

HKU project funded under the NSFC/RGC Joint Research Scheme

## **Practical Quantum Dynamics Simulation – Theory and Application**

Principal Investigator (Hong Kong):

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Project Summary:

Quantum computers have the potential to solve classically intractable problems, revolutionising fields like physics, chemistry, materials science, and data science. Despite significant progress in developing efficient quantum simulation algorithms and their applications over the past few decades, current quantum simulation research often relies on simplified theoretical models, faces challenges in experimental implementations, and lacks considerations of practical applications to realistic problems. To bridge this gap, the project aims to focus on advancing the theory and application of quantum dynamics simulation, with the overarching goal of enhancing the practicality of quantum computing.

From a theoretical standpoint, the project will study the development of new Hamiltonian simulation algorithms and introduce systematic theoretical tools for analyzing variational quantum simulations. From an application perspective, the project will investigate the potential uses of quantum simulation in studying the time evolution of quantum many-body systems, examining the static properties of quantum systems, and solving important classical problems in information technology.

This project aims to deepen our understanding of the fundamental theory of quantum computing, establish the groundwork for applying quantum computing in various fields, and ultimately propel the practicality of quantum computing for solving realistic problems. The project will bridge the gap between theory and application and pave the way toward unlocking the transformative potential of quantum computing.

港大「聯合科研資助基金計劃」項目

**實用化量子動力學類比：理論與應用**

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項目簡介：

量子動力學模擬是量子計算的重要研究方向之一，在量子算法設計和量子計算應用中扮演關鍵作用。然而，量子動力學模擬算法研究仍過於理論化和模型化，算法實現對量子計算硬件要求較高，同時缺乏在實際具體問題中的應用討論。為了推動量子計算的實用化，本項目聚焦量子動力學模擬的理論與應用。在理論方面，本項目將結合經典--量子混合計算思想提出和改進當前哈密頓量模擬算法，同時提出變分量子模擬算法的系統理論分析工具，建立高效的、具有理論保障的量子動力學模擬算法基礎理論。在應用方面，本項目研究量子動力學模擬在量子多體系統的動力學演化、量子系統的靜態特徵提取和經典問題三個方面中的應用，結合基礎理論、具體問題、算法實現和資源估計，構建實用化量子動力學模擬應用的可行性理論。本項目將加深對量子計算

基礎理論的理解，為量子計算在量子物理學、信息科技、材料科學、化學、醫學等方向的應用奠定基礎，推動量子計算的實用化。