Press release **For immediate release**

HKU physicists make a stride closer in the quest for quantum materials through better measurement of quantum entanglement

February 14, 2022

A research team from the Department of Physics, the University of Hong Kong (HKU) has developed a new algorithm to measure entanglement entropy, advancing the exploration of more comprehensive laws in quantum mechanics, a move closer towards actualisation of application of quantum materials.

This pivotal research work has recently been published in one of the most prestigious journals in physics – *Physical Review Letters*.

Quantum materials play a vital role in propelling human advancement. The search for more novel quantum materials with exceptional properties has been pressing among the scientific and technology community.

2D Moire materials such as twisted bilayer graphene are having a far-reaching role in the research of novel quantum states such as superconductivity which suffers no electronic resistance. They also play a role in the development of "quantum computers" that vastly outperforming the best supercomputers in existence.

But materials can only arrive at "quantum state" , i.e. when thermal effects can no longer hinder quantum fluctuations which trigger the quantum phase transitions between different quantum states or quantum phases, at extremely low temperatures (near Absolute Zero, -273.15°C) or under exceptional high pressure. Experiments testing when and how atoms and subatomic particles of different substances "communicate and interact with each other freely through entanglement" in quantum state are therefore prohibitively costly and difficult to execute.

The study is further complicated by the failure of classical LGW (Landau, Ginzburg, Wilson) framework to describe certain quantum phase transitions, dubbed Deconfined Quantum Critical Points (DQCP). The question then arises whether DQCP realistic lattice models can be found to resolve the inconsistencies between DQCP and QCP. Dedicated exploration of the topic produces copious numerical and theoretical works with conflicting results, and a solution remains elusive.

Mr Jiarui ZHAO, Dr Zheng YAN, and Dr Zi Yang MENG from the Department of Physics, HKU successfully made a momentous step towards resolving the issue through the study of quantum entanglement, which marks the fundamental difference between quantum and classical physics.

The research team developed a new and more efficient quantum algorithm of the Monte Carlo techniques adopted by scientists to measure the Renyi entanglement entropy of objects. With this new tool, they measured the Rényi entanglement entropy at the DQCP and found the scaling behaviour of the entropy, i.e. how the entropy changes with the system sizes, is in sharp contrast with the description of conventional LGW types of phase transitions.

"Our findings helped confirm a revolutionised understanding of phase transition theory by denying the possibility of a singular theory describing DQCP. The questions raised by our work will contribute to further breakthroughs in the search for a comprehensive understanding of unchartered territory," said Dr Zheng Yan.

"The finding has changed our understanding of the traditional phase transition theory and raises many intriguing questions about deconfined quantum criticality. This new tool developed by us will hopefully help the process of unlocking the enigma of quantum phase transitions that has perplexed the scientific community for two decades," said Mr Zhao Jiarui, a PhD who came up with the final fixes of the algorithm.

"This discovery will lead to a more general characterisation of the critical behaviour of novel quantum materials, and is a move closer towards actualisation of application of quantum materials which play a vital role in propelling human advancement." Dr Meng Zi Yang remarked.

Quantum entanglement entropy and quantum materials

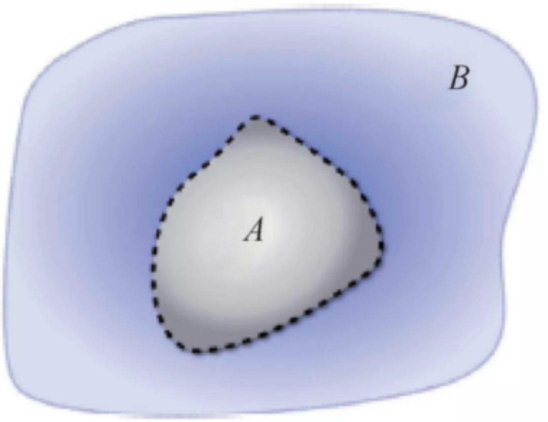

Image 1. A quantum system with subsystem A and its compliment B.

For a quantum state, particles in subsystem A are entangled with particles in subsystem B through quantum entanglement. The quantum entanglement entropy is to measure how much particles in a subsystem A are entangled with the rest of particles in the system. Quantum entanglement is a universal feature for quantum materials and thus can be regarded as a fingerprint for various of quantum materials.

