

Improved certification of Bell-operator correlations via optimization

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Bell nonlocality is an intrinsic feature of quantum mechanics, which can be detected via the violation of Bell inequalities. It is therefore a fundamental question to certify Bell nonlocality from experimental data. Here we present an optimization framework to detect Bell-operator correlations by exploring flexible mappings between Bell inequalities and Hamiltonians corresponding to the Bell operators. We show that several Hamiltonian models can be mapped to new inequalities with improved classical bounds compared to the original one, enabling a more robust certification of Bell-operator correlations. From the other direction, we investigate the mapping from fixed Bell inequalities to Hamiltonians, aiming to maximize quantum violations while considering experimental imperfections. As a practical application, we experimentally exploit this method in an XXZ-like honeycomb-lattice model utilizing over 70 superconducting qubits. The successful application of this technique, together with the combination of the two directions to form an optimization loop, may open new avenues for developing more practical and noise-resilient certification techniques for Bell-operator correlations and enable broader experimental explorations.

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I. INTRODUCTION

Nonlocality, characterized by correlations that cannot be explained within a local hidden-variable framework, is among the most mysterious and fundamental features of the quantum world [1]. This property can be revealed via the violation of a Bell inequality [2–4], where measurements on entangled quantum systems yield correlations surpassing the classical reach. Following early demonstrations, primarily on optical platforms [5–8], loopholes such as the detection and locality loopholes have been carefully addressed [9,10], culminating in loophole-free experiments across several platforms,

including nitrogen-vacancy centers [11], photons [12–14], neutral atoms [15], and more recently superconducting circuits [16]. Apart from its fundamental importance, nonlocality is also a crucial resource for applications: It enables device-independent information processing such as quantum cryptography [17–19], randomness amplification [20–22], and self-testing [23] and it supports unconditional computational advantages [24,25].

With larger quantum devices available in laboratories, the focus has shifted to accessing nonclassical correlations in many-body systems. In this regime, fully device-independent, loophole-free Bell tests [11–16] remain out of reach, and experiments typically infer Bell-type signatures from restricted measurement data, often involving collective observables; this has enabled demonstrations in, e.g., Bose-Einstein condensates [26] and spin-squeezed atomic ensembles [27]. Since such analyses rely explicitly on quantum mechanics and additional modeling assumptions, it is useful to distinguish between (i) Bell nonlocality in the device-independent loophole-free sense [17] and (ii) Bell correlations in many-body settings, where certification depends on restricted

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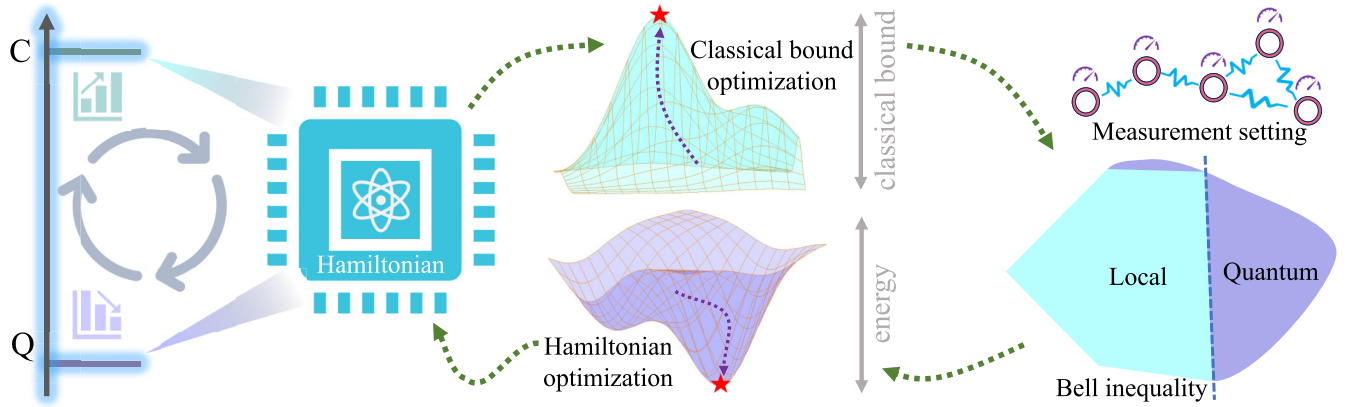


