysis of the correlation functions demonstrates the capability of using one unified neural network ansartz to discover distinct phases of a quantum many-body system with remarkably high accuracy, in contrast to the traditional method of using separate ansatzes for each phase and comparing which ansatz has the lowest energy.
- Our study paves the way for physically-motivated neural network wavefunctions to be developed and applied to other challenging continuum systems in quantum materials.

Nano-terahertz Spacetime Mapping of Surface Plasmon Polariton in Strongly Interacting Dirac Fluids



Suheng Xu, Yutao Li, Rocco A. Vitalone, Ran Jing, Aaron J. Sternbach, Shuai Zhang, Julian Ingham, Milan Delor, James. W. McIver, Matthew Yankowitz, Raquel Queiroz, Andrew J. Millis, Michael M. Fogler, Cory R. Dean, James Hone, Mengkun Liu, D.N. Basov
https://arxiv.org/ftp/arxiv/papers/2311/2311.11502.pdf

Scientific Achievement

We have pioneered a novel time-resolved nano-spectroscopic methodology, termed nano-terahertz spacetime mapping. This innovative approach allows us to track the propagation of electron-photon quasiparticles over nanometer distance at femto-second time scales. We utilized the newfound capabilities to visualize the electronic interactions in monolayer graphene which hosts strongly interacting Dirac fluids.

Significance and Impact

Quasiparticle interference (QPI), arguably, is one of the most informative methods for probing interactions in quantum materials originally developed by scanning tunneling experimentalists. We proposed an entirely new version of QPI. First, the quasiparticles we employ are electron-photon quasiparticles rooted in tera-Hertz photons hybridized with Dirac electrons. Second, we explore the interference textures in space-time coordinates (bottom panels) gaining access to entirely new observables.

Research Details

- We developed the polaritonic spacetime methodology
- We studied the polaritonic cavity modes from room temperature to cryogenic temperatures and revealed the existence of long-lived polaritonic quasiparticles, exhibiting a remarkable lifetime of 5 picoseconds.
- We demonstrated the polaritonic renormalization in the Dirac fluids and quantified the electronic interaction strengths by measuring the chemical potential dependent group velocity and lifetime.

The development of space-time metrology is supported as part of Programmable Quantum Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), under award DE-SC0019443". Research on electronic interactions in graphene is supported by DOE-BES DE-SC0018426.

Relative Contributions

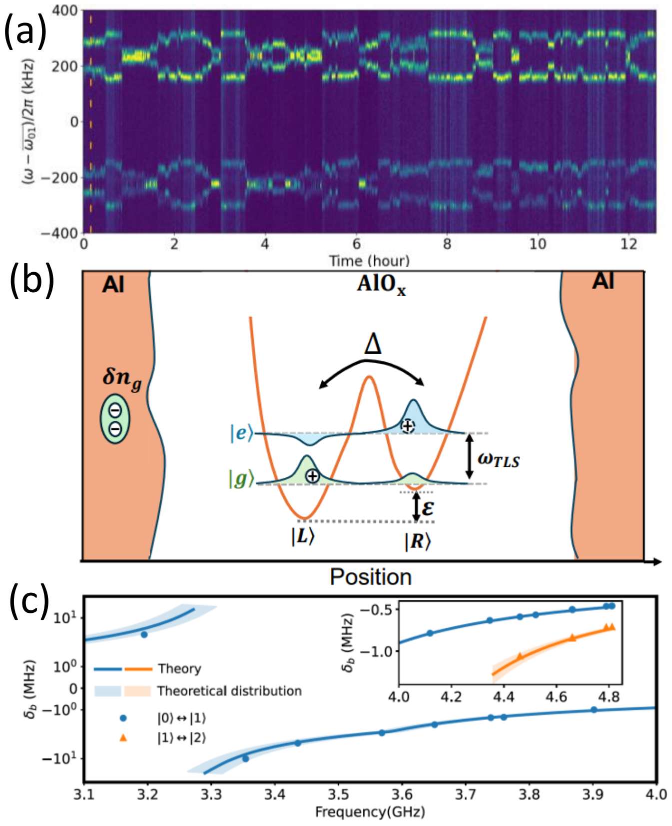
This work was supported, in part, by the U.S. Department of Energy (DOE) Office of Science, National Quantum Information Science Research Center, Co-design Center for Quantum Advantage (C^2QA) under contract no. DE-SC0012704.

