Quantum hardware simulating four-dimensional inelastic neutron scattering

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Finite-size spin systems could constitute key elements in future spintronics devices [1–5], long-lasting nano-scale memories [6] or scalable and noise-resilient quantum computing platforms [7–9]. They are also natural test-beds for investigating peculiar quantum phenomena [10]. Inelastic Neutron Scattering is the technique of choice to model these systems. Indeed, it enables an atomic-scale characterization of the molecular eigenstates [11], which can provide unambiguous fingerprints of the spin cluster [12, 13] and can be used to quantify entanglement in supramolecular complexes [14]. However, the full potential of molecular magnetism is still largely unexploited, because large molecules and complex supramolecular structures can be controllably synthesized [15–18], but are poorly understood. In fact, their large Hilbert space precludes the simulation of their dynamics and the interpretation of spectroscopic measurements.

Here we show that quantum computers [19–22] can efficiently solve this issue. By simulating prototypical spin systems on the IBM quantum hardware [22], we extract dynamical correlations and the associated magnetic neutron cross-section. From this information we then obtain the degree of entanglement in eigenstates. The synergy between developments in neutron scattering and processors containing few dozens of qubits will enable a big step forward in the design of spin clusters for fundamental and technological applications.

Huge investments have been devoted in the last years to the realization of new powerful neutron sources (such as the European Spallation Source), which in the near future will enormously enlarge experimental capabilities. For instance, the powerful but demanding 4-dimensional inelastic neutron scattering (4D-INS) approach [11, 12, 14], exploiting measurements of the scattered intensity as a function of both the transferred energy ($E$) and momentum ($Q$), will greatly benefit from the large increase of the neutron flux in these new facilities. These technological progresses pave the way to the characterization of larger and more complex spin systems, such as already synthesized rings of potential qubits [15], highly frustrated clusters [16, 17] or giant spin cycles close to a quantum critical point [18].

In order to understand the spin dynamics of these systems from INS experiments, we need to compute the magnetic neutron cross-section ($T = 0$) [23]:

$$I(Q, E) \propto \sum_{i,j} F_i(Q) F_j^*(Q) \sum_{\alpha,\beta=\pm 1} \sum_p \left( \delta_{\alpha,\beta} - \frac{Q_\alpha Q_\beta}{Q^2} \right) \langle 0|s_i^\alpha|p\rangle\langle p|s_j^\beta|0\rangle e^{-iQ R_{ij}} \delta(E - E_p).$$

(1)

Here $F_i(Q)$ is the (known) magnetic form factor for ion $i$, $|0\rangle$ and $|p\rangle$ are the ground and excited molecular eigenstates with energies $E_0 = 0$ and $E_p$ and $R_{ij}$ are the relative positions of the magnetic ions with spin components $s_i^\alpha$. The excitation energies $E_p$ and the products of spin matrix elements $\langle 0|s_i^\alpha|p\rangle\langle p|s_j^\beta|0\rangle$ are the Fourier frequencies and coefficients of dynamical spin-spin correlations functions:

$$C_{ij}^{\alpha\beta}(t) = \langle s_i^\alpha(t)s_j^\beta(t) \rangle_0 = \sum_p \langle 0|s_i^\alpha|p\rangle\langle p|s_j^\beta|0\rangle e^{-iE_p t}. \quad (2)$$

These are the key ingredients for computing $I(Q, E)$ and constitute the hard task for classical computers. Indeed, the calculations of $C_{ij}^{\alpha\beta}(t)$ for many interesting molecules is presently inconceivable.

