Quantum many-body states: A novel neuromorphic application

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ABSTRACT

Emergent phenomena in condensed matter physics, such as superconductivity, are rooted in the interaction of many quantum particles. These phenomena remain poorly understood in part due to the computational demands of their simulation. In recent years variational representations based on artificial neural networks, so called neural quantum states (NQS), have been shown to be efficient, ie. sub-exponentially scaling, representations. However, the computational complexity of such representations scales not only with the size of the physical system, but also with the size of the neural network. In this work, we use the analog neuromorphic BrainScaleS-2 platform to implement probabilistic representations of two particular types of quantum states. The physical nature of the neuromorphic system enforces an inherent parallelism of the compuation, rendering the emulation time independent of the used network size. We show the effectiveness of our scheme in two settings: First, we consider a hallmark test for "quantumness" by representing a quantum state that violates the classical bounds of the Bell inequality. Second, we show that we can represent the large class of stoquastic quantum states with fidelities above 98% for moderate system sizes. This offers a novel application for spike-based neuromorphic hardware which departs from the more traditional neuroscience-inspired use cases.

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1 INTRODUCTION

The properties of materials are determined by the interactions between many electrons and are described by the laws of quantum mechanics on the microscopic level. The inherent complexity of these laws makes it challenging to predict emergent macroscopic material properties from first principles. Examples include the electronic structure of molecules, topological states of matter, or high temperature superconductivity. Many of these phenomena can be modeled by spin-1/2, or qubit, systems, i.e. ensembles of two-state particles. Conceptionally, quantum states can be represented either using the wave function formalism $|\psi\rangle = \sum_i c_i |\psi_i\rangle$ or the density matrix formulation. Here $|\psi_i\rangle$ represent a choice of basis states and $c_i \in \mathbb{C}$ are coefficients determining their contribution to the system's state $|\psi\rangle$. The number of c_i's is given by the size of the system's state or Hilbert space k^n, where k is the number of states per body and n the number of bodies in the system. Already for the spin-1/2 system ($k = 2$) this requires an exponential number of coefficients to be known. In practice, the interest lies in describing a specific state, or at least states from a specific class, for example the ground state of a system. This introduces properties that can be exploited to find a compressed state representation. Recently, neural-network-based approaches have been shown to be able to efficiently provide an effective representation such quantum states [2]. These methods essentially implement a priority sampling of the most relevant $|\psi_i\rangle$ in order to keep the computational complexity of expectation value calculations limited. For these methods, fast sampling represents an essential prerequisite for their usefulness.

We use the analog neuromorphic system BrainScaleS-2 to implement a probabilistic representation of quantum states. The physical nature of our system renders the speed of the sample generation independent of the size of the neural network used [1]. We demonstrate the feasibility of our scheme on two types of quantum states: First, we learn the prototypical Bell-state of two spin-1/2 particles and show that the representation can violate the classical bounds of the Bell observable $|\mathcal{B}| \leq 2$. Second, we represent stoquastic quatum states, i.e. states which can be represented by real coefficients $c_i \in \mathbb{R}$ and use these representations to find ground states, i.e., states of least energy, for the transverse-field Ising model (TFIM).

2 NEUROMORPHIC IMPLEMENTATION

BrainScaleS-2 (Fig. 1b) provides up to 512 leaky integrate-and-fire (LIF) neurons with a maximum fan-in of 256 pre-synaptic partners per circuit. Under high-frequency Poisson stimulus, networks of

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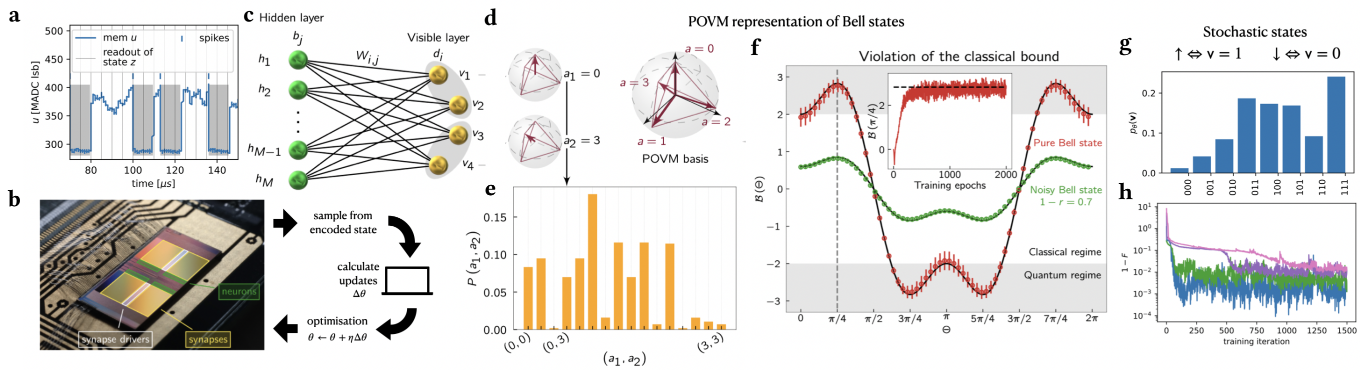

