Toward NMR Quantum Reservoir Computing

Makoto Negoro, Kosuke Mitarai, Kohei Nakajima, and Keisuke Fujii

Abstract Reservoir computing is a framework used to exploit natural nonlinear dynamics with many degrees of freedom, which is called a reservoir, for a machine learning task. Here we introduce the NMR implementation of quantum reservoir computing and quantum extreme learning machine using the nuclear quantum reservoir. The implementation utilizes globally controlled dynamics of nuclear spin qubits in solid state and it has been demonstrated.

The physical implementation of quantum information processing has been extensively studied with various quantum systems (Nielsen and Chuang 2000; Ladd et al. 2010). Any physical realization of the quantum computer must satisfy the following criteria: (1) a scalable physical system with well-characterized qubits, (2) the ability to initialize the state of the qubits, (3) a *universal* set of quantum gates, (4) long relevant decoherence times, much longer than the gate-operation time, and (5) a qubit-specific measurement capability (DiVincenzo 2000). To this day, there have been many proposals of implementations which satisfy these criteria, such as superconducting qubits, semiconductor quantum dots, trapped atoms, photonics, and nuclear magnetic resonance (NMR). One of the most promising candidates is the superconducting qubit system. In 2019, Google has announced a quantum computer employed

M. Negoro (✉) · K. Mitarai · K. Fujii
Center for Quantum Information and Quantum Biology, Osaka University, Toyonaka, Osaka 560-8531, Japan
e-mail: negoro@qc.ee.es.osaka-u.ac.jp

K. Fujii
e-mail: fujii@qc.ee.es.osaka-u.ac.jp

M. Negoro · K. Mitarai · K. Nakajima · K. Fujii
JST PRESTO, Kawaguchi, Saitama 332-0012, Japan

K. Mitarai · K. Fujii
Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan

K. Nakajima
Graduate School of Information Science and Technology, The University of Tokyo, Bunkyo-Ku, 113-8656 Tokyo, Japan

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with 53 superconducting qubits (Arute et al. 2019) with which they have claimed to achieve *quantum computational supremacy* (Preskill 2012). Arrays of atoms trapped in the vacuum have also gained attention as good candidates for large-scale quantum computing and simulation (Mazurenko et al. 2017; Bernien et al. 2017; Zhang et al. 2017). However, it is not yet clear that these implementations will ultimately be successful.

NMR quantum information processing (QIP) has been proposed in 1996 by Chuang et al. (Gershenfeld and Chuang 1997) and Cory et al. (1997). In this approach, we use nuclear spins in a molecule as qubits. In a static magnetic field, spin-1/2 particles have two energy levels, each corresponding to the states parallel ($|\uparrow\rangle$) and anti-parallel ($|\downarrow\rangle$) to the magnetic field. These two quantum states can be used as $|0\rangle$ and $|1\rangle$ of a qubit. An organic molecule, which can have many nuclei with spin-1/2, forms a many-qubit system that can be used for QIP purposes. A usual NMR sample has a macroscopic ensemble of identical copies of such a many-qubit system. The ensemble-nature of NMR allows the direct measurement of an observable. Qubits are controlled by applying oscillating magnetic fields at radiofrequency. Gate operations between two qubits can be implemented by utilizing the naturally existing interaction between the spins. As NMR spectroscopy has been applied for analysis of materials for over 60 years, vast knowledge to control nuclear spins has been accumulated (Slichter 1990). Early day proof-of-principle QIP experiment is performed with NMR, owing to the nice controllability of the many-qubit system. It is hoped that future progress of macromolecular and supramolecular technology will make it possible to array Avogadro number of spins in two or three dimensions, let alone far more than 10^9 spins, which is required for fault-tolerant quantum computation to outperform classical computation (Jones et al. 2012).