- S.X., R.A.V., R.J., M.K.L., and D.N.B. received support for the THz-SNOM development through C^2QA.
- D.N.B. conceived of the study.
- M.K.L. and D.N.B. designed and developed instrumentations for space-time imaging
- S.X. recorded the near-field data with assistance from R. A. V., R. J., A. J. S. and S. Z.;
- Y.L. prepared the samples, with guidance from J. H and C. R. D;
- S.X. performed theoretical calculations and numerical simulations, with assistance from R. J., J. I., R. Q., A. J. M., M. M. F.;
- S.X. analyzed the data with assistance from R. A. V., R. J., A. J. S, S. Z., M. D., J. W. M, M. Y., A. J. M, M. M. F, M. L.;
- S.X. and D.N.B. wrote the manuscript with input from all the coauthors.

What We Did

- This is a new development based on the home-built cryogenic terahertz scanning near-field optical microscopy (SNOM), which enabled probing of the nano-electromagnetic response of materials in the terahertz frequency range. The present study visualized the traveling of electron-photon quasiparticles and unveiled the strong electronic interactions in a Dirac fluid. The manuscript is now posted on arXiv (arXiv:2311.11502)
- In the present study we measured dynamics of moving polaritonic wave packets in monolayer graphene. Motions of a plasmon polaritons are recorded on (1+1)d maps with ultrafine spacetime pixels.
- We developed theoretical models for calculating polaritonic group velocities and polaritonic lifetime based on graphene's ac conductivity. The models fully captures the experimental observations in both Fermi liquid and Dirac fluid regimes at distinct temperatures.
- We conducted a temperature-dependent study of polaritonic cavity modes and demonstrated a remarkably long polaritonic lifetime of up to 5 picoseconds at 55K.
- We studied how electronic interactions in the Dirac fluid altered the polaritonic dynamics. The polaritonic renormalization is most prominent at the charge neutral point, where plasmon polaritons are sustained by an equal density of thermally activated electrons and holes. The renormalization manifests itself in the reduced group velocity and polaritonic lifetime, both of which depend on the carrier densities. We were able to quantitatively extract electronic scattering rate and fine-structure constant of graphene, which serves as a measure of electronic interaction strength in graphene.

Observation of Discrete Charge States of a Coherent Two-level System in a Superconducting Qubit



Observe TLS-induced offset charge fluctuations.
(a). Spectroscopy data of the $|0\rangle \leftrightarrow |1\rangle$ transition of the qubit. (b). Schematic representation of the TLS-induced offset charge in the Josephson junction tunnel barrier. (c). TLS-induced dispersive shift δ_b as a function of the transmon frequency. The solid line is the theoretical prediction of the full Hamiltonian form of the qubit-TLS interaction. [2401.12183.pdf (arxiv.org)]

Scientific Achievement

We present unambiguous observations of the discrete charge states of a TLS in strong dispersive coupling to a superconducting qubit, which suggests that 1/f charge noise and microwave dielectric loss may indeed share a similar microscopic origin.

Significance and Impact

This study of a TLS provides direct evidence to the existence of a coherent tunnelling charge within the Al/AlOx/Al Josephson junction. From measurements of qubit-TLS coupling over up to 2 GHz of detuning, we characterize the full Hamiltonian form of the qubit-TLS interaction.