Here we propose this strategy: (i) use the quantum computer (QC) to simulate $C_{ij}^{\alpha\beta}(t)$; (ii) extract the excitation energies and products of matrix elements by fitting $C_{ij}^{\alpha\beta}$ or by performing a classical Fourier transform; and finally (iii) calculate the neutron cross-section on a classical computer by combining the coefficients obtained in (ii) with known quantities such as form factors and positions of the ions. The core step of this procedure is the simulation of target molecule dynamics to evaluate $C_{ij}^{\alpha\beta}(t)$ (see below), which on classical computers is limited to few dozens of spins, even in the simplest case of spins 1/2. Conversely, such simulation is exponentially more efficient on a QC [24]. The procedure can then be repeated for different sets of Hamiltonian parameters, thus providing a method to fit

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INS data of complex spin systems.

To experimentally test this scheme, we compute with IBM chips the INS cross-section for prototype kinds of spin clusters. The so-obtained results show that the procedure is effective and will be extended to larger systems when improved QCs become available. Experiments are performed on a 5- (ibm2x4) and 16-qubit (ibmq5x) superconducting processors [25] composed of fixed-frequency Josephson-junction-based transmon qubits [26]. Qubit control and readout are achieved using individual superconducting coplanar waveguide (CPW), while another set of CPW resonators (quantum buses), organized as in Figs. 1a and 4a for the 5- and 16-qubit devices provide the necessary inter-qubit connectivity. To avoid thermal excitation and dephasing, the qubits are cooled down to 25 mK in a dilution refrigerator and thus initialized in their ground state (see Methods). All the experiments were run with a large number of measurements (8192) to reduce noise on the chip.

The benchmark molecules are characterized by the Hamiltonian \( H \) (2, 3):

\[
H = \sum_{i=1}^{N-1} \left[ J_p \left( s_i^x s_{i+1}^x + s_i^y s_{i+1}^y \right) + \sum_{i=1}^{N} g_i s_i^z \right] + B \sum_{i=1}^{N} g_i s_i^z.
\]

As recently demonstrated [14], the 4D-INS approach allows one to quantify entanglement in effective spin dimers. This is achieved by applying a sizable magnetic field \( B \gg |J_p| \), such that the ground state is factorized \( |↓↓\rangle \) and can be exploited as a reference to investigate entanglement in the excited states. Indeed, modulations in the \( I(Q) \) of each transition directly reflect...
the concurrence of the corresponding excited state (see below). Hence, we exploited the ibmqx4 chip (sketched in Fig. 1a) to extract the dynamics and compute the neutron cross-section of spin dimers characterized by different sets of parameters: $J_p = J_z = J$, $g_1 = g_2 = g$ (Heisenberg model, molecule 1), $J_p = J_z = J$, $g_1 \neq g_2$ (Heisenberg model with two inequivalent ions, molecule 2) and $J_p = 0$, $J_z = J$, $g_1 \neq g_2$ (Ising model, molecule 3). Besides showing that $I(Q, E)$ strongly depends on the Hamiltonian parameters, these experiments enable us to investigate different degrees of entanglement in the dimer eigenstates.

The quantum circuit used to compute dynamical correlation functions is reported in Fig. 1b and exploits an ancillary qubit ("a") to measure correlations between logical qubits 1 and 2 [27]. After initialization of the qubits in the ground state $|0\rangle = |↓↓\rangle \equiv |11\rangle$ and of the ancilla in $|0\rangle$, the simulation of the time evolution induced by $\mathcal{H}$ is sandwiched between a controlled-$\alpha$ and a controlled-$\beta$ gate (\(\alpha, \beta = x, y, z\)) in which the ancilla acts as a control of qubit $i$. Finally, the value of $\omega_{ij}^\alpha$ is obtained by measuring $\langle s_i^x \rangle = \langle s_i^x \rangle + i\langle s_i^y \rangle$. The simulation of the time evolution induced by the target cluster Hamiltonian $U(t) = e^{-i\mathcal{H}t}$ is obtained by decomposing the time interval into small steps $\tau = t/n$ and then applying the Suzuki-Trotter formula (see Methods).

