Simulation of a quantum algorithm implemented in a single nitrogen vacancy center of diamond on IBMQ

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***Abstract*— Hybrid quantum systems based on diamond, such as the nitrogen vacancy (NV) centers, have potential to be used in quantum computation both due to long coherence times exhibited by nuclear spins and fast manipulation possible for electron spins. We run a quantum algorithm implemented in a single nitrogen vacancy center in diamond on IBMQ back ends to demonstrate the importance of having access to quantum devices via the cloud. In comparison with experimental investigations, we implement Grover's algorithm using Qiskit, and run on a simulator and device. The results we obtain are consistent with theoretical expectations and actual physical implementations.**

I. INTRODUCTION

One of the key application for quantum computation is to simulate quantum physics phenomenon [1]. Electron and nuclear spins associated with defects in solids provide natural hybrid quantum registers. Fully-controlled registers of multiple spins hold great promise as building blocks for quantum networks and fault-tolerant quantum computing [2]. The defect electron spin enables initialization and readout of the register and coupling to other (distant) electron spins, whereas the nuclear spins provide well-isolated qubits and memories with long coherence times. Superconducting quantum computers are prospective for the simulation of the dynamics of spin models. The important advantage of these machines is that they are programmable, so that different spin models can be simulated in the same chip, as well as various initial states can be encoded into it in a controllable way. This opens an opportunity to use superconducting quantum computers in studies of fundamental problems of statistical physics such as the absence or presence of thermalization in the free evolution of a closed quantum system depending on the choice of the initial state as well as on the integrability of the model. Programmable quantum computers have an advantage that the dynamics of different spin models can be modeled via unitary evolution using the same chip [3, 4]. Another positive aspect is that various initial conditions including entangled states of spins can be implemented thanks to the individual addressability of physical qubits in quantum computers. Therefore, it is also possible to analyze the dependence of the evolution on the initial conditions. Note that spin models are also directly applicable to study magnetic properties of various materials, see, e.g., so that quantum simulation of these models can have an impact on material science as well. Various physical systems, such as NMR, trapped atomic ions, optics and superconducting systems have been implemented efficient algorithms like Grover's and Shor's [5, 6]. In this work, we take advantage of quantum computers now available via the cloud [7, 8] to digitally simulate and demonstrate the reliability of this approach.

II. GROVER'S ALGORITHM

Grover's algorithm is an unstructered search algorithm on a database to find the item of interest. We first initialize the states to be in n-quantum register

$$|0\rangle^{\otimes n} = |0\rangle \tag{1}$$

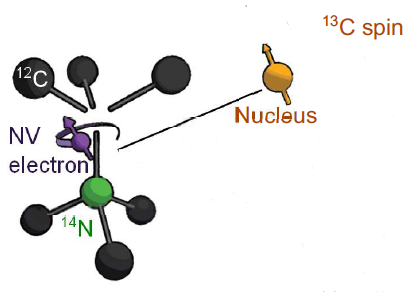
Putting the system into an equal superposition of states

$$H^{\otimes}|0\rangle = \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} |x\rangle \tag{2}$$

where $N = 2^n$ is the size of the database, $|x\rangle$ is the basis state of the system and n is the number of qubits. We implement the oracle O which performs the phase flip operation on the target state. The algorithm produces a quadratic speedup of complexity $O(\sqrt{N})$.

III. IMPLEMENTATION APPROACH

We consider the interaction of a single nitrogen vacancy center interacting with the carbon-13 nucleus spin in Figure 1 [9]. We first perform the initialization of the electron spin and carbon-13 spin using specific gates. This is followed by the quantum search algorithm and then reconstruct the target state using tomography. The target state of interest is $|01\rangle$. The phase flip operation [10] that is applied consists of four gates two of which are the Pauli X rotation and two U_1 phase gates. The sequence of these gates are shown in



spins.png

Fig. 1: Weakly coupling of nitrogen-vacancy (NV) electron spin to ^{13}C nuclear spin.

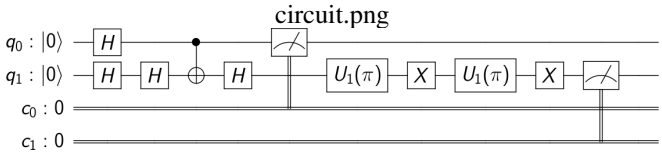


Fig. 2: Gate sequence of quantum search algorithm for the target state $|01\rangle$.

The Hamiltonian of the nv center and the ^{13}C spin is given by

$$H = A_{\|} S_z I z + A_{\perp} S_z I_x + \omega_L I_z \tag{3}$$

where $S_z, I_{x,z}$ are the electron and carbon nuclei spin operators, $A_{\|,\perp}$ are the parallel and perpendicular hyperfine coupling between the electron and nitrogen-14 spins.

IV. RESULTS

We simulate the circuit on a simulator in ibmq to reconstruct the target quantum state $|01\rangle$ as shown in Figure 3 and 4 below. There is a 0.97 probability of measuring the target state $|01\rangle$ although other states such $|00\rangle, |11\rangle, |10\rangle$ can be measured by changing the phase flip operation consisting of the Pauli x-rotation gate and the phase gates U_1 to be applied at a particular qubit.

