Energy materials and thermoelectric conversion, Quantum computing, Nano-structured device design

New developments in quantum many-body systems through the integration of quasicrystal property research and quantum algorithm development

Department of Physics, Graduate School of Science

Associate Professor Nayuta Takemori

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Abstract

We propose a novel interdisciplinary research that bridges the gap between **quasicrystal materials science** and **quantum algorithm development** to create new directions in quantum many-body physics. Quasicrystals—structures that lack translational periodicity yet possess long-range order—exhibit unique electronic, thermal, and transport properties absent in conventional crystals. Simultaneously, quantum algorithms tailored to strongly correlated systems remain a frontier in quantum information science. In our approach, we aim to elucidate the physical properties of quasicrystalline systems via first-principles modeling and numerical simulation, while developing efficient quantum algorithms to simulate large-scale correlated quasicrystal models beyond classical feasibility. The synergy of materials insight and quantum computation offers a two-way feedback: physical models guide algorithmic design, and algorithmic advances unlock new regimes of material prediction and control.

Background & Results

Quasicrystals, first discovered in the 1980s, exhibit long-range order without periodicity, challenging traditional crystallography. Their aperiodic structures give rise to unconventional thermal and electronic properties, with potential applications in thermoelectrics and quantum technologies. However, theoretical understanding remains limited, particularly in the presence of strong correlations and interactions.

Meanwhile, quantum algorithms for many-body systems are rapidly developing, yet applying them to nonperiodic and strongly interacting systems remains challenging.

In this work, we explore a hybrid approach, integrating theoretical modeling of correlated quasicrystalline systems—including structures with hyperuniform order—with quantum algorithmic techniques for efficient characterization. Our goal is to establish a framework that connects aperiodic materials science with emerging quantum computational methods, paving the way for future breakthroughs in both fundamental understanding and practical simulation capabilities.

Significance of the research and Future perspective

This research lies at the intersection of quantum materials and quantum information science, aiming to establish new foundations for the computational exploration of aperiodic systems. By combining insights from quasicrystal physics with advances in quantum algorithms, we seek to enable: (i) principled modeling of thermally and electronically unconventional materials, (ii) scalable simulation strategies for nonperiodic, strongly correlated systems, and (iii) feedback between material theory and algorithm design.

Future directions include extending our methods to more complex geometries and model classes, while incorporating quantum-classical hybrid approaches and resource-efficient algorithmic techniques. Rather than offering immediate solutions, our work contributes a conceptual and computational framework with long-term relevance for both fundamental science and potential applications.

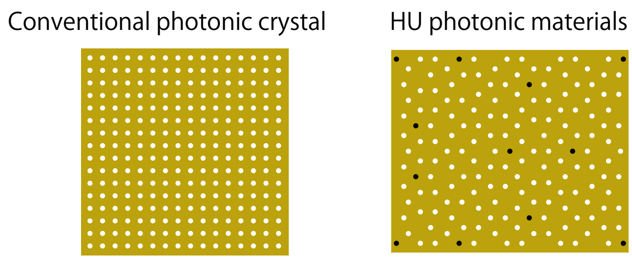

Figure 1. Designing optical control materials via quasiperiodicity and hyperuniformity

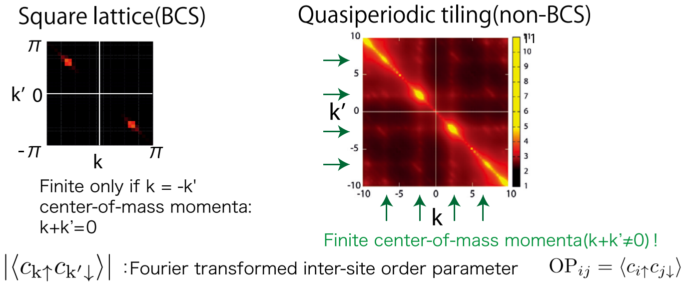

Figure 2. Finite center-of-mass momentum pairs in quasicrystals: beyond conventional theory

Patent

Treatise

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