The real (red circles) and imaginary (blue) parts of $\mathcal{C}^{\alpha\beta}_{ij}(t)$ evaluated with ibmqx4 chip for molecule 1 are reported in Fig. 1c. In this case, all terms in $\mathcal{H}$ commute and the correct time-evolution is already obtained with a single Trotter step ($n = 1$). These results are in excellent agreement with the exact behavior, calculated by diagonalizing $\mathcal{H}$ (Figs. S3-S7). Energies $E_p$ and coefficients $\langle 0|s_i^\alpha|p\rangle|s_j^\beta|0\rangle$ entering the cross-section are extracted fitting the time-dependence with a combination of constant and oscillating $e^{-iE_p}\tau^i$ terms (Eq. 2) (see Methods). In particular, while $\omega - \omega$ correlations are constant, we find that $\omega - \omega$ ones have two Fourier components. The extracted coefficients are reported in the caption of Fig. 1 and Table S1 and are in excellent agreement with exact values (indicated in squared brackets). We have reported here only relevant terms for the neutron cross-section, while the others are shown in the SI.

The resulting neutron cross-section $I(Q_x, Q_y, Q_z = 0, E)$ is shown in Fig. 1d. Modulations of the neutron intensity as a function of $Q_x$ at the two energy-cuts correspond-

**FIG. 2:** Correlation functions and INS cross-section for molecule 2. a, $C^{ij}_{II}(t)$ computed on ibmqx4 for molecule 2 ($B_{g1} = 10J$, $B_{g2} = 12.5J$). To minimize the digital error, we exploit the second order expansion reported in Fig. 1b with $n = 2$ up to $J t = 2.0$ and $n = 4$ for $2.0 < J t \leq 6.0$. This allows us to simulate multiple beats in the oscillations of $C^{II}_{II}(t)$, which are then reproduced periodically. These oscillations are captured by fitting the points simulated on the chip with a combination of two sinusoidal functions. The parameters obtained from the fit are $\omega_1/J = 9.50(5)[9.40]$, $\omega_2/J = 12.10(8)[12.10]$, $\langle |0|s_1^x|1\rangle^2 = 0.24(2)[0.24]$, $\langle |0|s_1^y|2\rangle^2 = 0.02(1)[0.01]$, $\langle |0|s_1^z|1\rangle^2 = 0.02(1)[0.01]$, $\langle |0|s_2^y|2\rangle^2 = 0.24(2)[0.24]$, $\langle 0|s_2^x|1\rangle|s_2^z|0\rangle = -0.05(1)[-0.05]$, $\langle 0|s_2^x|1\rangle|s_2^z|0\rangle = 0.05(1)[0.05]$. Exact values obtained from Hamiltonian diagonalization are reported in squared brackets. The agreement is very good. b, Inelastic neutron scattering cross section $I(Q_x, Q_y, Q_z = 0, E)$ evaluated from the parameters listed above. Compared to Fig. 1d, the $Q$-modulation is smoother, indicating a smaller entanglement between the two ions.

