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Quantum control and quantum computing

Hsi-Sheng Goan
NATIONAL TAIWAN UNIVERSITY
1, ROOSEVELT RD., SEC. 4
TAIPEI CITY, , 10617
TWN

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Hsi-Sheng Goan

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14. ABSTRACT
Project 20IOA033: Quantum Control and Quantum Computing Abstract: The goal of this project of “Quantum control and quantum computing” is to develop theoretical descriptions for various important issues and challenges in quantum control, quantum information processing, quantum machine learning, quantum chemistry, and quantum optimization from which design proposals
for novel applications will follow, accompanied by fundamental insights into quantum nanoscience. The specific research topics and results obtained in the period of 2021/09-2023/03 described in this report can be categorized into three parts: (A) Quantum Computation for Quantum Chemistry: (1) Qubit-efficient encoding scheme for quantum simulations of electronic structure, (2)
Accurate and efficient quantum computations of molecular properties, (B) Quantum Machine Learning: (1) Quantum reinforcement learning with a hybrid tensor network-variational quantum circuit (TN-VQC) architecture, (2) Single-qubit quantum agent and output reuse for quantum deep reinforcement learning, and (C) Quantum Optimization and Ising Model Problems: (1) Hybrid
Gate-Based and Annealing Quantum Computing for Large-Size Ising Problems. Keywords: Quantum Computing, Quantum Computational Chemistry, Quantum Machine Learning, Quantum Optimization, Variational Quantum Circuit, Vaiational Quantum Eigensolver, Ising Model Problems

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Project 20IOA033: Quantum Control and Quantum Computing

The goal of this project of "Quantum control and quantum computing" is to develop theoretical descriptions for various important issues and challenges in quantum control, quantum information processing, quantum machine learning, quantum chemistry, and quantum optimization from which design proposals for novel applications will follow, accompanied by fundamental insights into quantum nanoscience.

We describe below briefly the research results obtained for the project in the period of 2021/09-2023/03. The specific research topics and results described in this report can be categorized into three parts: (A) Quantum Computation for Quantum Chemistry, (B) Quantum Machine Learning and (C) Quantum Optimization and Ising Model Problems. We summarize the main result in each research topic below.

- **Quantum Computation for Quantum Chemistry**:

1. **Qubit-efficient encoding scheme for quantum simulations of electronic structure**

   Simulating electronic structure on a quantum computer requires encoding of fermionic systems onto qubits. Common encoding methods transform a fermionic system of N spin-orbitals into an N-qubit system, but many of the fermionic configurations do not respect the required conditions and symmetries of the system so the qubit Hilbert space in this case may have unphysical states and thus cannot be fully utilized. We propose a generalized qubit-efficient encoding (QEE) scheme that requires the qubit number to be only logarithmic in the number of configurations that satisfy the required conditions and symmetries. For the case of considering only the particle-conserving and singlet configurations, we reduce the qubit count to an upper bound of $O(m \log_2 N)$, where m is the number of particles. This QEE scheme is demonstrated on an H_2 molecule in the 6-31G basis set and a LiH molecule in the STO-3G basis set using fewer qubits than the common encoding methods. We calculate the ground-state energy surfaces using a variational quantum eigensolver algorithm with a hardware-efficient ansatz circuit. We choose to use a hardware-efficient ansatz since most of the Hilbert space in our scheme is spanned by desired configurations so a heuristic search for an eigenstate is sensible. The simulations are performed on IBM Quantum machines and the Qiskit simulator with a noise model implemented from an IBM Quantum machine. Using the methods of measurement error mitigation and error-free linear extrapolation, we demonstrate that most of the distributions of the extrapolated energies using our QEE scheme agree with the exact results obtained by Hamiltonian diagonalization in the given basis sets within chemical accuracy. Our proposed scheme and results show the feasibility of quantum simulations for larger molecular systems in the noisy intermediate-scale quantum (NISQ) era. The research results have been published in Phys. Rev. Research in 2020 [1].

