Beyond AI Project
Analysis of materials' quantum properties using AI
(Quantum ID: Exploiting "Quantum Fingerprintings" of materials with AI)

Project Leader
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The goal of this project is to extract information hidden in complex quantum properties and quantum fluctuations, which appear in microscopic physical systems governed by quantum mechanics, using artificial intelligence (AI). The concrete research achievements are summarized below.

1. Deciphering quantum fingerprints in electric conductance using AI [1]

We have made the AI-assisted analysis of complex fluctuations in electric conductance (the reciprocal of resistance) that manifest in microscopic electric conduction in metals. In the minuscule metals with the nanometer size, the electrons responsible for electrical conduction obey quantum mechanics, demonstrating properties of both particles and waves, leading to quantum interference phenomena similar to the interference of water waves. The atomic-level impurities and lattice defects in the micro-metal lead to the interference between the wave functions, which are scattered from the impurities (or defects) and reflected at the edges of the metal. As a result, when the magnitude of the magnetic field applied to the metal changes, the electric conductance exhibits a highly complex pattern of fluctuations in response. This complex pattern is essentially originated from quantum mechanics, and unlike the random thermal fluctuations of the classical world, it retains microscopic information such as the positions of impurities in micro-metals, thus being termed as a 'quantum fingerprint'. However, due to its complexity, the standard procedure has been to analyze these fluctuation patterns by averaging, making it challenging to decode the hidden microscopic information. In this research, we successfully extract information about quantum interference of wave functions in micro-metals from the quantum fingerprints using AI. More specifically, we dealt with micro-metals incorporating various impurity arrangements by numerically solving the Schrödinger equation for electrons, allowing us to determine interference patterns of the wave functions and derive the magnetic field-dependent electric conductance. We start with the machine learning on image data of these interference patterns based on a Variational Autoencoder (VAE), enabling us to extract their characteristic features in a latent space (Feature Extraction Network). Subsequently, we trained a deep neural network to estimate the characteristic features extracted by the VAE from the quantum fingerprints in electric conductance (Geometry Generative Network). This approach enabled us to successfully reconstruct microscopic quantum information such as impurity positions and interference patterns from the quantum fingerprint in the micro-metals. (See Fig. 1)