**FIG. 3:** Quantifying entanglement a-c. Inelastic neutron scattering spectra for molecules 1-3 as a function of the normalized transferred energy (integrated over the whole $Q$-range). Here $q = (g_1 + g_2)/2$. d-f, $Q_x, Q_y$-dependence of peak I at $Q_z = 0$ for the three examined molecules (left panels), and corresponding $Q_y = 0$ cuts (right panels), evidencing a decreasing modulation of the scattered intensity with decreasing concurrence ($C = 1.0(1), 0.4(1), 0.0(1)$ for molecule 1, 2, 3 respectively), which is directly extracted from a fit of the $I(Q_x, Q_y = 0, Q_z = 0, E = E_1)$ data.
FIG. 4: Dynamical correlation functions and INS spectrum of a spin trimer. a, Sketch of the spin trimer structure (equilateral triangle with edge 5 Å) and of its mapping on ibmqx4 and ibmqx5 chips, with qubits 1-3 encoding the spin trimer and an ancilla (a) for measurements. Due to their different topology, ibmqx4 is used for nearest-neighbor correlations $C^2_{12}(t)$, while ibmqx5 for next-to-nearest-neighbor $C^3_{123}(t)$. b, Scheme of ibmqx5 chip, with labels on the qubits employed in our experiments. c, Quantum circuit to compute $C^3_{123}(t)$. Trotter decomposition is required, due to non-commuting terms $s_1 \cdot s_2$ and $s_2 \cdot s_3$, leading to evolution operators $U_{12}(\tau) = e^{-iJ_{s_1} s_2 \tau}$ and $U_{23}(\tau) = e^{-iJ_{s_2} s_3 \tau}$ for each time step $\tau = t/n$. d, Dynamical auto-correlations (real part) for the two inequivalent ions 1 ($C^2_{11}$) and 2 ($C^2_{12}$) and cross-correlations between nearest-neighbor ($C^2_{22}$) and next-to-nearest-neighbor ($C^3_{23}$) spins, fitted with a superposition of three frequencies: $\omega_1/J = 8.5(1)[8.5]$, $\omega_2/J = 9.5(1)[9.5]$, $\omega_3/J = 10.0(1)[10.0]$. The other parameters of the fit are: $|\langle 0|s_1^x|1\rangle|^2 = 0.04(3)[0.0425]$, $|\langle 0|s_2^x|1\rangle|^2 = 0.14(2)[0.125]$, $|\langle 0|s_3^x|1\rangle|^2 = 0.08(3)[0.0825]$, $|\langle 0|s_1^x|0\rangle|^2 = 0.23(5)[0.2300]$, $|\langle 0|s_2^x|0\rangle|^2 = 0.02(3)[0.000]$, $|\langle 0|s_3^x|0\rangle|^2 = 0.09(3)[0.0825]$, $|\langle 0|s_1^x|0\rangle|^2 = 0.05(3)[0.0425]$, $|\langle 0|s_2^x|0\rangle|^2 = 0.13(1)[-0.125]$, $|\langle 0|s_3^x|0\rangle|^2 = 0.08(3)[0.0825]$. Exact values are indicated in squared brackets, showing a good agreement. e, $I(E)$ spectrum, $I(Q_x,Q_y)$ maps and associated precession pattern of the individual spins at energies corresponding to the three peaks.

The agreement between measured and calculated Fourier coefficients (see caption of Fig. 2 and Table S1) is still very good, even if the number of gates used for molecule 2 is much larger than in 1. Experiments performed with the parameters of cluster 3 lead to completely monochromatic oscillations of the auto-correlation functions and negligible cross-correlations. Extracted coefficients are listed in Table S1.

The $Q$-dependence of the neutron spectra is strictly related with entanglement in the eigenstates [14]. Hence, the present experiments allow us to extract the concurrence $C$, a measure of entanglement [29] (see Methods). Figure 3 shows a comparison of the spectra calculated for the three dimers. The energy-dependence (first column) is similar in the three cases. Conversely, the $I(Q_x,Q_y)$ maps and the corresponding cuts for $Q_y = 0$ (reported in panels (d-f) for peak 1) are much more informative. A clear decrease in the amplitude of the $I(Q_z)$ modu-
lations fingerprints a decrease of entanglement. Indeed, by fitting these oscillations (red dots) with the analytical expression reported in the Methods (black line), we obtain $C = 1.0(1), 0.4(1), 0.0(1)$ for molecule 1, 2, 3, in agreement with exact calculations from Hamiltonian diagonalization.