Figure 1: **(a) Dynamics of sampling neurons. After a spike the neuron is considered to be active $z = 1$ (shaded area, $z = 0$ otherwise). (b) The BrainScaleS-2 chip used to represent the desired quantum states and the associated hardware-in-the-loop training scheme. (c) Layered network structure used for all experiments. The distribution over the visible layer $p(v)$ is parametrized by the connectivity matrix W and represents the quantum state $|\psi\rangle$. (d) Positive-operator-valued measure (POVM) representation of quantum states. POVM labels $a^n \in \{0, 1, 2, 3\}^n$ are associated with the sampled binary states $z \in \{0, 1\}^{2n}$. (e) Example of a sampled distribution $p(z)$. (f) Final neuromorphic representation of a pure Bell state (red) and a noisy state (green). Depending on the measurement angle Θ, the chosen Bell observable exceeds the classical bound $|\mathcal{B}(\Theta)| \leq 2$ (shaded area). The inset shows the convergence over the course of the training. (g) For the stoquastic state representation, the probability of each observed binary state $z \in \{0, 1\}^n$ directly represents the wave function coefficients c_i of the quantum state $|\psi\rangle$. (h) Resulting (quantum) infidelities of the learned ground states over the course of the training for different system sizes ($N = 3, 5, 7, 9$).**

such neurons have been shown to approximately sample from Boltzmann distributions $p(z) = \frac{1}{Z}\exp\left(-\frac{1}{2}z^t W z - b^t z\right)$ [6]. Their membrane potential u then implements a random walk with network-input-dependent target values (see Fig. 1a). We interpret the neuronal state as active ($z = 1$) immediately after a spike when the neuron is refractory and as inactive ($z = 0$) otherwise.

Using a hierarchical network topology (Fig. 1c) we use the visible layer to represent the quantum state. The connections to the hidden layer are trained such that the network samples from the correct distribution over visible states $p(v)$. We employ an iterative learning scheme, where for each iteration we first perform a sampling run on hardware, then transfer all the recorded spikes to an host computer, collect the distribution $p(v, h)$ and calculate the corresponding gradients. Using these we update the configuration parameters of the system Θ and continue with the next iteration.

2.1 Bell States

For the Bell state $\left|\psi^+\right\rangle = \left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\right)/\sqrt{2}$ we use a positive-operator-valued measures (POVM) [5] representation: A POVM – for a single spin – is a choice of 4 informationally-complete measurements $\vec{e}_i$ such that all states can be represented by $\vec{\phi} = \sum_{i=0}^{3} a_i e_i$ with $\sum a_i = 1$. We associate the four basis vectors e_i with binary states $z \in \{0, 1\}^2$. The coefficients a_i then correspond to the probability $p(z)$ which allows a reformulation of all physical observables as expectation values over $p(z)$. Using the knowledge of the correct target distribution p_{target}, we implement a Hebbian learning scheme with gradients calculated as $\Delta W_{ij} = \left\langle v_i h_j \right\rangle_{\text{target}} - \left\langle v_i h_j \right\rangle_{\text{model}}$, where we recover the target correlations by reweighting the observed correlations: $\left\langle v_i h_j \right\rangle_{\text{target}} = \left\langle \frac{p_B(\vec{v})}{p(\vec{v};\mathcal{W})} v_i h_j \right\rangle$. This allows us the update calculation based on a single hardware configuration, which would otherwise introduce significant runtime overhead [3].

Since we can thereby represent the complete state $\left|\psi^+\right\rangle$, we can perform any measurement on it. In particular, looking at the Bell observable $\mathcal{B}(\theta) = E_{0,\theta} + E_{0,-\theta} + E_{2\theta,\theta} + E_{2\theta,-\theta}$ we see that our representation consistently and correctly violates the classical limit for particular measurement angles (for a pure Bell state, Fig. 1f red).

2.2 Stoquastic States

Ground states of stoquastic Hamiltonians have non-negative real wavefunction coefficients $c_i \in \mathbb{R}$. This allows us to directly identify the (square-root) of the probability of each state as c_i: $|\psi_\theta\rangle = \sum_{\{v\}} \sqrt{p_\theta(v)}\,|v\rangle$, where we identify $z = 1$ ($z = 0$) with $|\uparrow\rangle$ ($|\downarrow\rangle$) (Fig. 1g).

Here, we suppose that we do not have a priori access to the target state $|\psi\rangle$, but rather have to find it by optimizing an observable. For ground state search, this requires minimizing the energy of the state: $E_\theta = \langle\psi_\theta| H |\psi_\theta\rangle$. For the transverse field Ising model (TFIM) Hamiltonian this results in the update rules: $\Delta W_{ij} \propto \left\langle \left(E^{\text{loc}}_{\vec{v}} - E_\theta\right) z_i z_j \right\rangle_{p_\theta(\vec{z})}$, which we can again evaluate based on a single hardware run (see [4] for details). For the investigated moderate system sizes ($N \leq 10$) we obtain fidelities $> 98\%$ (Fig. 1h). The performance degrades slightly for larger systems, which most likely originates in the requirement of longer sampling times for which the system is currently not set up.

3 CONCLUSIONS

We demonstrated the feasibility of realizing different quantum state representation schemes using a spike-based implementation on neuromorphic hardware. Both the POVM represenation and the ground states can be well approximated such that a reliable estimation of the relevant expectation values is possible. The physical nature of BrainScaleS-2, i.e, the implementation of the spiking neural system as electronic circuits, makes the runtime independent of the size of the used system. This allows our method to scale to larger systems, thereby uncovering the emulation of quantum many-body states as a potential application for (spike-based) neuromorphic systems.

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