The NMR quantum computer has succeeded in implementing Shor's algorithm using 7 qubits (Vandersypen et al. 2001), quantum simulation using 7 qubits (Negrevergne et al. 2005), and quantum machine learning (Biamonte et al. 2017) using 4 qubits (Li et al. 2015). However, the *pseudo-initialization technique* (Cory et al. 1997) used in these implementations is not scalable, which blocks the exponential speedup of the quantum algorithms. The state with partially initialized spins in these implementations is inevitably separable, that is, they do not have entanglement (Braunstein et al. 1998). In order to efficiently solve BQP (bounded error quantum polynomial time) type problems like factoring, a scalable initialization technique of nuclear spin qubits is required. Nuclear spins are only slightly polarized even in the strong magnetic fields conventionally used in NMR spectroscopy at room temperature because the magnetic energy of nuclear spin is much smaller than the thermal energy. One of the scalable initialization schemes is to use dynamic nuclear polarization (DNP) which is operated at very low temperature in solids (A. Abragam, M. Goldman, Nuclear Magnetism: Order and Disorder (Clarendon Press 1982). Solid state NMR quantum information processing experiments have also been studied. Solid state nuclear spin qubits have a long coherence time (Ladd et al. 2005) and have already been controlled with high fidelity although not initialized (Ryan et al. 2008; Alvalez et al. 2015). The initialization technique is not still compatible with high-fidelity control to this day, which motivates us to seek a way to benefit

from the solid state NMR quantum computer with partially polarized qubits without pseudo-initialization.

A class of problems that can be solved scalably by quantum computers with partially polarized states is called DQC1 (deterministic quantum computation with 1 qubit) (Knill and Laflamme 1998). Recently, it has been proven theoretically that DQC1 is unsimulatable with classical computers under stable complexity conjectures (Morimae et al. 2014). Owing to the theoretical progress, now we can provide a roadmap to scale up the NMR quantum computer by first showing the quantum computational supremacy with partially polarized spins, DQC1 type, then with initialized spins. There are various oligomers and polymers with more than 50 spins. The simulation of ensemble dynamics of more than 50 qubits is computationally hard for classical computers whether the state is initialized or partially polarized. Quantum simulation experiments (Alvalez et al. 2015) have demonstrated that the controllable dynamics of partially polarized nuclear spins in molecular solids can be highly complex as more than 1000 spins are quantum mechanically correlated.

We experimentally demonstrated how to exploit such complex quantum dynamics of a nuclear spin ensemble for machine learning (Negoro et al. 2018). To this end, a quantum reservoir framework (QRC) is employed (Fujii and Nakajima 2017). Reservoir computing provides a framework for exploiting nonlinear dynamics with many degrees of freedom, called a reservoir, for machine learning (Maass et al. 2002; Jaeger and Haas 2004; Varsraeten et al. 2007). It was first proposed as an echo-state network or liquid-state machine (Maass et al. 2002; Jaeger and Haas 2004), where a conventional neural network is used as a reservoir, but its internal dynamics are randomly prefixed and only the linear readout weights are optimized to learn a nonlinear task. This black-box property allows for the use of actual physical systems that employ photonics (Vandoorne et al. 2013), spintronics (Torrejon et al. 2017), or soft robotics (Nakajima et al. 2015), as well as qubits (Fujii and Nakajima 2017). Originally proposed implementation of QRC requires the initialized spins and also the on-demand initialization in the protocol, which are not yet possible in actual experiments. To avoid this difficulty, we proposed a slightly modified algorithm together with the experimental realization (Negoro et al. 2018). Here we introduce the experimental proposal.

Figure 1a shows the physical implementation of a quantum reservoir consisting of nuclear spins with a partially polarized state in a molecular solid. In this implementation, all B spins are controlled with the same oscillating magnetic field, which results in a *global control* scheme (Benjamin and Bose 2003), where each of B spins is controlled in an equivalent way. At the first sight, this scheme might seem not sufficient for the universal quantum computation, but nonetheless, it has been shown that universal quantum circuits can be implemented with global control (Benjamin and Bose 2003; Lloyd 1993). Topological error correction can also be implemented with global control and on-demand initialization of qubits (Fujii et al. 2014). As a proof-of-principle experimental demonstration, we have performed non-temporal tasks using the natural quantum dynamics of the quantum reservoir, which we also refer to as quantum extreme learning machine (QELM), a quantum counterpart of extreme learning machine (see also another chapter written by Fujii and Nakajima