The models

To test the efficiency and superior power of the algorithm and demonstrate the distinct difference between the entanglement entropy of normal QCP between DQCP, the research team chose two representative models — the J_1-J_2 model hosting normal O(3) QCP and the J-Q_3 model hosting DQCP, as shown in Image 2.

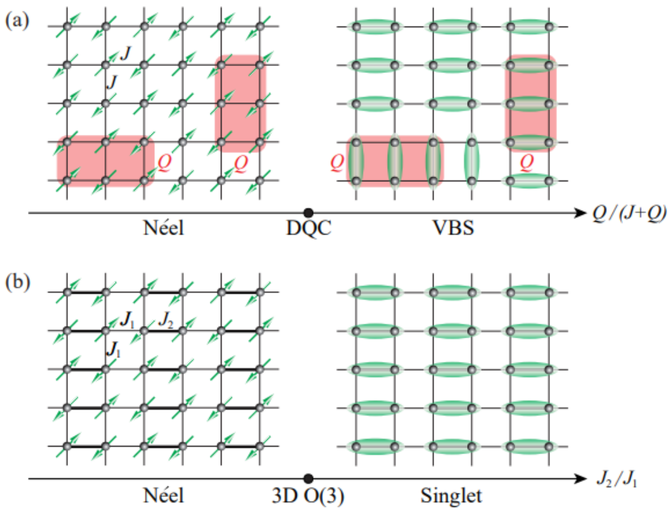

Image 2. The two lattice models: (a) For J-Q_3 model, the Q term characterises the strength of the six-site plaquette correlation (pink-shaded area), and the J term characterises the strength of nearest neighbour correlation. (b) For J_1-J_2 model, J_1 and J_2 separately identify the correlation strength between two kinds of nearest neighbours. , The J-Q_3 model hosts a DQCP when adjusting the ratio of Q term and J term, and the J_1-J_2 model hosts a O (3) QCP as the ratio of J_1 and J_2 is appropriately tuned.

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Nonequilibrium increment algorithm

Based on previous methods, the research team created a highly paralleled increment algorithm. As illustrated in Image 3, to the main idea of the algorithm is to divide the whole simulation task into many smaller tasks and uses massive CPUs to parallelly execute the smaller tasks thus greatly decreasing the simulation time. This improved method helped the team to simulate the two models previously mentions with high efficiency and better data quality.

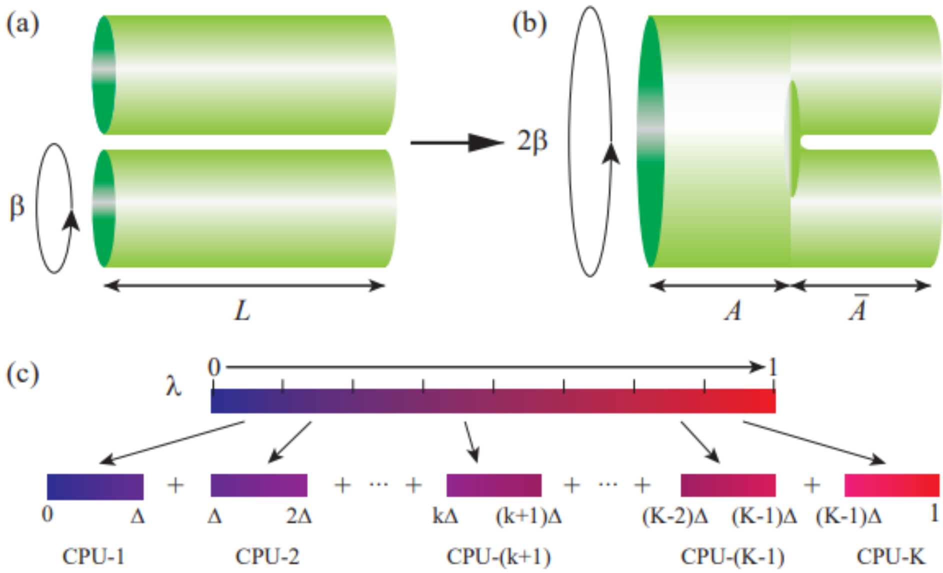

Image 3. The schematic diagram of the QMC diagram and the nonequilibrium increment method.

Findings

With the nonequilibrium increment method, the research team successfully obtain the second Rényi entanglement entropy $S_A^{(2)}$ at QCP and DQCP of the two models for different system sizes. The data is shown in Image 4, and one can find from the insets that when deducting the leading term(area law contribution from the entanglement boundary) the signs of the sub-leading term clearly distinguish the QCP (negative in J_1-J_2 model,) and DQCP (positive in J-Q_3 model). This finding rules out the possibility of the description of DQCP based on a unitary assumption and raises several intriguing questions about the theory of DQC. This discovery is likely to lead to a more general characterisation of the critical behaviour of novel quantum materials.