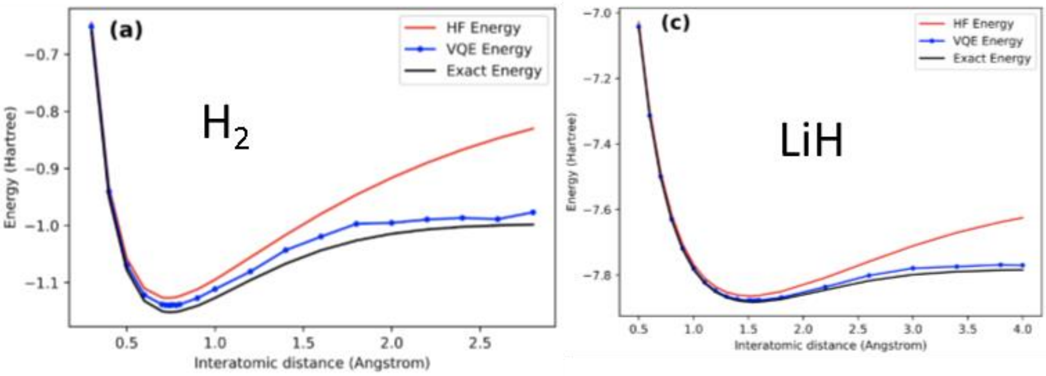

Fig. 1: Potential energy surfaces of an H2 molecule in the 6-31G basis set and a LiH molecule in the STO-3G basis set. The red curves were obtained using the Hartree-Fock method and the black curves represent the exact energy surfaces obtained by diagonalization of the Jordan-Wigner (JW) qubit Hamiltonian with classical algorithms. The blue curves were the extrapolated energies over three different CNOT gate counts with the energies of each CNOT gate count being averaged over ten sets of VQE experiments and with 104 shots for each iteration using a qubit-efficient encoding (QEE) qubit Hamiltonian. The simulations were performed on the QASM simulator with a noise model implemented from the calibration data of IBM quantum device ibmq_santiago.

2. Accurate and efficient quantum computations of molecular properties

Quantum chemistry calculation is considered as the most compelling application for quantum computing. However, this is technically limited to only small molecules due to the limitations on the number of qubits and the depth and complexity of computational circuits available in nowadays quantum computers. Consequently, reducing the number of required qubits is necessary to make quantum computation of molecular systems practical. Currently, the minimal contracted Gaussian basis set is commonly used in benchmark studies because it requires the minimum number of spin orbitals and thus the minimal number of qubits; nonetheless, the accuracy is generally low and thus cannot provide useful predictions. We demonstrate that a minimal basis set constructed from Daubechies wavelet basis can yield accurate results through a better description of the molecular Hamiltonian, while keeping the number of spin orbitals minimal. With the improved Hamiltonian through Daubechies wavelets, we calculate vibrational frequencies for H_2 and LiH using quantum-computing algorithm to show that the results are in excellent agreement with experimental data. This is an unprecedented demonstration of quantum computation with accuracy comparable with that of the full configuration interaction (FCI) method using a large basis set, whereas the computational cost is merely the same as that of a minimal basis set calculation. We also perform numerical experiments on a quantum simulator with a noise model implemented from a real quantum machine. We demonstrate that most of the error-mitigated data agree well with the exact FCI results within chemical accuracy. Thus, our work provides an efficient and accurate scheme for quantum computations of molecular systems, and for the first time demonstrates that predictions in agreement with experimental measurements are possible to be achieved with quantum resources available in near-term quantum computers.

The research results have been published in PRX Quantum in 2020 [2].