FIG. 1. Illustration of the optimization scheme executed between Bell inequalities and Hamiltonians. We begin by parametrizing both Bell inequalities and measurement settings, and a Bell inequality where the quantum measurement observables replace the measurements forms an equivalent Hamiltonian $\mathcal{H}$. For a specified spin Hamiltonian, by keeping $\mathcal{H}$ fixed and equal to this spin Hamiltonian, we search through the parameter space to find Bell inequalities with higher classical bounds (upper half). For a specified Bell inequality, with experimentally measured correlators, we can also optimize the measurement settings to find lower quantum values (lower half). This process forms a loop and can be executed iteratively to maximize the gap between the classical bound and the quantum value until it converges.

measurement access and additional assumptions. A fruitful approach in this regime is to adopt an energy perspective: A Bell inequality together with a choice of local measurements defines a Bell operator, which in some cases can be identified with a local many-body Hamiltonian [28–31]. Here we focus on this intermediate regime between loophole-free Bell non-locality and collective many-body Bell correlations, where we can assume individual addressability of the parties, which we term Bell-operator correlations [31].

In practical many-body scenarios, experimental noise poses a major obstacle to certifying Bell-operator correlations [26–30,32–34]. Prepared states may deviate from the ideal target, and the observed energy may fail to cross the classical bound associated with a given inequality. A central question is therefore whether Bell-operator correlations can still be certified even when experimental data fail to violate a preselected Bell inequality. Recently, an optimization method was introduced [35] to systematically identify the optimal inequality that maximizes the classical-quantum gap for the observed correlations from the entire set of Bell inequalities in a given scenario.

In this work we propose an iterative optimization framework that exploits flexible mappings between Bell inequalities and Hamiltonians (Bell operators) to improve certification without requiring prior knowledge of the complete inequality set. The core idea is to alternately refine the Bell expression and the associated quantum strategy (state or measurement settings), thereby enlarging the gap between the classical bound and quantum value, as schematically illustrated in Fig. 1. Within this framework, the detection of Bell-operator correlations can be approached in two complementary ways: (i) by raising the classical bound via an optimization of the inequality coefficients for a fixed Hamiltonian and (ii) by lowering the quantum value through an optimization of measurement settings for a fixed inequality.

We apply this framework to Hamiltonians connected to Bell inequalities from previous works [29,31], including a variant of Gisin’s elegant inequality [29,36]. We show that the same target Hamiltonian can be mapped to new

inequalities with substantially improved classical thresholds. As an experimental demonstration, we implement a variational quantum algorithm to prepare low-energy states of an XXZ-like honeycomb-lattice model on a 73-qubit superconducting processor. In the original setting, the quantum value does not violate the classical bound beyond the statistical uncertainty due to experimental noise, whereas an optimized inequality certifies Bell-operator correlations using the same measurement data. The search procedure is model dependent (qubits, a specified Hamiltonian structure, and Bloch-sphere parametrized measurements), while the resulting Bell inequalities are device independent in the formal sense. However, the experimental demonstration here is not loophole-free and therefore does not constitute a fully device-independent test.

II. PRELIMINARIES

We fix notation for Bell expressions and the associated Bell operators and introduce the Hamiltonian mapping used throughout the paper. We consider a Bell inequality written as $\mathcal{I} \geq \beta_C$, where $\mathcal{I}$ is a linear combination of correlators and β_C is the classical bound, the smallest obtainable value of $\mathcal{I}$ if we adhere to a local hidden-variable model. Throughout, we adopt an energy-witness convention: A violation of the Bell inequality corresponds to obtaining an expectation value of the associated Bell operator below the classical bound, i.e., quantum correlations are certified when the measured expectation value of the implied energy crosses the classical bound from above to below.