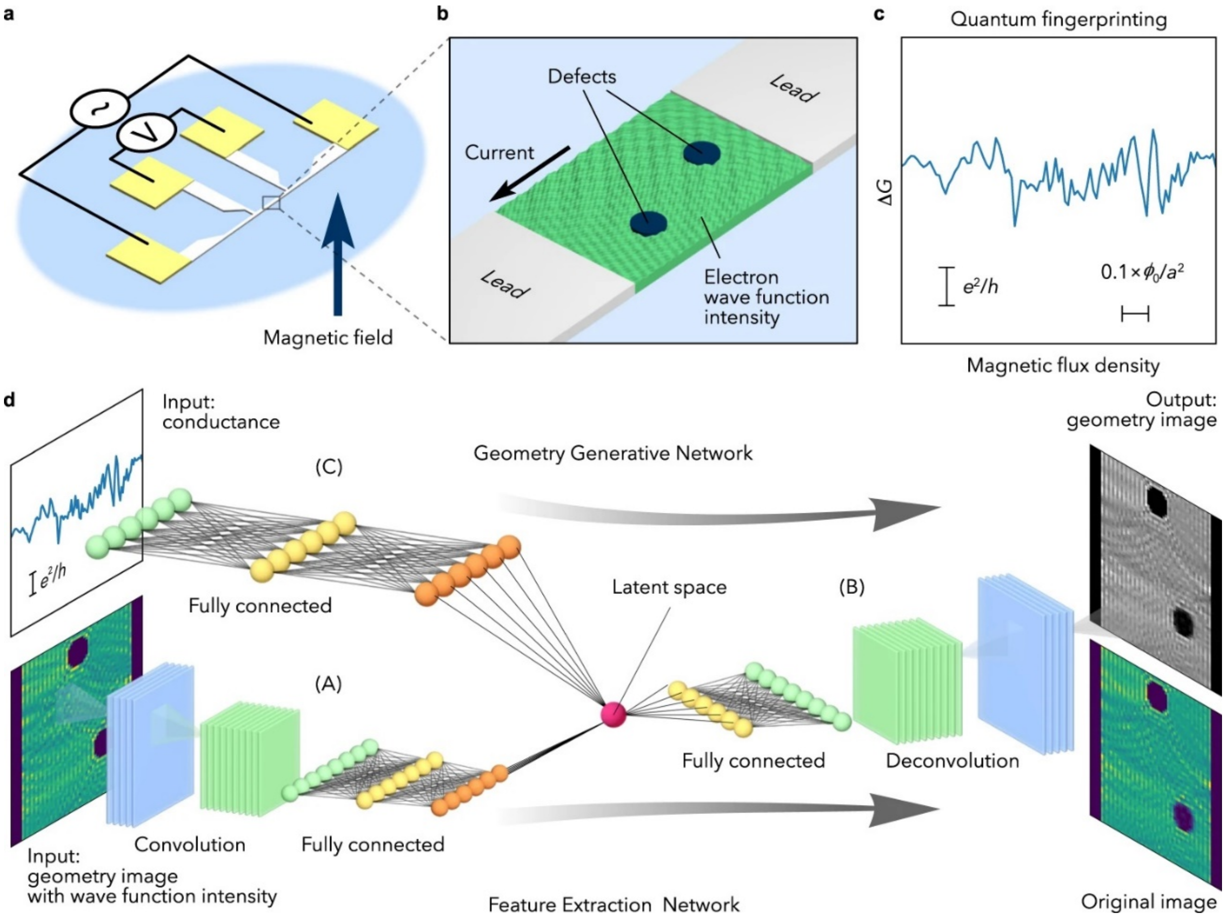

Fig.1 : Schematic image of deciphering quantum fingerprints in electric conductance [1].

2. Quantum circuit distillation using AI [2]

We utilize AI in research on fluctuations that appear in the output of quantum computations performed by quantum computers and lead to errors in computations. Quantum operations performed on quantum bits (qubits), the basic units of a quantum computer, are governed by quantum mechanics, and it is known to be extremely challenging to achieve precise quantum operations due to various external disturbances. The frequency of errors increases with the number of quantum operations required for quantum computation, leading to greater fluctuations in the output results, which make meaningful computations impossible. In this research, we performed reinforcement learning in AI for the ideal relationship between inputs and outputs for the quantum circuits (sequences of quantum operations) used in quantum computations. This allowed us to discover new quantum circuits that achieve (almost) the same outputs as well-known quantum circuits but are composed of fewer quantum operations. The discovered quantum circuit, with fewer quantum operations compared to conventional ones, can exhibit smaller errors in the final output. Implementing this new quantum circuit using superconducting qubits in an actual quantum computer has successfully led to output results with fewer errors compared to conventional circuits in quantum computations. (See Fig.2)