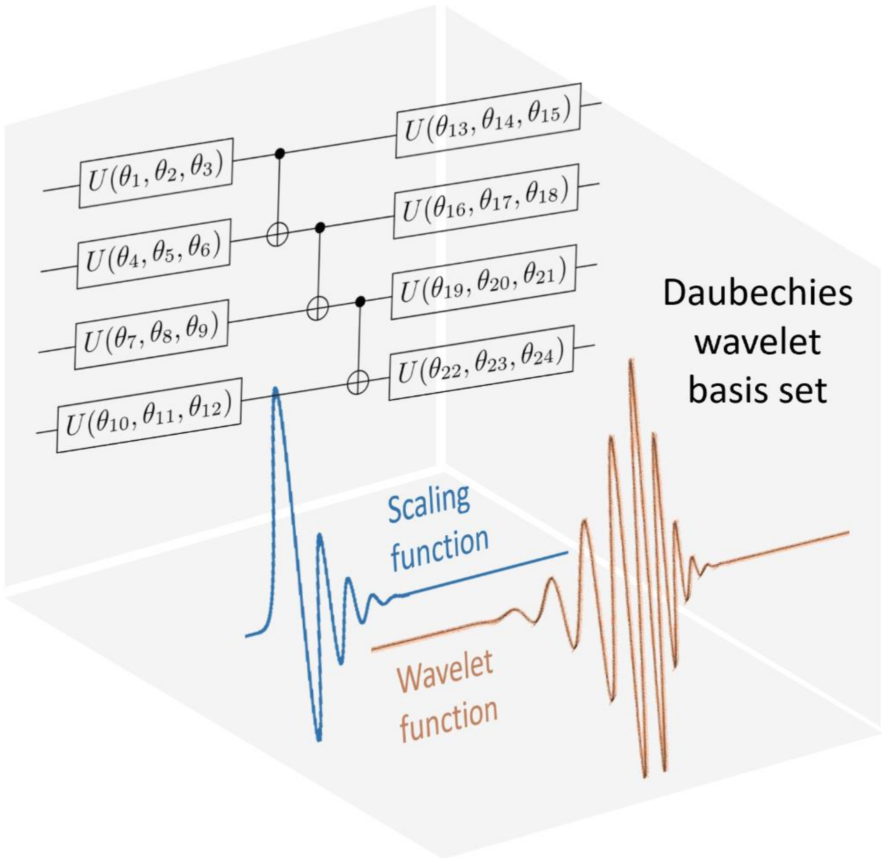

Fig. 2: Schematic illustrations of the two fundamental functions, a scaling function $\varphi(x)$ and a wavelet function$\psi(x)$, in the wavelet theory to construct the minimal basis Daubechies wavelet molecular orbitals, as well as the heuristic quantum circuit ansatz in the variational eigensolver algorithm for quantum computation of molecular properties..

- **Quantum Machine Learning (QML):**

1. **Quantum reinforcement learning with a hybrid tensor network-variational quantum circuit (TN-VQC) architecture**

Recent advances in classical reinforcement learning (RL) and quantum computation point to a promising direction for performing RL on a quantum computer. However, potential applications in quantum RL are limited by the number of qubits available in modern quantum devices. Here, we present two frameworks for deep quantum RL tasks using gradient-free evolutionary optimization. First, we apply the amplitude encoding scheme to the Cart-Pole problem, where we demonstrate the quantum advantage of parameter saving using amplitude encoding. Second, we propose a hybrid framework where the quantum RL agents are equipped with a hybrid tensor network-variational quantum circuit (TN-VQC) architecture to handle inputs of dimensions exceeding the number of qubits. This allows us to perform quantum RL in the MiniGrid environment with 147-dimensional inputs. The hybrid TN-VQC architecture provides a natural way to perform efficient compression of the input dimension, enabling further quantum RL applications on noisy intermediate-scale quantum devices. The research results have been published in Mach. Learn.: Sci. Technol. in 2020 [3].

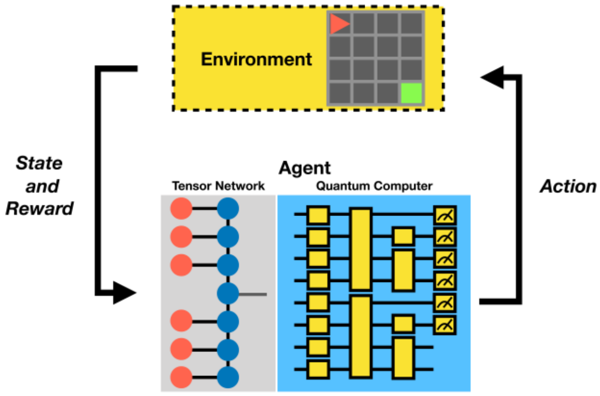

Fig. 3: Hybrid TN-VQC agent for the MiniGrid environment. In this framework, the observation or state, which is of a dimension exceeding the capabilities of available QCs, is first compressed into a vector via the trainable matrix product states (MPS). Compressed representation is then encoded into the VQC for further training. Action is chosen based on the output of the VQC. In this work, we train this TN-VQC model in an end-to-end fashion.

