Annual Report (PhD Student)

University of Genoa, Italy

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Training Activities:

Course / Topic	Instructor	Institute	Dated
Python for Scientists - LINK	Prof. Andrea Lira Loarca	DICCA, UniGe	Mar 2024 ~ April 2024
Introduction to the Foundations of quantum mechanics and Applications	Prof. Paolo Solinas Prof. Pierantonio Zanghi	Dep of Physics, UniGe	Feb 2023 ~ Mar 2023
Interfacing gravity and Quantum Physics - LINK	Martinez, Hugget, Elder, Bose, Sanpera, Dvali, Ulbricht, overstreet, Northup	VCQ & TURIS Summer School 2024	Sep 2024 ~ Sep 2024
Quantum Optics	Prof. Dario Ferraro	Dep of Physics, UniGe	April 2024 ~ May 2024
Advanced Computational Physics	Prof. Riccardo Ferrando Prof. Diana Nelli	Dep of Physics, UniGe	June 2024 ~ July 2024
Research Project			
Practical Hands-on Related Software including python			
Future Research Activities and Plans			

Other Training Activities:

Course / Topic	Institute/By/Tool	From-to
Q-Bronze Quantum Computing and Programming workshop – LINK	Organized by Q-Slovenia	April 2024-April 2024
Specific Training for office staff-Low-risk	INFN	July 2024-July 2024
General Training of safety and health	INFN	July 2024-July 2024

Research Project

1. Introduction- Quantum Computer and Optimization

Quantum computing helps to solve tasks like simulating complex problems or large linear algebra problems that are impossible for conventional computers. Despite the challenges posed by noisy, intermediate-scale quantum computers, hybrid quantum-classical algorithms offer a practical compromise. These include the Quantum Approximate Optimization Algorithm (QAOA) and Variational Quantum Eigen solver (VQE). These methods optimize a cost function

by mapping it onto a quantum circuit, whereas a classical processor progressively adjusts parameters in response to the quantum measurements. However, the limited number of qubits and noise in the quantum circuits create a need for more resource-efficient ways to improve performance. Here, we offer an alternate approach to directly estimate the derivatives of the observable by connecting the system with the detector after measurement, the detector phase stores the information about the observable, its gradient, or the high derivatives. This method, known as quantum non-demolition measurement **(QNDM)**, reduces the circuit iterations required for optimization algorithms like gradient descent and Newton optimization.

2. Comparison of Direct Measurement (DM) and Quantum Non-Demolition Measurement (QNDM) Approaches

This work compares two methods to determine a quantum system's lowest energy state: Direct Measurement **(DM)** and Quantum Non-Demolition Measurement **(QNDM)**. In variational quantum algorithms, both methods are used to improve molecular simulations, such as those for lithium-hydrogen (Li-H) and lithium-lithium (Li_2) molecules. While **DM** has been a widely studied algorithm in the quantum optimization literature, **QNDM** provides a new computing strategy that leverages higher derivatives in a single run of a quantum circuit to reduce the computing resources required.

DM computes the cost function and its gradient by querying specific elements of the Hamiltonian. Quantum circuits are executed in **DM** to obtain the expectation values and the parameter shifts, after which the parameter-shift rule is used to compute the gradient. It requires different measurements for each parameter, leading to a more computationally hefty approach as the circuit grows more complex, especially in highly qubit-limited systems or where high-accuracy results are desired.

The unique feature of Quantum Non-Demolition Measurement **(QNDM)** is that the quantum detector is coupled to the system; thus, you can obtain information about the phase derivative of the observable, and it will be performed during the measurements.

This approach provides access to both the gradient and all higher-order derivatives directly from a single run of a single circuit, thereby reducing the number of repetitions we need to perform. **QNDM** is helpful in optimization algorithms, like gradient descent, because it speeds up convergence by skipping the need for extra measurements for each gradient calculation.

3. Methodology

The **QNDM** method connects a quantum system with a quantum detector, which gathers information about the observable gradient in its phase during a system-detector interaction. This happens through a few key steps:

1. **System-Detector Coupling:** The quantum system evolves under a unitary operator based on Hamiltonian parameters. While they interact, the system state is “frozen,” allowing the detector’s phase to store information about the desired derivative of the observable.
2. **Detector Measurement:** The quasi-characteristics function, which shows the accumulated phase of the detector, gives us the gradient of the cost function with less computational demands.

3. **Implementation with Qiskit for Molecule Optimization:** For practical use, the **QNDM** method was tested on molecular systems, including Lithium-Hydrogen (Li-H) and Lithium-Lithium through **Qiskit**. The process includes:
    i. **Constructing the Hamiltonian:** The Hamiltonian becomes a sparse Pauli operator, prepared for the quantum states of Li-H and Li-Li molecules.
    ii. **Quantum Circuit Setup:** Layered parameterized quantum circuits are built using rotation and entangling gates, optimized by **QNDM**.
    iii. **Gradient Calculation and Optimization: QNDM** calculates gradients effectively to iteratively lower the Hamiltonian energy, the molecule's ground-state energy.

    This approach was compared with the Direct Measurement **(DM)** technique, showing that **QNDM** can reach similar accuracy but needs less circuit depth and fewer measurements, highlighting its practical implementation in optimizing quantum tasks.

4. Future Research Activities and Plans

This idea involves simulating different molecular systems to determine their ground state energies. We want to use two techniques for quantum measurement, quantum Non-Demolition Measurement **(QNDM)** and Direct Measurement **(DM)**, to estimate and optimize the Hamiltonian energy efficiently. Using both **QNDM** and **DM** methods, we're trying to do some gradient-based optimization on the Hamiltonian, which should help us minimize energy and better estimate the ground state energy for each molecule.

Dated: 06/11/2024