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Article

Experimental study of Forrelation in nuclear spins

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ABSTRACT

Correlation functions are often employed to quantify the relationships among interdependent variables or sets of data. Recently, a new class of correlation functions, called Forrelation, has been introduced by Aaronson and Ambainis for studying the query complexity of quantum devices. It was found that there exists a quantum query algorithm solving 2-fold Forrelation problems with an exponential quantum speedup over all possible classical means, which represents essentially the largest possible separation between quantum and classical query complexities. Here we report an experimental study probing the 2-fold and 3-fold Forrelations encoded in nuclear spins. The major experimental challenge is to control the spin fluctuation to within a threshold value, which is achieved by developing a set of optimized GRAPE pulse sequences. Overall, our small-scale implementation indicates that the quantum query algorithm is capable of determining the values of Forrelations within an acceptable accuracy required for demonstrating quantum supremacy, given the current technology and in the presence of experimental noise.

1. Introduction

With the ability of creating exponential number of superposition of states, quantum computation provides an unprecedented computational power over classical computation. For example, Shor's factoring algorithm [1], the Harrow-Hassidim-Lloyd (HHL) algorithm [2], and other progresses in quantum simulation [3–5] provide strong evidences that quantum computation can gain exponential speed-up in practical problems. Apart from computational decision problems, quantum devices can be exploited for other classically-intractable computational tasks, including sampling distributions of some quantum systems [6–10]. As a result, one may expect to gain "quantum supremacy" [11] in relatively-simple quantum devices in the near future.

Although these results are promising, complete and rigorous proofs supporting claims of gaining quantum supremacy are still unavailable. Recalling that for the case of Shor's algorithm, we have not excluded the possibility of the existence of a polynomial-time classical algorithm for the factoring problem. For the HHL algorithm, which is BQP-complete, it remains to be determined if quantum computation is indeed more powerful than classical computation, or technically, if it is true that BQP $\supset$ BPP. Here BPP (bounded-error probabilistic polynomial time) is the class of decision problems solvable by a probabilistic Turing machine in polynomial time with an error probability of at most 1/3 for all instances and BQP (bounded-error quantum polynomial time) is the quantum analogue of the complexity of BPP in computational complexity theory. Furthermore, the success of the sampling algorithms is founded on several conjectures in the theory of classical computational complexity. Even though boson-sampling devices are capable of creating an exponentially large superposition of quantum states, the transition amplitudes can still be estimated by classical devices within additive errors [12].

On the other hand, query complexity, which counts the number of queries of black-box functions (i.e., without knowledge of the internal structure), provides further evidence supporting quantum speed-up over the classical counterparts. For example, Grover's search algorithm [13], the Deutsch-Jozsa algorithm [14] and Simon's algorithm [15] are all characterized in the context of query complexity.

Recently, Aaronson and Ambainis [16] introduced a new concept in query complexity, called Forrelation, which characterizes the multi-fold correlations among different boolean functions. It was found that a quantum computer is capable of solving 2-fold Forrelation problems within a constant $O(1)$ number of queries.

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However, classical computers require an exponential number of queries. The difference of the query complexity between quantum and classical methods is shown to be a maximally-achievable separation with quantum methods (see also Refs. [17–19]). Furthermore, multiple-fold Forrelation problems are as hard as quantum computation [16], i.e., BQP-complete.

Here we report the first experimental study of the 2-fold and 3-fold Forrelations in a system of nuclear spins, where the NMR quantum circuit for 2-fold Forrelation involves only 2 queries of the black box functions, but classically, it takes a total of 8 queries for an exact result. Similarly, 3 queries are needed for the NMR implementation of 3-fold Forrelation, while 12 queries are needed classically if memory is given for the black-box functions; otherwise it can go up to 192 classical queries.

However, we note that the measurement results come directly from the NMR signals, but a standard implementation of the quantum circuit involves probabilistic measurement outcomes. Furthermore, similar to other experimental demonstrations of Deutsch-Jozsa algorithms [20,21], the applied NMR pulse sequence depends on the knowledge of the functions, which are not strictly "black boxes". Therefore, the current experimental results cannot be taken as a direct proof for demonstrating quantum supremacy, which is relevant only in the large-N limit.

The purpose of the experiment is to investigate whether a small-size prototype experiment can produce Forrelation within the accuracy required for demonstrating the quantum advantages (above the threshold 3/5 or below the threshold 1/100), given the current technology and in the presence of experimental noise. In particular, our experimental fluctuation for the spin measurement has to be controlled within 1%. These experimental results allow us to identify the places one can improve for scaling up the size of the experiment in future.

2. Forrelation

Given k Boolean functions, $f_1 \equiv f_1(x_1), \cdots, f_k \equiv f_k(x_k)$, each with n variables, i.e., $x_j \in \{0,1\}^n \to \{-1,1\}$, the k-fold Forrelation, $\Phi_k \equiv \Phi_{f_1 f_2 \ldots f_k}$, of these functions is defined as follows,

$$\Phi_k \equiv \sum_{x_1,x_2,\ldots} \frac{e^{i\phi(x_1,x_2,\ldots)}}{2^{(k+1)n/2}} f_1(x_1) f_2(x_2) \cdots f_k(x_k), \tag{1}$$

where $e^{i\phi(x_1,x_2,\ldots)} \equiv (-1)^{x_1 \cdot x_2}(-1)^{x_2 \cdot x_3} \cdots (-1)^{x_{k-1} \cdot x_k}$, and $x \cdot y$ indicates the bitwise inner product between the n-dimensional binary vectors x and y. The total number of possible assignment is $N = 2^n$. Essentially, 2-fold Forrelation is simply the inner product between a boolean function and the Fourier transform of another boolean function, i.e.,

$$\Phi_{f,g} \equiv \frac{1}{2^{3n/2}} \sum_{x,y \in \{0,1\}^n} (-1)^{x \cdot y} f(x) g(y). \tag{2}$$