The mapping between Bell inequalities and Bell operators (Hamiltonians) is generally not one to one [29,37]. First, for a fixed Bell inequality, different choices of local measurement settings generally lead to different Bell operators and thus to different effective Hamiltonians. For example, in the Clauser-Horne-Shimony-Holt (CHSH) inequality [3], varying the relative angles between the two dichotomic observables at each site changes the resulting Bell operator. Second, whenever a given Hamiltonian admits an interpretation as a Bell operator, it can typically be realized by multiple Bell

inequalities with suitably chosen measurements. As a simple illustration, the same two-qubit interaction Hamiltonian proportional to $\sigma_x^{(1)}\sigma_x^{(2)} + \sigma_z^{(1)}\sigma_z^{(2)}$ can be embedded into distinct CHSH-type Bell expressions by different assignments of measurement labels and local basis rotations.

For concreteness, we first describe a bipartite $(m_1, 2, m_2, 2)$ scenario, where party A (B) performs one of m_1 (m_2) measurements and each measurement has two outcomes. The general Bell operator of this scenario can be written as

$$\mathcal{B}_{\text{gen}} = \sum_{x_1, x_2=0}^{m_1-1, m_2-1} \sum_{k_1, k_2=0}^1 \alpha_{x_1, x_2}^{(k_1, k_2)} A_{x_1}^{(k_1)} B_{x_2}^{(k_2)}, \quad (1)$$

where $A_{x_1}^{(k_1)} = \sum_{a=0}^1 (-1)^{ak_1} F_{x_1, a}$ is the discrete Fourier transform of a positive-operator-valued measure $\{F_{x_1, a}\}_{a=0}^1$ representing the measurement on party A in the basis x_1 ; $B_{x_2}^{(k_2)}$ for party B is defined similarly. Note that $[A_{x_1}^{(k_1)}, B_{x_2}^{(k_2)}] = 0$ for $x_1 \in [m_1] = \{0, 1, \dots, m_1 - 1\}$, $x_2 \in [m_2] = \{0, 1, \dots, m_2 - 1\}$, and $k_1, k_2 = 0, 1$ since they act on different systems. Moreover, the term $A_{x_1}^{(k_1)} B_{x_2}^{(k_2)}$ reduces to the local term $B_{x_2}^{(k_2)}$ when $k_1 = 0$ and similarly to $A_{x_1}^{(k_1)}$ when $k_2 = 0$. In this paper we exclude single-body terms, and therefore we impose $\alpha_{x_1, x_2}^{(0,0)} = \alpha_{x_1, x_2}^{(1,0)} = \alpha_{x_1, x_2}^{(0,1)} = 0$ and retain only the $(k_1, k_2) = (1, 1)$ sector. Accordingly, we drop the superscripts and write $A_{x_1} \equiv A_{x_1}^{(1)}$ and $B_{x_2} \equiv B_{x_2}^{(1)}$. Finally, by fixing the Bell operator $\mathcal{B}_{\text{gen}}$, one can build a corresponding Hamiltonian $\mathcal{H}_{\text{gen}}$ such that $\mathcal{H}_{\text{gen}} \equiv \mathcal{B}_{\text{gen}}$. Further details on the Bell-operator–Hamiltonian mapping are given in Appendix A.

III. ITERATIVE OPTIMIZATION FRAMEWORK

In this section we propose an iterative optimization framework that exploits flexible mappings between Bell inequalities and Hamiltonians (Bell operators) to improve certification, without requiring prior knowledge of the complete inequality set. The core idea is to alternately refine the Bell expression and the associated quantum strategy (state preparation and/or measurement settings), thereby increasing the separation between the classical bound and quantum value, as illustrated in Fig. 1. Operationally, the scheme proceeds in two complementary directions. First, for a fixed target Hamiltonian identified with a Bell operator, we search for an equivalent Bell inequality whose classical bound is as high as possible, making a violation easier to observe in the presence of noise. Second, for a fixed Bell inequality and a fixed set of experimentally estimated correlators, we optimize the measurement settings used to evaluate that inequality so as to minimize the observed quantum value. Importantly, while the resulting Bell inequalities are valid in a device-independent sense for the specified Bell scenario, the search procedure used to generate them is model dependent: Throughout we assume qubits, a fixed target Hamiltonian structure, and local measurement observables parametrized on the Bloch sphere.