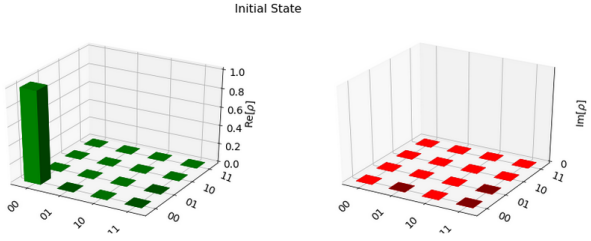


Fig. 3: Density matrices for the initial state $|00\rangle$.

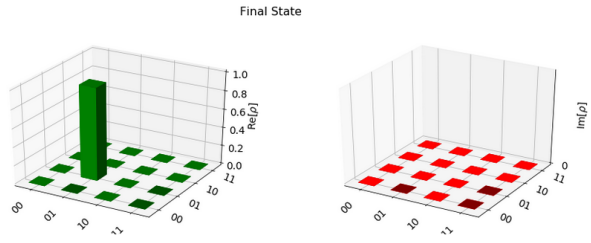


Fig. 4: Measured density matrices the target state $|01\rangle$.

For fidelity, F = 1 - gate errors we obtained the final state $|01\rangle$ fidelity of 0.83 $\pm$ 0.02 after the quantum search.

V. CONCLUSION

We simulate the implementation of Grover's search algorithm in a hybrid quantum computer based on NV center in diamond. We extend the simulation to include noise models and gate optimizations using tools provided on Qiskit. Our work shows that it is possible and more efficient to study, test and evaluate hybrid quantum circuits using quantum devices available on the cloud. Moreover, from this effort we envisage that open source software platforms like Qiskit can be improved to link with spin based physical devices. By utilizing the cloud interface, experiments could be specified, tested (both in the ideal case and with simulated errors), and then run to output noisy (but expected) results. Quantum simulation is one of the primary short- to mid-term goals of many research groups focusing on quantum computation. The potential advances that even a modest quantum simulator would unleash are substantial in a broad range of fields, from material science (high temperature superconductors and magnetic materials) to quantum chemistry. Quantum simulations are particular promising for simulating fermionic many-body systems and their phase transitions, where the "sign problem" limits efficient classical numerical approximation techniques. Larger quantum simulators could tackle problems in lattice QCD that currently consume a sizable fraction of scientific computing power, while quantum simulations of quantum chemistry have wide-ranging applications reaching as far as the design of molecules for new drugs. We have seen that the theoretical foundations have been laid quite comprehensively, providing detailed methods for efficient quantum simulators, and calculations that confirm their viability.

Ideally, this work will help motivate others to make use of the online hardware and software produced by IBM. Moreover, due to the individual addressability of physical qubits of the chip, one can create various initial conditions (different from Hamiltonian eigenstates) and to study the influence of these conditions on the free evolution of the system. The choice of models is linked to the topologies of the quantum chips as well as to gate errors we have chosen spin models with the arrangement of spins and interactions between them, which are in one-to-one correspondence with the quantum chips and available two-qubit gates between physical qubits of the chips. Although the reported results can be relatively easily found explicitly or using classical computers, scaling towards chips with many physical qubits, improved coherence times and reduced CNOT errors might lead to the resolution of problems which can hardly be solved using more traditional approaches. Indeed, in order to study the dynamics from first principles, one needs to know all eigenstates of a given Hamiltonian. The number of eigenstates, in general, increases exponentially with the increase of the particle number. Therefore, even quantum computers of medium sizes, which can appear in the near future, might be of practical importance for the modeling of dynamics of quantum systems. Even if errors will be still too large to simulate the dynamics untractable on classical computers, an implementation of advanced error correction codes should ultimately allow for such a modeling.

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REFERENCES

[1] K. L. Brown, W. J. Munro, and V. M. Kendon, "Using quantum computers for quantum simulation," *Entropy*, vol. 12, no. 11, pp. 2268–2307, 2010.

[2] L. Childress and R. Hanson, "Diamond nv centers for quantum computing and quantum networks," *MRS bulletin*, vol. 38, no. 2, pp. 134–138, 2013.

[3] A. Zhukov, S. Remizov, W. Pogosov, and Y. E. Lozovik, "Algorithmic simulation of far-from-equilibrium dynamics using quantum computer," *Quantum Information Processing*, vol. 17, no. 9, p. 223, 2018.

[4] F. Mazhandu, K. Mathieson, C. Coleman, and S. Bhattacharyya, "Experimental simulation of hybrid quantum systems and entanglement on a quantum computer," *Applied Physics Letters*, vol. 115, no. 23, p. 233501, 2019.

[5] J. Zhang, S. S. Hegde, and D. Suter, "Efficient implementation of a quantum algorithm in a single nitrogen vacancy center of diamond," *arXiv preprint arXiv:1911.06371*, 2019.

[6] M. Amico, Z. H. Saleem, and M. Kumph, "An experimental study of shor's factoring algorithm on ibm q," *arXiv preprint arXiv:1903.00768*, 2019.

[7]

[8] Q. Textbook, *Qiskit Textbook*, 2018.

[9] Y. Qiu, W. Xiong, L. Tian, and J. You, "A hybrid quantum system: Coupling spin ensembles via superconducting flux qubits," *arXiv preprint arXiv:1401.3095*, 2014.

[10] J. Gao, F. Sun, and C. W. Wong, "Realizing quantum controlled phase-flip gate through quantum dot in silicon slow-light photonic crystal waveguide," *arXiv preprint arXiv:0803.1017*, 2008.