Importantly, an exact determination of 2-fold Forrelation $\Phi_{f,g}$ is a computationally-hard problem for classical devices, which can be justified by the following challenge [16]: given a pair of Boolean functions f and g, suppose it is known that either (1) $|\Phi_{f,g}| \leq 1/100$ or (2) $\Phi_{f,g} \geqslant 3/5$ is true, all classical methods require an exponential number $\Omega(\sqrt{N}/\log N)$ of queries to the black-box functions, but quantum computers can finish the task with a constant number of queries. The separation between the quantum and classical query complexity is (almost) possibly largest one can achieve [16].

Quantum circuits for solving 2-fold and 3-fold Forrelation problems [16] are shown in Fig. 1. For 2-fold Forrelation problems, there are 2 query operators O_{f_1} and O_{f_2}, which map each input basis state $|x\rangle$ to $f_1(x)|x\rangle$ and $f_2(x)|x\rangle$ respectively, i.e., $O_{f_k}|x\rangle = f_k(x)|x\rangle$.

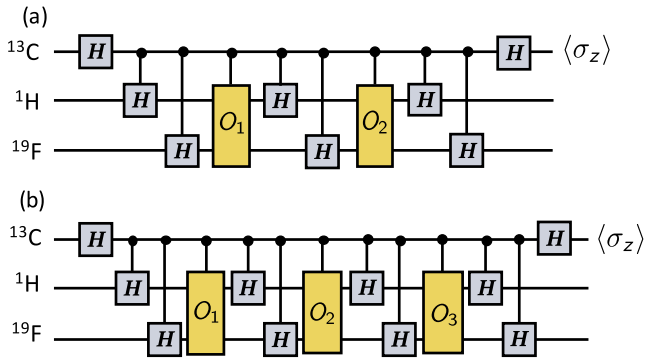

Fig. 1. (Color online) Quantum circuit for probing (a) 2-fold and (b) 3-fold Forrelation problems. The system is prepared at state $|000\rangle$. $O_1 \equiv O_{f_1}, O_2 \equiv O_{f_2}$, and $O_3 \equiv O_{f_3}$ are query operators that map states $|x\rangle$ to $f_1(x)|x\rangle, f_2(x)|x\rangle$, and $f_3(x)|x\rangle$ respectively, where $f_1(x), f_2(x), f_3(x) \in \{1, -1\}$.

3. Experimental background

Nuclear magnetic resonance (NMR) is a reliable technology for studying small-to-medium size quantum information experiments [22,23], and quantum simulation [24–28]. Motivated by the needs of studying quantum information, many sophisticated techniques of controlling nuclear spins have been developed.

Here all the experiments are carried out at room temperature (295 K) on a Bruker Avance III 400 MHz spectrometer and the ^{13}C labelled Diethyl-fluoromalonate dissolved in $d6$ acetone is used as a 3-qubit NMR quantum information processor. The structure and Hamiltonian parameters of Diethyl-fluoromalonate are shown in Fig. 2a where ^{13}C, ^{1}H and ^{19}F nuclear spins respectively act as an ancillary qubit and two work qubits. Moreover, the internal Hamiltonian of the system is given by

$$H_{\text{int}} = \sum_{i=1}^{3} \pi \nu_i \sigma_z^i + \sum_{j<k,=1}^{3} \frac{\pi}{2} J_{jk} \sigma_z^j \sigma_z^k, \tag{3}$$

The whole experimental procedure consists of three parts: (1) state initialization, (2) realization of the quantum algorithm for solving 2 (or 3)-fold Forrelation problem, and (3) readout of the expectation value of σ_z^1 of the ancillary qubit ^{13}C, which is equal to the Forrelation, i.e.,

$$\langle \sigma_z^1 \rangle = \Phi_k, \tag{4}$$

for any $k \geqslant 2$. We note that for the NMR quantum computing, the whole system, starting from the thermal equilibrium state, can be converted to the pseudo-pure state (PPS) [29,30] $\rho_{000} = (1-\varepsilon)I/8 + \varepsilon|000\rangle$, using the spatial average technique [31]. To check the success of preparing the PPS, a full quantum state tomography (QST) [32] is carried out. The fidelity between the density matrix prepared in experiment (ρ_{exp}) and the target one in theory (ρ_{th}) is given by the following expression,

$$F(\rho_{\text{exp}}, \rho_{\text{th}}) \equiv \text{tr}(\rho_{\text{exp}} \rho_{\text{th}}) / \sqrt{\text{tr}(\rho_{\text{exp}}^2)\text{tr}(\rho_{\text{th}}^2)}. \tag{5}$$

A spectrum of the PPS observed on ^{13}C is shown in Fig. 3a. The real parts of the initial state are shown in the last figure as ρ_0. Overall, the initial state can be well prepared in our setup; the fidelity can reach up to 96.9%.

4. Experimental details

To solve the k-fold Forrelation problem, a quantum circuit is designed to obtain Forrelation $\Phi_k \equiv \Phi_{f_1,\ldots,f_k}$ by measuring the