A. From Hamiltonians to Bell inequalities

We first consider the task of adapting measurement settings to obtain Bell inequalities whose classical bounds are as high as possible for a fixed target Hamiltonian. To search for better

measurement operators, we begin with the parametrization of quantum measurement settings of the different parties. A single-qubit measurement $\vec{n} \cdot \vec{\sigma}$, where $\vec{n}$ denotes the measurement direction and $\vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$ denotes the Pauli basis, can be visualized in the Bloch sphere shown in Fig. 2. In this way, the parametrized measurements of party A can be written as $A_i = \vec{n}_i \cdot \vec{\sigma}$, where $\vec{n}_i$ specifies the measurement and contains parameters that can be variationally tuned. The measurements B_i for party B can be defined analogously. In this formalism, we build a parametrized mapping between the Bell inequality and the Bell operator: For all measurements, we denote the above parameters determining the respective vectors $\vec{n}_i$ collectively by θ .

Given a fixed Hamiltonian $\mathcal{H}$, we first decompose it into Pauli strings

$$\mathcal{H} = \sum_{p \in P_N} c_p p, \quad (2)$$

where P_N is the set of all Pauli strings operating on N sites and p is the Pauli string. For the unnormalized Pauli basis used here, $c_p = 2^{-N} \text{Tr}(p\mathcal{H})$. We use $\vec{h}$ to collectively denote the coefficients c_p in the Pauli basis, and use a vector $\vec{\alpha}$ to represent the coefficients of the Bell inequality [cf. Eq. (1)]. For the bipartite two-body sector, the components of $\vec{h}$ are $h_{ij} = \frac{1}{4} \text{Tr}[(\sigma_i \otimes \sigma_j) \mathcal{H}]$ for Pauli-axis indices $i, j \in \{x, y, z\}$, whereas the Bell coefficients are α_{x_1, x_2} for measurement-setting indices x_1, x_2 . Due to the connection between the Bell inequality and the operator, we obtain a set of linear equations

$$\mathbf{T}(\theta) \cdot \vec{\alpha} = \vec{h}, \quad (3)$$

where the two vectors are linearly connected by a matrix $\mathbf{T}(\theta)$ as a function of measurement parameters θ . Here $\mathbf{T}(\theta)$ is constructed from local qubit observables $A_i = \vec{n}_i \cdot \vec{\sigma}$ (and similarly for B_j) and therefore encodes the model assumptions.

Our objective in the Hamiltonian to inequality direction is to maximize the classical bound $\beta_C(\vec{\alpha})$ over the measurement parameters θ , subject to the constraint $\mathbf{T}(\theta)\vec{\alpha} = \vec{h}$ in Eq. (3). The explicit construction of $\mathbf{T}(\theta)$ for $(m_a, 2, m_b, 2)$ scenarios and its block structure are given in Appendix A. This equation may be underdetermined depending on the number of measurements in the Bell scenario. Upon obtaining a solution for the inequality determined by $\vec{\alpha}$, the corresponding classical bound can be computed, for instance, by exhaustive enumeration of all local deterministic strategies, ensuring that the final expression defines a valid Bell inequality for the given scenario. A general expression of $\mathbf{T}(\theta)$ as a matrix and its dependence on the Bell setting can also be found in Appendix A [37].