This scheme is now extended to a spin trimer (Fig. 4a) with Heisenberg nearest-neighbors interactions ($J_1 = J$ and $g_1 = g$ in Eq. 3). We exploit two chips which, thanks to the different coupling topology (Fig. 4a), allow us to probe both nearest-neighbors (on ibmqx4) and next-to-nearest-neighbor correlation functions (on ibmqx5, outlined in panel b). The quantum circuit employed to extract dynamical correlations in the trimer is reported in Fig. 4c, while the resulting $C_{xx}^{ij}$ are displayed in panel d and in the SI, fitted with three oscillating functions. Due to the larger number of gates, we have here used a Trotter decomposition with $n = 2$, which allows us to extract the correct Fourier coefficients (see the caption of Fig. 4) and to accurately compute the INS spectrum. The latter is shown in panel e and is very close to that obtained by diagonalizing $\mathcal{H}$ (see Fig. S22). These results are remarkable, because the number of gates make the computation time rather close to the measured coherence times of the superconducting qubits (see Tables S3-S4).

We stress that the total time required for the simulation of, e.g., a spin chain of length $N$ does not increase for $N > 3$, since the simulation of odd ($s_{2i-1} \cdot s_{2i}$) and even ($s_{2i} \cdot s_{2i+1}$) bonds can be performed in parallel. Computations in small or zero applied field can be performed for a generic geometry in the same way, by exploiting the variational eigensolver procedure described in Ref. [22] to find the initial state. At last, the same scheme can be used for clusters with spins $s > 1/2$ (see Methods).

By performing experiments on ibmqx4 and ibmqx5 chips, we have demonstrated that available quantum computers can be used to efficiently calculate the INS cross-section of finite-size spin systems. We show that accurate time-correlation functions can be obtained using state-of-the-art (non error-corrected) devices. While our simulations are still limited by the performance of available qubits, they could be extended with forthcoming technological progresses to a number of spins that cannot be managed by classical devices, opening up new avenues for the characterization of large scale INS experiments. These results, combined with remarkable developments occurring in neutron scattering facilities, open new prospects in the design and understanding of spin systems.

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Author contributions

A.C., F.T. and M.G. used the IBM chips to implement gate sequences. Analysis of the experimental results was made by A.C., F.T., D.G., I.T. and S.C.. Classical calculations have been performed by A.C. and F.T.. P.S., I.T., D.G. and S.C. conceived the work and discussed the results with other coauthors. A.C. and S.C. wrote the manuscript with inputs from all coauthors.

Competing interests

The authors declare no competing interests.

Additional information

is available for this paper at

Methods

Experimental implementation of the gates. The ibmqx4 5-qubit processor is described schematically in Fig. 1a. All 5 transmon qubits are coupled individually with CPW resonators used for both qubit control and readout. Two additional shared CPW resonators are used to couple the central qubit, a, with all other qubits (1 to 4) as well as qubit 2 with 4, and 1 with 3. The second quantum processor used in this work, ibmqx5, is composed of 16 transmon qubits organized as depicted in Fig. 4b. In this case, only four qubits (a, 1, 2 and 3 in Fig 4b) are used in order to achieve the desired connectivity reported in Fig.4a, which cannot be obtained using the ibmqx4 device of Fig. 1a.

The qubits are controlled by microwave pulses that are sent from the electronics operating at room temperature to the quantum chip through attenuated coaxial lines. Single qubit gates are operated at their specific fixed frequencies ω_{i} for i=1,2,3,4 in ibmqx4 and i=a,1,2,3 in ibmqx5 as specified on IBM QX webpage. Two-qubit cross-resonance gates are obtained by driving a selected qubit Q_{a} (characterized by a fixed frequency ω_{a}) at the frequency ω_{p} of the target qubit. For both quantum processors, the pairs of control-target qubits are defined by the coupling map in Figs. 1a and 4a. The state of each qubit is measured at its readout resonator frequency; the reflected readout signals are amplified first by a Josephson parametric converter followed by HEMT amplifiers operating at 4K.