2. **Single-qubit quantum agent and output reuse for quantum deep reinforcement learning**

We provide concrete numerical evidence that the sample efficiency (the speed of convergence) of quantum RL could be better than that of classical RL, and for achieving comparable learning performance, quantum RL could use much (at least one order of magnitude) fewer trainable parameters than classical RL. Specifically, we employ the popular benchmarking environments of RL in the OpenAI Gym, and show that our quantum RL agent converges faster than classical fully-connected neural networks (FCNNs) in the tasks of CartPole and Acrobot under the same optimization process. We also successfully train the first quantum RL agent that can complete the task of LunarLander in the OpenAI Gym. Our quantum RL agent only requires a single-qubit-based variational quantum circuit without entangling gates, followed by a classical neural network (NN) to post-process the measurement output. Finally, we could accomplish the aforementioned tasks on the real IBM quantum machines. To the best of our knowledge, none of the earlier quantum RL agents could do that. The research results have been summarized as a manuscript posted in e-preprint arXiv [4].

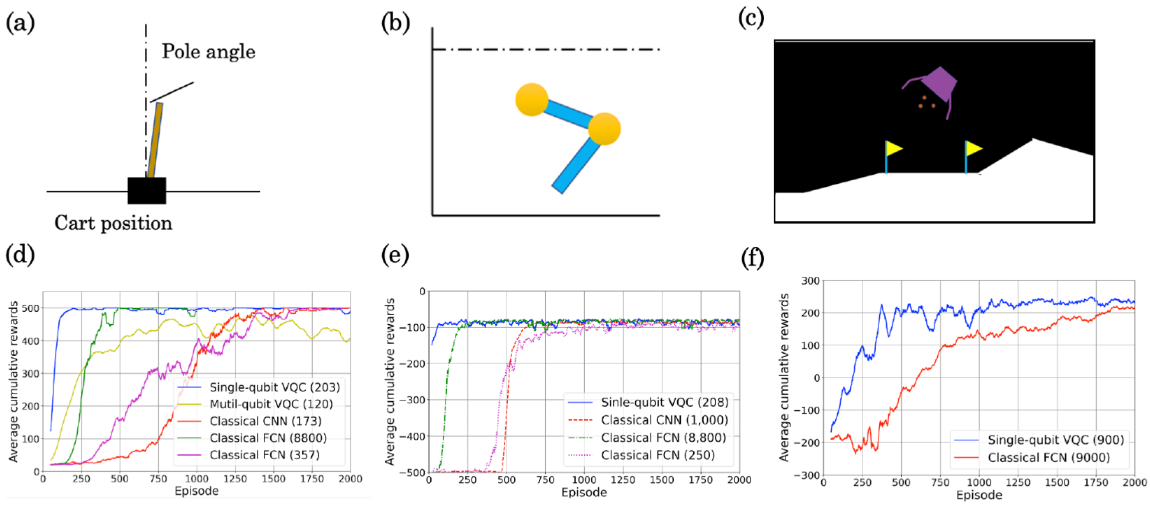

Fig. 4. Illustrations and performances of the single-qubit variational quantum circuit (VQC) using single-qubit systems with output reuse strategy, classical fully-connected neural network (FCN) and convolutional neural network (CNN) in the reinforcement learning (RL) optimization process for (a)(d) CartPole, (b)(e) Acrobot, and (c)(f) LunarLander problems. The numbers in the parentheses of different models are the total trainable parameters used in these models, respectively. The x-axis is the number of episodes and the y-axis represents the average cumulative reward, averaged over the last 20 episodes, at that episode. The CartPole and Acrobot experimental results are averaged over _ve runs and the LunarLander result is the best one in 10 runs. The sample efficiency follows approximately the relationship of Single-qubit VQC > classical FCN ≈ classical CNN > Multi-qubit VQC.