To formalize this problem as an optimization task, we define the cost function as the classical bound to be maximized, i.e., $\mathcal{L} = \mathcal{C}(\theta)$, where $\mathcal{C}(\theta)$ represents the classical bound obtained from the inequality implied by Eq. (3) for a given set of measurement parameters θ . By maximizing the cost function, we aim to find the optimal measurement parameters that yield the highest possible classical bound. The reason we only track the classical bound is that the quantum value associated with a fixed Hamiltonian is already determined here, so the only way to enlarge the quantum-to-classical separation is to tighten the classical bound. In other words, a higher classical

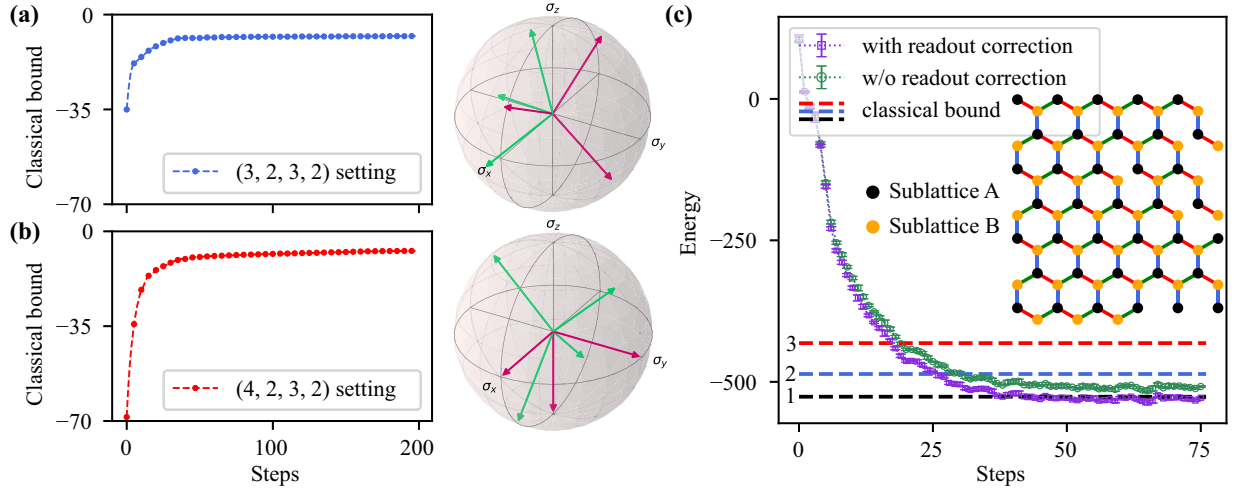


FIG. 2. Mappings from fixed spin Hamiltonians to Bell inequalities. (a) and (b) Optimized classical bounds as a function of training steps, where the Bloch sphere on the right side exhibits the measurement settings corresponding to the highest classical bound. Cyan and pink arrows denote measurement observables of parties *A* and *B*, respectively. (a) Parties *A* and *B* with three dichotomic measurements with outputs ± 1 . (b) Parties *A* and *B* with four and three dichotomic measurements with outputs ± 1 , respectively. (c) Experimental variational quantum optimization for the two-dimensional honeycomb model with 73 superconducting qubits. We present the measured energy of the model Hamiltonian with respect to training steps and the original classical bound [dashed line 1 is from Eq. (4)]. The optimized classical bound is shown as dashed line 2 for (a) and dashed line 3 for (b). The error bars denote the standard deviation over repeated estimates; each measurement configuration contains 1000 shots.

threshold directly translates into an improved inequality for subsequent quantum violations. This optimization problem can be handled by gradient-based optimization algorithms. Here we apply gradient ascent with the Adam optimizer.

B. From Bell inequalities to Hamiltonians

We have studied optimizable mappings from Hamiltonians to Bell inequalities, which can make Bell-operator correlations easier to certify in realistic, noisy experiments. We now turn to the complementary direction that is most relevant once experimental data are fixed: For a given Bell inequality, we optimize the measurement settings to lower the evaluated quantum value.