It is important to mention that all non-elementary quantum operations (e.g. Toffoli and SWAP gate) need to be decomposed into elementary operations of the fundamental gate set (Bloch sphere rotations and CNOT gates) prior coding them in the IBM processors (see SI). We finally note that CNOT gates can only be implemented between two connected qubits with a fixed orientation that defines control and target qubits (arrows in Figs. 1a and 4a).

Fitting dynamical correlation functions. C^{αβ}_{ij}(t) are fitted with a combination of oscillating functions:

\[
C^{αβ}_{ij}(t) = \sum_{p} \left[ A^{αβ}_{ij}(ω_p) + i B^{αβ}_{ij}(ω_p) e^{-iω_p t} \right]
= \sum_{p} \left[ A^{αβ}_{ij}(ω_p) \cos ω_p t + B^{αβ}_{ij}(ω_p) \sin ω_p t \right] + i \sum_{p} \left[ B^{αβ}_{ij}(ω_p) \cos ω_p t - A^{αβ}_{ij}(ω_p) \sin ω_p t \right].
\] (4)
Here we have recast the Fourier coefficients \((0|s^α_i|p)\langle ps^β_j|0\rangle = A_{ij}^{αβ}(ω_η) + iB_{ij}^{αβ}(ω_η)\) in order to separate the real and imaginary parts of \(C_{ij}^{αβ}(t)\), corresponding to the second and third line of Eq. (1). Some general conditions impose constraints on the parameters of the fit. In particular, \(C_{αα}^{αα}(0)\) must be real and positive, because it corresponds to a sum of squared absolute values. This allows us to correct for a dephasing in the measured values of \(C_{ij}^{αβ}(t)\), without making any assumption on the specific form of the target eigenstates. Indeed, the real and imaginary parts of the raw correlation functions \(C_{ij}^{αβ}(t)\) are found to be mixed, if compared to the exact calculation. This is related to a systematic error in the implementation of single qubit \(R_x\) and \(R_y\) rotations. However, this dephasing can be easily corrected by multiplying \(\bar{C}_{ij}^{αβ}(t)\) in the whole time domain for a phase factor, such that \(C_{αα}^{αα}(0) = e^{iω_η α} \bar{C}_{αα}^{αα}(0)\) is imposed to be real. The measured behavior of \(C_{ij}^{αβ}(t)\) should also be corrected for an overall attenuation of the experimental oscillations due to the combined effect of measurement errors and decoherence. To fix this scaling factor, which depends on the parameters of the fit. In particular, \(C_{αα}^{αα}(0)\) are independent of time (thus not contributing to the inelastic cross-section). At last, the results fulfill axial and permutation symmetries of the target Hamiltonian, when present. The former leads to equivalence between \(\bar{C}_{ij}^{αβ}(t)\) and \(\bar{C}_{ji}^{αβ}(t)\) contributions, the latter between \(\bar{C}_{ij}^{αβ}(t)\) and \(\bar{C}_{αα}^{αα}(t)\). Since \(\bar{C}_{ij}^{αβ}(t)\) involves a larger number of gates and is thus more error prone than \(\bar{C}_{ij}^{αβ}(t)\), leading to more noisy correlation functions, we used only \(\bar{C}_{ij}^{αβ}(t)\) for calculating the final cross-section (see comparison in the SI).

\[ \langle \sigma_i^α | p | \sigma_j^β \rangle = 0, \]\n
\[ \sum_k C_{kk}^{αα}(0) = \sum_k C_{kk}^{αα}(0) = 1, \]\n
with \(\mathcal{H}_1 = B(g_1 s^x_i g_2 s^x_j)\) and \(\mathcal{H}_2 = J_\sigma (s^x_i s^x_j + s^y_i s^y_j) + J_\sigma s^z_i s^z_j\) indicating one- and two-body terms of the target spin Hamiltonian.