- **Quantum Optimization and Ising Model Problems**:

1. **Hybrid Gate-Based and Annealing Quantum Computing for Large-Size Ising Problems**

One of the major problems of most quantum computing applications is that the required number of qubits to solve a practical problem is much larger than that of today's quantum hardware. We propose an algorithm, called large-system sampling approximation (LSSA), to solve Ising problems with sizes up to $N_{\mathrm{gb}}2^{N\mathrm{g}_{\mathrm{b}}}$ by an N_{gb}-qubit gate-based quantum computer, and with sizes up to $N_{\mathrm{an}}2^{N\mathrm{g}_{\mathrm{b}}}$ by a hybrid computational architecture of an N_{an}-qubit quantum annealer and an N_{gb}-qubit gate-based quantum computer. By dividing the full-system problem into smaller subsystem problems, the LSSA algorithm then solves the subsystem problems by either gate-based quantum computers or quantum annealers, optimizes the amplitude contributions of the solutions of the different subsystems with the full-problem Hamiltonian by the variational quantum eigensolver (VQE) on a gate-based quantum computer, and determines the approximated ground-state configuration. We apply the level-1 approximation of LSSA to solving fully-connected random Ising problems up to 160 variables using a 5-qubit gate-based quantum computer, and solving portfolio optimization problems up to 4096 variables using a 100-qubit quantum annealer and a 7-qubit gate-based quantum computer. We demonstrate the use of the level-2 approximation of LSSA to solve the portfolio optimization problems up to 5120 ($N_{\mathrm{gb}}2^{2N\mathrm{g}_{\mathrm{b}}}$) variables with pretty good performance by using just a 5-qubit (N_{gb}-qubit) gate-based quantum computer. The completely new computational concept of the hybrid gate-based and annealing quantum computing architecture opens a promising possibility to investigate large-size Ising problems and combinatorial optimization problems, making practical applications by quantum computing possible in the near future. The research results have been summarized as a manuscript posted in e-preprint arXiv [5].

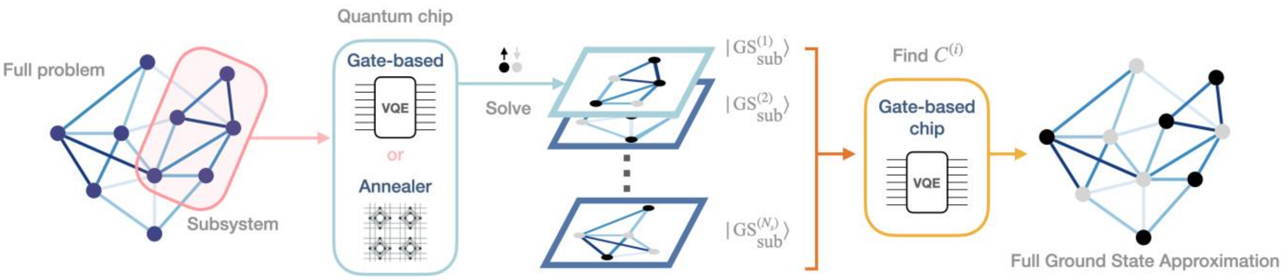

Fig. 5. Schematic flow chart of LSSA. After a procedure of random grouping of the spin variables from the full-system problem to form subsystems, the subsystem ground-state problems are solved by gate-based or annealing quantum chips. The resulting subsystem ground states are used to construct a trial state vector |Swc⟩ with

undetermined coefficients (amplitudes), and then the variational quantum eigensolver (VQE) is used to find the optimal coefficients.

We have managed to carry out our investigation of the project. At the moment, three papers have been published in scientific journal and two in the e-preprint arXiv. As a result of execution of the project, our understanding and knowledge towards quantum information processing, quantum chemistry, quantum machine learning and quantum optimization have advanced significantly. We acknowledge the support from the US Air Force Office of Scientific Research under award number FA2386-20-1-4033.

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