In practice, after preparing the entangled states, we certify Bell-operator correlations by measuring a predefined set of correlators and using their outcomes as the experimental observations. Due to experimental noise, these correlators may not yield a violation for a chosen inequality. The Bell-inequality to Hamiltonian direction addresses precisely this situation: The correlators are already measured, and we only adjust how they are combined. Using Eq. (3), fixing the inequality coefficients $\vec{\alpha}$ while varying the measurement parameters θ induces a family of Hamiltonians $\mathcal{H}(\vec{\alpha}, \theta)$. Since the correlator values are treated as fixed experimental inputs, we do not solve any ground-state problem; instead, we reweight the measured correlators to obtain the smallest possible value compatible with the chosen inequality parametrization. Formally, for Pauli-axis indices $i, j \in \{x, y, z\}$, we define the measured two-body Pauli correlators as

$$c_{ij} = \langle \sigma_i \otimes \sigma_j \rangle = \text{Tr}[\rho(\sigma_i \otimes \sigma_j)].$$

We collect these correlators in the row vector

$$\vec{c} = (c_{xx}, c_{xy}, c_{xz}, c_{yx}, \dots, c_{zz}),$$

using the same Pauli-axis ordering as the components of $\vec{h}$. Thus, for fixed $\vec{\alpha}$, our objective is to minimize

$$\mathcal{E}(\theta) = \vec{c} \cdot \vec{h}(\theta) = \vec{c} \cdot \mathbf{T}(\theta) \cdot \vec{\alpha}$$

over θ , where optimization methods such as gradient descent can be applied.

IV. BENCHMARK: A VARIANT OF GISIN'S ELEGANT INEQUALITY

The basic Bell inequality model we consider here is a variant [29] of Gisin's elegant Bell inequality [36]. This setting describes a bipartite scenario, where party *A* has four dichotomic measurements with outcomes ± 1 and *B* has three with outcomes ± 1 . Parametrized by Δ , this inequality is expressed as

$$\begin{aligned} \mathcal{I}_G(\Delta) = & A_0 B_0 + A_1 B_0 - A_2 B_0 - A_3 B_0 + A_0 B_1 - A_1 B_1 \\ & + A_2 B_1 - A_3 B_1 + \Delta(A_0 B_2 - A_1 B_2 - A_2 B_2 + A_3 B_2) \\ \geq & -2|\Delta| - |\Delta + 2| - |\Delta - 2|, \end{aligned} \quad (4)$$

where the bound is -8 for $\Delta = 2$. We will use this setting for both numerical and experimental explorations. For this inequality, by assigning four measurements

$$\begin{aligned} A_0 &= \frac{\sigma_x + \sigma_y + \sigma_z}{\sqrt{3}}, & A_1 &= \frac{\sigma_x - \sigma_y - \sigma_z}{\sqrt{3}}, \\ A_2 &= \frac{-\sigma_x + \sigma_y - \sigma_z}{\sqrt{3}}, & A_3 &= \frac{-\sigma_x - \sigma_y + \sigma_z}{\sqrt{3}} \end{aligned} \quad (5)$$

to party *A* and three measurements

$$B_0 = \sigma_x, \quad B_1 = \sigma_y, \quad B_2 = \sigma_z \quad (6)$$

to party B , we obtain a Bell operator in the form of a two-body Hamiltonian

$$\mathcal{H}_G = \frac{4}{\sqrt{3}}(\sigma_x^{(1)}\sigma_x^{(2)} + \sigma_y^{(1)}\sigma_y^{(2)} + 2\sigma_z^{(1)}\sigma_z^{(2)}), \quad (7)$$

where $\sigma_x^{(i)}$, $\sigma_y^{(i)}$, and $\sigma_z^{(i)}$ are Pauli operators acting on the qubit indexed by i . This Hamiltonian has a ground-state energy of approximately -9.24 , lower than the classical bound of -8 . Thus, by preparing the ground state of this model on hardware, we can experimentally certify Bell-operator correlations.