### Inelastic Neutron Scattering

For each examined spin excitation, the extracted \(Q\)-dependence of the inelastic neutron cross-section gives important informations about the structure of the eigenstates involved in the transition. For instance, transitions between states belonging to different total spin multiplets are characterized by a minimum in \(I(Q)\) for \(Q \to 0\). This is evident in the modulations displayed in Fig. 1d, where peak I corresponds to an inter-multiplet transition between the ground state triplet and the excited singlet, while peak II represents a transition within triplet states, namely the ground \(|↓↓\rangle\) and the excited \(\vec{Q}(|↓↓\rangle + |↑↑\rangle)\). This is consistent with the positive sign of \(J\) in the target Hamiltonian, leading to a singlet state lower in energy than the triplet.

The information on eigenstates in reciprocal \((E, Q)\) space is equivalent to a description in terms of time and position variables. Indeed, the \(Q\)-dependence of a peak at energy \(E_p\) is directly related to the spatial pattern of the spins preceding around \(z\) with frequency \(E_p\), after a resonant perturbation has brought a molecule from its ground state into a superposition state with a small component on the corresponding excited state [12]. These patterns are represented by the vectors \(\langle s^α_i(t) \rangle, \langle s^β_j(t) \rangle, \langle s^α_i(t) \rangle \rangle\) schematically depicted in the insets of Figs. 1, 3 and 4. In particular, the two excitations shown in Fig. 1d are an inter-multiplet transition (I, with the \(x - y\) components of the two spins preceding in phase opposition) and a giant spin excitation (II, with the two spins rigidly precessing conserving the same total-spin modulus of the ground state). Conversely, peak III of Fig. 4e represents an excitation in which only the two external spins 1 and 3 are preceding, while peak III is another intra-multiplet giant spin excitation.

### Concurrence from INS spectrum of spin dimers

The two-qubit entanglement can be quantified by means of the concurrence \((C)\) [29]. For pure two-qubit states \(|p\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle, C = 2|ad - bc|\). In the present cases, we have found \(C_{ij}^{αβ}(t)\) independent of time and hence \(d = 0\) in the excited states corresponding to the two calculated INS peaks. By inserting the expression of \(|p\rangle\) in Eq. (1), we get

\[ I(Q_s) \propto F_1(Q_s)F_2(Q_s) \left[ |b|^2 + |c|^2 + 2|bc|^2 \cos Q_s R - 2\text{Im}(bc^*)\sin Q_s R \right] \quad (5) \]

where \(R_{12} = Bx\). Hence, the parameters \(b\) and \(c\) (and, consequently \(C = 2|bc|\)) can be obtained from a fit of \(I(Q_s)\). We note that the presence of only two peaks in Fig. 3a-c implies \(a = 0\).

### Simulation of spin clusters with \(s > 1/2\)

The simulation of Hamiltonians involving \(s > 1/2\) spins (and the related calculation of dynamical correlation functions) can be performed by encoding the state of each spin into that of 2s qubits. For instance, we can exploit four qubits \(\sigma_1,...,\sigma_4\) to encode a pair of interacting spins \(s_{1,2} = 1\), i.e. \(s^α_1 = (\sigma^α_1 + \sigma^α_2) / 2\) and \(s^α_2 = (\sigma^α_2 + \sigma^α_3) / 2\). Then the calculation of dynamical correlation functions on the target Hamiltonian can be recast in terms of correlation functions on pairs of physical qubits:

\[ \langle s^α_i(t)s^β_j(t) \rangle = \frac{1}{4} \left[ \langle \sigma^α_i(t)\sigma^β_i(t) \rangle + \langle \sigma^α_i(t)\sigma^β_j(t) \rangle + \langle \sigma^α_j(t)\sigma^β_i(t) \rangle + \langle \sigma^α_j(t)\sigma^β_j(t) \rangle \right] \]

which can be directly evaluated using the QC.
Data availability.
All the data and simulations that support the findings of this study are available from the corresponding author upon reasonable request.

Code availability.
The custom Python scripts for the quantum hardware and original codes are available from the corresponding author upon reasonable request.