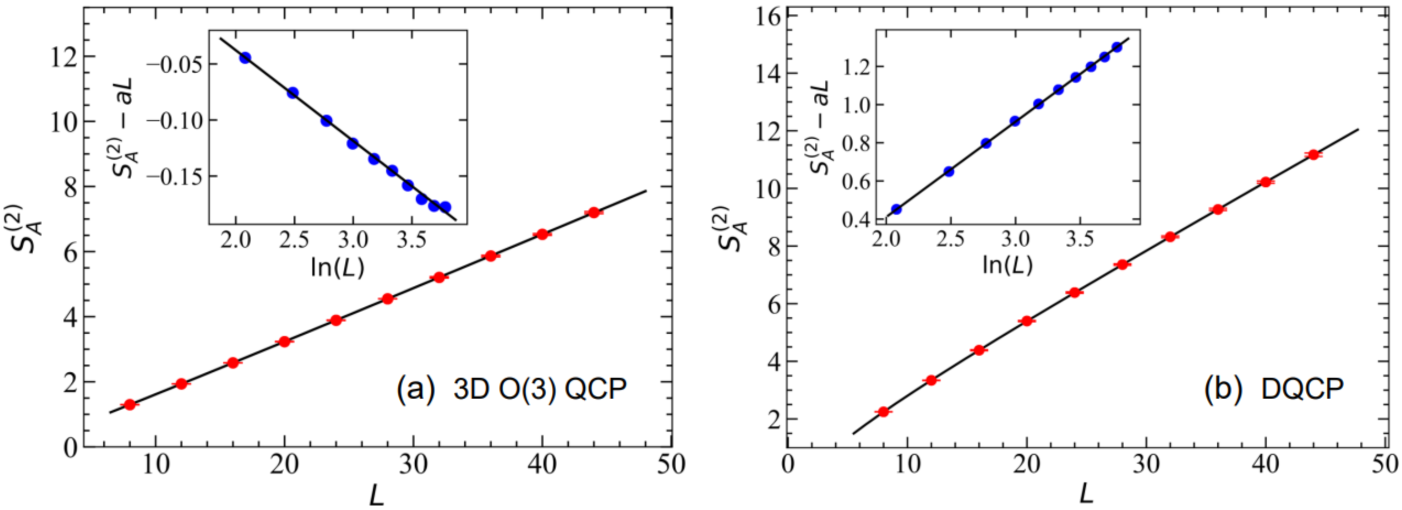

Image 4. Second Rényi entanglement entropy $S_A^{(2)}$ for (a) J_1-J_2 antiferromagnetic columnar dimer model at QCP and (b) J-Q_3 model which hosts DQCP. The insets of (a) (b) show the subleading log-corrections acquires a opposite sign for the two cases.

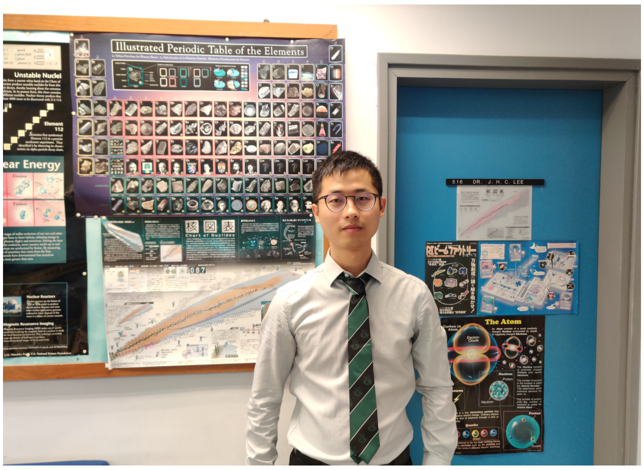

Image 5. Mr Jiarui ZHAO, a PhD student from Department of Physics from HKU, came up with this new algorithm of computing the quantum entanglement on a trip in the subway.

About the research

Mr Jiarui ZHAO is the first author of the journal paper. He is a PhD student from the Department of Physics, HKU, under the supervision of Dr Zi Yang Meng.

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The journal paper can be accessed from here:
https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.128.010601

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