Research Details

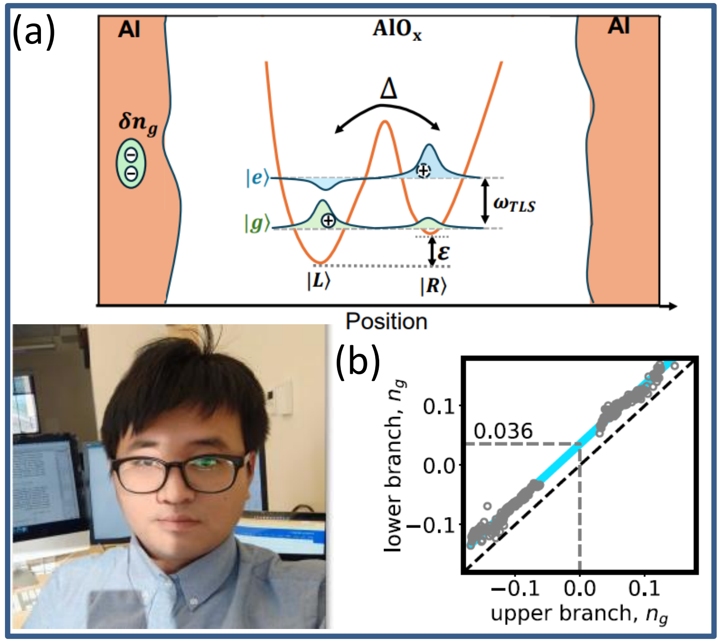
- We observe random telegraphing switching (RTS) between two qubit frequencies in addition to its dependence on charge parity, and the offset charge n_g associated with each frequency branch consistently differ by $\delta_{n_g} \approx 0.036$, which indicates discrete charge states of a coherent dielectric TLS
- Combining measurements in the strong dispersive and resonant regime, we quantify both transverse and longitudinal coupling of the TLS-qubit interaction, which further indicates that for similar long-lived dispersively-coupled TLS at lower frequencies (e.g., 0.1-1 GHz), its thermal excitations would directly lead to RTS of 10's of kHz without invoking TLS-TF interactions
- We further perform joint tracking of TLS transitions and quasiparticle tunneling dynamics and find no intrinsic correlations.

This work was mainly supported by the Co-design Center for Quantum Advantage (C^2QA) under contract number DE-SC0012704. Transmon qubits were fabricated and provided by the SQUILL Foundry at MIT Lincoln Laboratory, with funding from the Laboratory for Physical Sciences (LPS) Qubit Collaboratory.

Relative Contributions

- **The work was mainly supported by the U.S. Department of Energy, Office of Science, National Quantum Information Science Research Center, Co-design Center for Quantum Advantage (C^2QA) under contract No. DE-SC0012704.**
- **C^2QA participants performed the bulk of the research. B. L., Y. W., C. W. performed work under C^2QA to provide:**
  - Experimental measurements in both strong dispersive and resonant regime, quantifying both transverse and longitudinal coupling of the TLS-qubit interaction(BL, YW)
  - Experimental measurements in joint tracking of TLS transitions and quasiparticle tunneling dynamics(BL, YW, TS)
  - Interpretation of results and manuscript writing (all authors)
  - Problem statement and scientific direction (CW)
- **Transmon qubits were fabricated and provided by the SQUILL Foundry at MIT Lincoln Laboratory, with funding from the Laboratory for Physical Sciences (LPS) Qubit Collaboratory.**

C²QA Spotlight on Progress – Baojie Liu, U of MA - Amherst



Observe TLS-induced offset charge fluctuations.
(a). The TLS-induced offset charge in the Josephson junction tunnel barrier. The TLS is modelled as a tunnelling charged particle in a double-well potential. (b). Charge offsets of lower ($|e\rangle$) and upper ($|g\rangle$) states extracted from qubit data of the $|0\rangle \leftrightarrow |1\rangle$ transition of the qubit showing a difference of 0.036 (in units of 2e). The resultant qubit frequency consists of four distinct values corresponding to the $|g, e\rangle$ states of the TLS and the charge parity states of the qubit.

Progress/Achievement in Technical Areas of Interest

University of Massachusetts Amherst postdoc Baojie Liu has contributed to a new tool to distinguish different operator forms of qubit-TLS interaction. Furthermore, he has built a framework to observe the TLS-induced offset charge and monitor the TLS-parity jumping in experiment.