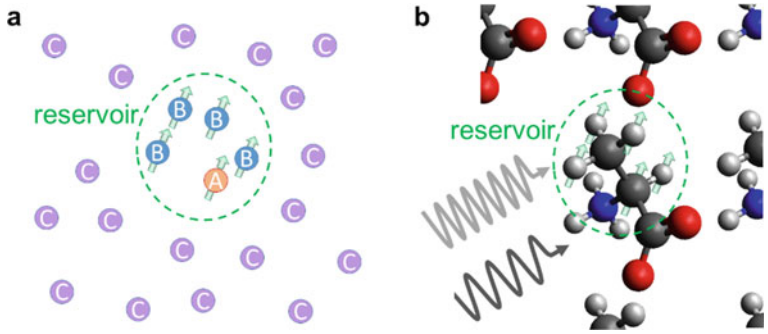

Fig. 1 NMR quantum reservoir (**a**) and its implementation with *l*-alanine (**b**)

in this book) (Butcher et al. 2013). Related quantum algorithms have been recently proposed (C.M. Wilson et al. 2018; Halvicek et al. 2019). In the experimental demonstration of QELM, we used isotopically labeled *l*-alanine (Negoro et al. 2018). This molecule has four ^{1}H spins and one ^{13}C spin, both of which have spin-1/2. We diluted it into a single crystal of $^{2}H_7$-*l*-alanine which has 7 ^{2}H spins as shown in Fig. 1b. ^{1}H, ^{13}C, and ^{2}H spins correspond to B, A, and C spins, respectively, and ^{1}H and ^{13}C spins are used as reservoir.

The quantum circuits of QELM and QRC are shown in Fig. 2. The quantum gate U, which is the source of nonlinearity of the output from the reservoir, is implemented as a time evolution that naturally arises from the interaction among the spins. Throughout the execution of the quantum circuit, the C spins do not interact with A and B spins. Accordingly, the ensemble reservoir is well isolated. In order to control the reservoir dynamics for input, we employed the selective rotation of A (Fig. 2a) or the global rotation of B spins (Fig. 2b). Input data can be fed into the reservoir using the selective rotation of A (Fig. 2a) or the global rotation of B spins (Fig. 2b). Our experimental demonstration uses the circuit of Fig. 2b. The initial state of QELM is a partially polarized state and that of QRC is initialized. In addition, the B spin is initialized by interacting with initialized bath spins, as implemented in Ryan et al. (2008), before every input (Fig. 2c).

QELM is a framework to perform non-temporal nonlinear tasks such as classification and pattern recognition with finite inputs. In the demonstration of QELM (Negoro et al. 2018), we consider the learning problem of a nonlinear function $y = f(s)$ using K training data sets including an input stream with the length of L, $\{s_{l,k}\}$ ($s_{l,k} \in [0,1]$), and corresponding teacher t_k. The input is processed by M cycles of the time evolution U, each of which is followed by the ensemble measurement of A spins. We repeat L series of the input process and cycles of evolution for each of K instances of the input $\{s_{l,k}\}$. Thus, we get a total of LM signals $x_{l,m}^{(k)}$ for a given input instance $\{s_{l,k}\}$. The output from the machine is defined as a weighted sum of the LM signals $x_{l,m}^{(k)}$:

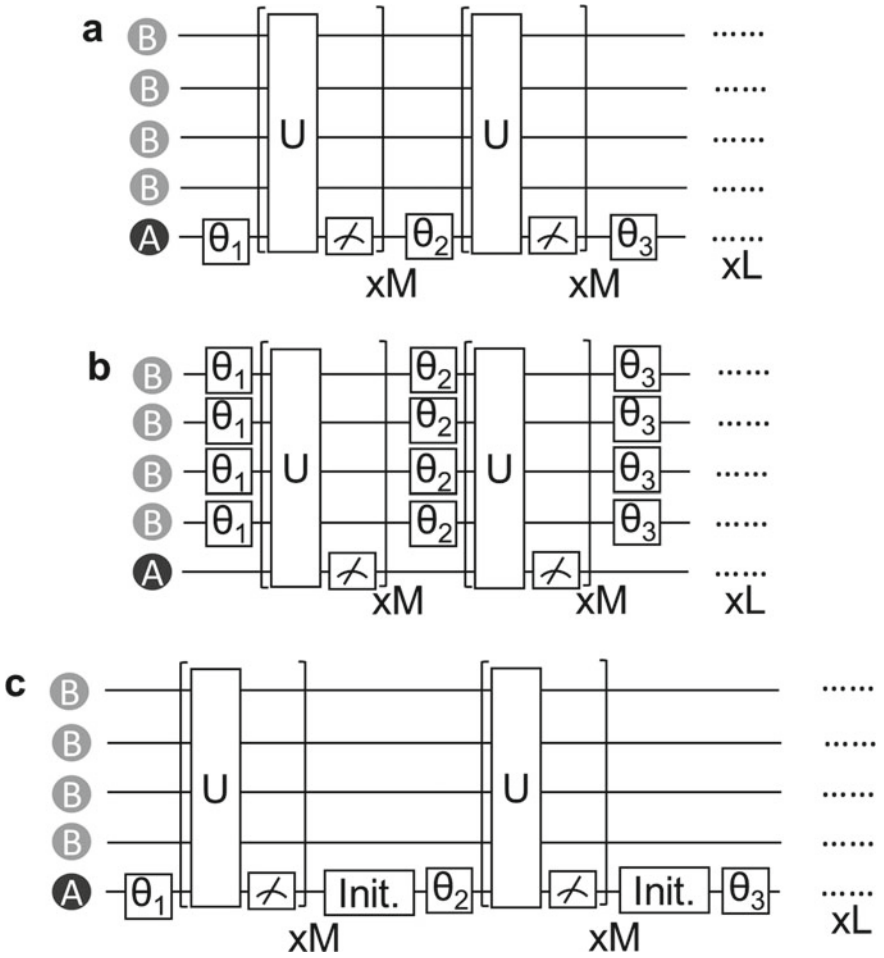

Fig. 2 Quantum circuits of QELM with selective rotation (**a**) and global rotation (**b**) and QRC (**c**)

$$y_k = \sum_{m=1}^{M} \sum_{l=1}^{L} W_{l,m} x_{l,m}^{(k)}, \tag{1}$$

where W is an LM-dimensional weight vector. After taking signals from K sets of training data, W is determined so as to minimize the mean squared error, $\Sigma_k (t_k - y_k)^2$.

We evaluated the computational capabilities of this QELM implementation with two benchmark tasks under a binary sequential input. One is the input recognition task, which measures how well each input is reconstructed from the quantum reservoir dynamics. Another is the parity check task, which tests how well the machine can perform a nonlinear transformation of the input. We found our implementation can perform both of the two. We further demonstrate to train the machine to compute

Table 1 Performance of learning functions

	MSE	# of error
2bit XOR	1.97×10^{-2}	0
3bit XOR	2.83×10^{-2}	0
4bit XOR	1.99×10^{-1}	3
NAND	2.26×10^{-2}	0
1bit Adder 0th order	2.26×10^{-2}	0
1bit Adder 1st order	2.01×10^{-2}	0
2bit Adder 0th order	4.36×10^{-2}	1
2bit Adder 1st order	2.02×10^{-1}	4
2bit Adder 2nd order	1.44×10^{-2}	0
Multiplication	2.32×10^{-3}	–
Division	5.22×10^{-4}	–
Nonlinear I	3.09×10^{-4}	–
Nonlinear II	7.64×10^{-3}	–

simple Boolean functions of input binary strings, which are nonlinear functions when the binary information is embedded into a continuous variable. The performance of learning functions measured by the mean squared error and the number of erroneous outputs are shown in Table 1. These experimental results are detailed and discussed in Negoro et al. (2018).

If we wish to perform QRC, we would have to initialize both qubits, namely in the above implementation, the C spins. For example, as mentioned earlier, nuclear spin qubits can be initialized by DNP which is performed at very low temperature of ~1 K (de Boer and Niinikoski 1974). For such a scheme, technological development for high-fidelity control at very low temperature is important (Cho et al. 2007). Alternatively, we can also develop and advance the initialization technique at room temperature (Tateishi et al. 2014), where nuclear spins can be controlled very accurately. In fact, we already have achieved the room-temperature initialization of up to 34% using photoexcitation of electrons (Tateishi et al. 2014). Initialization technique that is compatible with high-fidelity control is within reach. In Ryan et al. (2008), the error per gate is approximately 1% in solid state at room temperature. The other important direction is to boost computational power by increasing the number of the reservoir spins, as numerically demonstrated in Fujii and Nakajima (2017) and Nakajima et al. (2019).

Our implementation of the quantum reservoir and demonstration of nonlinear information processing therein pave the way for exploiting quantum computational supremacy in NMR ensemble systems for information processing with reachable technologies.

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