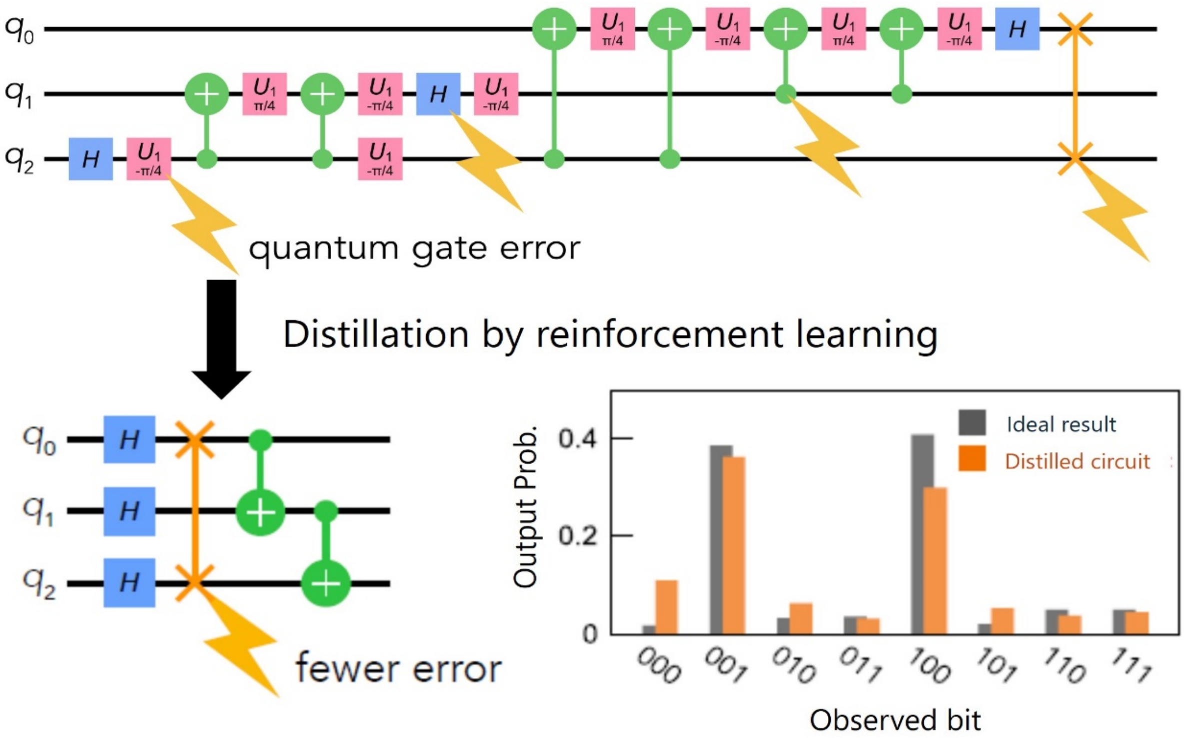

Fig.2 : Quantum circuit distillation of the inverse quantum Fourier transform of three qubits by reinforcement learning [2].

3. Quantum state tomography for magnons [3, 4]

We are conducting research using AI not only for known physical systems that exhibit quantum properties, but also exploring new quantum physical systems for the AI-assisted research in this project. One of these is the system of magnons, which are elementary excitations in magnetic materials. Magnons are fluctuations in the quantum spins of electrons responsible for magnetism and have played a crucial role in the field of spintronics, where next-generation, low-power-consumption devices utilizing spins are actively explored. To discern whether magnons exhibit quantum properties, it is essential to investigate the statistical distribution followed by the fluctuations of magnons. This necessitates extensive data acquisition and analysis of magnon fluctuations. In this research, we have successfully implemented a technique called state tomography for the first time concerning magnons, allowing the determination of the presence or absence of quantum properties in the states of magnons generated and controlled by magnetic fields and microwaves [3, 4]. This advancement enables the acceleration of exploration into various quantum states based on magnons and their potential applications in the future.

Selected papers :

[1] S. Daimon, K. Tsunekawa, S. Kawakami, T. Kikkawa, R. Ramos, K. Oyanagi, T. Ohtsuki and E. Saitoh, Nature Communications **13**, 3160 (2022). (https://doi.org/10.1038/s41467-022-30767-w)

[2] S. Daimon, K. Tsunekawa, R. Takeuchi, T. Sagawa, N. Yamamoto and E. Saitoh, arXiv:2309.01911[quant-ph]. (https://doi.org/10.48550/arXiv.2309.01911)

[3] Tomosato Hioki, Hiroki Shimizu, Takahiko Makiuchi, and Eiji Saitoh, Physical Review **B104**, L100419 (2021). (https://doi.org/10.1103/PhysRevB.104.L100419)

[4] Tomosato Hioki and Eiji Saitoh, Journal of Applied Physics **132**, 203901 (2022). (https://doi.org/10.1063/5.0123221)