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Where analogue and digital meet

Kai-Niklas Schymik

Realizing a useful quantum advantage on noisy intermediate-scale quantum hardware is challenging. A proposal now suggests a hybrid digital–analogue hardware-efficient approach for reconfigurable qubit platforms to simulate strongly interacting matter.

Simulating quantum chemistry and complex materials is one of the most promising applications of quantum computers. However, today's quantum hardware is noisy and intermediate-scale, making simulations of complex systems impractical due to the large circuit depths required. More hardware-efficient approaches are thus needed. Reporting in *Nature Physics*, Nishida Maskara and colleagues[1] have now proposed a hardware-efficient simulation toolbox based on recent advances in reconfigurable qubit platforms, which support non-local gates [2,3] and multi-qubit interactions [4,5].

Electronic structure problems of strongly correlated molecules and materials are of particular interest for quantum computing due to their high computational cost on classical devices. A common approach is to use a variety of spin models to capture properties of complex molecules, such as their low-lying electronic structure. However, classical numerical methods struggle at large system sizes when there is significant entanglement, making this an ideal application for programmable quantum simulators that can naturally handle large entanglement.

In recent years, model Hamiltonians with local connectivity have been studied on multiple analogue quantum simulation platforms. Yet, complex features such as higher-order interactions or non-locality have remained challenging to realize. A universal digital quantum computer could in principle simulate these features, but the number of gates required is beyond current hardware capabilities. Recent advancements in quantum hardware, however, opened up the possibility of realizing these features through a hybrid analogue–digital approach.

Maskara and colleagues built upon recent progress in reconfigurable qubit platforms, particularly neutral atoms in optical tweezer arrays. These platforms use individual atoms held by tightly focused laser beams and exploit Rydberg transitions to high energy levels to engineer interactions and perform computations. The first crucial ingredient of the proposal by Maskara and colleagues is the capability to entangle atoms and move them without loss of coherence to realize arbitrary non-local connectivity[2]. The second is the creation of multi-qubit gates by bringing atoms close together and entangling them with a combined laser excitation[5]. Although the team devised the approach with a focus on neutral atom architectures, it should also be extendable to other reconfigurable qubit platforms, such as trapped ion devices.

Their method encodes spin-S variables of the model Hamiltonian in the collective spin of a cluster of 2S qubits (Fig. 1a). Interactions are generated by moving pairs of qubits from different clusters together. The target Hamiltonian is engineered by alternating between the dynamics in the cluster and with qubit pairs from different clusters (Fig. 1b). Here, Maskara and colleagues drew inspiration from dynamical decoupling sequences in nuclear magnetic resonance (NMR) systems, which decompose complex interactions into far fewer gates than other standard procedures.

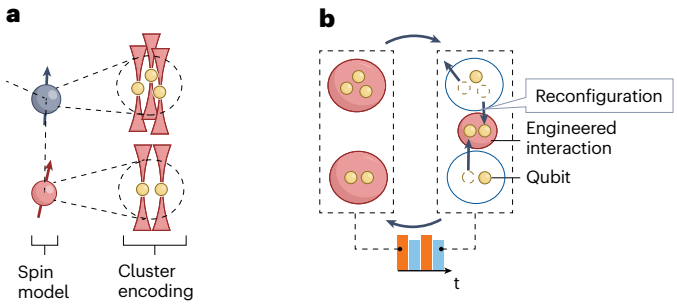

Fig. 1 | Hardware-efficient simulation of model spin Hamiltonians. a, A spin model (left) captures properties of a target molecule. The spin-S variables of the model are encoded in the collective spin of a 2S qubit cluster held in tightly focused laser beams (right). **b**, The target Hamiltonian is engineered by alternating between two evolutions, within the cluster and with pairs of qubits from different clusters. The qubits are reconfigured between each step. The evolution with qubits from different clusters implements interactions between encoded spin-S variables of the target Hamiltonian, while the evolution within the cluster projects back into the encoding space. The authors propose hardware-efficient ways of implementing the desired evolutions using multi-qubit laser excitations involving Rydberg states.

The analogue component of the simulation lies in the hardware-efficient implementation of multi-qubit interactions. The team showed that native interactions between the atoms can be transformed into the required form using numerical pulse engineering techniques. They considered two implementations: one using alternating diagonal phase gates and single-qubit rotations, and another with a dual driving scheme where both the single-qubit transition and the Rydberg transition are simultaneously used. The second scheme, in particular, is highly hardware-efficient and significantly extends the available simulation time.

Finally, Maskara and colleagues illustrated a use-case of their analogue–digital framework with a many-body spectroscopy algorithm. They calculated a spectral function, which in the chosen implementation is split between a classical computation and a quantum simulation to handle highly entangled expressions. The team demonstrated that the method can extract relevant chemical information of a transition metal complex involved in photosynthesis – the Mn_4O_5Ca core of the oxygen-evolving complex.

The work by Maskara and colleagues underlines the potential of reconfigurable qubit platforms for quantum simulation. Non-local and multi-qubit gates represent a promising route to solve interesting problems in a resource-efficient manner. Their proposal extends the

application toolbox to new types of Hamiltonians relevant to chemistry and material science, merging digital and analogue methods. Whether this framework is sufficient to achieve a useful quantum advantage on near-term hardware is yet to be seen. It could be interesting in the future to consider the compatibility of the approach with error mitigation techniques, or even logical qubit control.

Furthermore, the team uses pulse-optimization techniques — frequently used in NMR and quantum hardware to optimize gate fidelities — to tailor multi-qubit interactions to the desired form. Experimentally, these techniques are challenging, as optimization results can depend on the choice of figure of merit. Validating this procedure on quantum hardware will be crucial. In general, combining analogue and digital approaches, as well as feedback between classical and quantum hardware, remains essential for successful near-term quantum simulations.

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References

1. Maskara, N. et al. *Nat. Phys.* https://doi.org/10.1038/s41567-024-02738-z (2025).
2. Bluvstein, D. et al. *Nature* **604**, 451–456 (2022).
3. Moses, S. A. et al. *Phys. Rev. X* **13**, 041052 (2023).
4. Katz, O., Feng, L., Risinger, A., Monroe, C. & Cetina, M. *Nat. Phys.* **19**, 1452–1458 (2023).
5. Evered, S. et al. *Nature* **622**, 268–272 (2023).

Competing interests

The author declares no competing interests.