Significance and Impact

This study of a TLS provides direct evidence to the existence of a coherent tunnelling charge within the Al/AlOx/Al Josephson junction, which suggests 1/f charge noise and microwave dielectric loss may indeed share a similar microscopic origin.

Background and outlook

– Baojie Liu joined the Chen Wang lab at UMass in 2022, after obtaining his PhD from the Southern University of Science and Technology. His research prior to joining UMass has focused on quantum control in superconducting qubit and noise suppression for fault tolerance quantum computing using geometric phase.

– Baojie's current research mainly focus on elucidating decoherence mechanisms and implementing novel error corrected methods on superconducting device for the improvements of state preparation, qubit coherence, and single/two qubit-gate fidelity.

Baojie Liu, Yingying Wang, Tal Sheffer, Chen Wang. [arXiv:2401.12183 (2024)]
Work was performed at University of Massachusetts-Amherst for Co-design Center for Quantum Advantage

A New Class of Algorithms for Finding Short Vectors in Lattices Lifted from Co-dimension k Codes

Algorithm 1 Simple Version of Our Algorithm

```
list = {e_k}_{k=1}^d
v = Dual lattice vector in Z_P^d
Define π_0(w) := v · w.
Define

    reduce(v_a, v_b) = { v_b − [b/a]v_a  if [b/a] ≤ P^{1/(d−2)}
                       { v_a  otherwise.

where a = π_0(v_a) and b = π_0(v_b).
list = SortBy(list, π_0);
while π_0(list[1]) ≠ 0 and length(list) > 1 do
    newlist =
Table[reduce(list[n], list[n + 1]), {n, 1, length(list) − 1}];
    list = SortBy(newlist, π_0);
end while
Return list
```

Sketch of the new Lin-Shor lattice reduction algorithm (for classical computers) in its simplest form, showing key new ideas based on Euclid's algorithm and reduction using sorting.

Scientific Achievement

Breakthrough result which resolves an open Stephens-Davidowitz problem, to find an approximation scheme for the shortest-vector problem (SVP) which does not reduce to near-exact SVP

Significance & Impact

Accelerates solution of important shortest-vector in integer lattice problem, giving new mathematical insights into approaches for quantum money, post-quantum crypto, and coding theory

Details

- Builds on mathematical facts about certain lattices, discovered during work on quantum money
- Based on using the well-known Euclidean algorithm *en masse* to rapidly obtain a short lattice vector
- Achieves $O(d^2)$ runtime for d-dimensional lattices in useful parameter regimes
- Faster than the state-of-art LLL lattice reduction
- Empirically observed to find smaller lattices than SOTA algorithms

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Reference: 2401.12383.pdf (arxiv.org)
Authors: Robert Lin and Peter W. Shor
Work was performed at MIT and Harvard

HARVARD UNIVERSITY | Massachusetts Institute of Technology | C2QA Co-design Center for Quantum Advantage

Relative Contributions

- **The work was supported, in part, by the U.S. Department of Energy, Office of Science, National Quantum Information Science Research Center, Co-design Center for Quantum Advantage (C^2QA) under contract No. DE-SC0012704.**

  - Peter Shor (faculty) was funded by sources at MIT, including C^2QA.
  - The portion of this work which connected to ideas from quantum money was supported by C^2QA.

- **Robert Lin (graduate student) was funded from sources at Harvard.**

What We Did

- Robert Lin and Peter Shor introduce a new class of classical algorithms and algorithmic techniques for finding a short vector in lattices defined by certain error-correction codes.
- For lattices of the specified form, the new algorithm achieves superior runtime and finds smaller lattices than state-of-the-art algorithms.
- Lin and Shor resolve an open problem which was posed by Noah Stephens-Davidowitz in 2020, that of coming up with an approximation scheme for the shortest-vector problem (SVP) which does not reduce to near-exact SVP.
- An advantage of the Lin-Shor approach is that one may obtain short vectors even when the lattice dimension is quite large, e.g., 8000.
- For a given lattice modulo P, the Lin-Shor algorithm yields shorter vectors for larger lattice dimension d.

Our Team

With additional support from