This two-body Hamiltonian can be generalized to many-body systems, such as one-dimensional chains [29] and two-dimensional lattices [37], by applying appropriate couplings between different qubits. Note that the measurement assignments in Eqs. (5) and (6) are chosen for convenience to obtain an XXZ-style Hamiltonian in Eq. (7). By selecting different measurements while fixing the Hamiltonian, we can obtain a higher classical bound, which is easier to violate experimentally. Our first goal is therefore to identify such measurement settings. In the following sections, we use this family of Hamiltonians and associated Bell inequalities as a benchmark for both optimization directions, before turning to the experimental many-body implementation.

A. Numerical results

We first fix the Hamiltonian in Eq. (7) and apply the Hamiltonian to inequality optimization to obtain new inequalities with higher classical bounds. As mentioned in Sec. III, this search procedure is inherently model dependent, as it assumes qubit-level Hamiltonians together with measurement operators parametrized on the Bloch sphere.

Let the (m_a, d_a, m_b, d_b) Bell scenario denote that party A and B have m_a and m_b measurements with d_a and d_b outcomes, respectively. We consider two scenarios. In the first scenario, both parties have three dichotomic measurements with outputs ± 1 , i.e., the $(3,2,3,2)$ scenario. The corresponding full-probability local polytope has only one nontrivial facet class beyond the CHSH inequality [38,39]. These classifications provide a useful benchmark, while our method does not require a precomputed facet list. Since the present ansatz excludes marginal terms, facets containing them would require extending the mapping to include one-body contributions.

The Adam optimization is executed for 10^4 steps and the parameters corresponding to the highest classical bound are recorded as the final output. All optimization hyperparameters and initialization choices can be found in Appendix B. For each choice of θ , the fixed-Hamiltonian optimization obtains $\tilde{\alpha}$ from the constraint $\mathbf{T}(\theta)\tilde{\alpha} = \tilde{h}$ and evaluates the corresponding classical bound over local deterministic strategies; no simulated or experimental correlator data enter the search.

For the selected parameters, the optimization yields a classical bound of around -7.39 , notably higher than the original bound of -8 [cf. Fig. 2(a)]. The optimized inequalities obtained from our numerical procedure often contain floating-point coefficients with many decimals, which are cumbersome to display and may obscure the main message. For clarity, we round the coefficients to three decimal places and report

a representative inequality explicitly:

$$\begin{aligned} \mathcal{I}_{(3,2,3,2)} = & -1.864A_0B_0 + 3.049A_0B_1 + 2.272A_0B_2 \\ & + 0.070A_1B_0 - 1.822A_1B_1 + 1.766A_1B_2 \\ & - 1.932A_2B_0 - 1.413A_2B_1 - 0.563A_2B_2 \\ & \geq -7.39. \end{aligned}$$

To visualize the optimized measurements, we also use the Bloch sphere to exhibit the optimized measurement directions in Fig. 2(a).

For the second $(4,2,3,2)$ scenario, party A has four dichotomic measurements while B has three. The complete classification also remains small in this case, with five nontrivial facet classes up to relabelings [39]. The best value reached in the numerical run is approximately -6.56 , further improving the value obtained in the first scenario. Similarly, we report this representative optimized inequality with coefficients rounded to three decimals:

$$\begin{aligned} \mathcal{I}_{(4,2,3,2)} = & -0.001A_0B_0 + 1.625A_0B_1 - 1.627A_0B_2 \\ & - 1.623A_1B_0 - 0.008A_1B_1 + 1.636A_1B_2 \\ & + 1.633A_2B_0 - 0.001A_2B_1 + 1.638A_2B_2 \\ & + 0.006A_3B_0 - 1.633A_3B_1 - 1.649A_3B_2 \\ & \geq -6.56. \end{aligned} \quad (8)$$

We also apply the Hamiltonian-to-inequality optimization to Gisin's elegant inequality [36] [$\Delta = 1$ in Eq. (4)], for which $\mathcal{I}_{G0} \geq -6$ and the corresponding Bell operator is

$$\mathcal{B}_{G0} = \frac{4}{\sqrt{3}}(\sigma_x^{(1)}\sigma_x^{(2)} + \sigma_y^{(1)}\sigma_y^{(2)} + \sigma_z^{(1)}\sigma_z^{(2)}) \quad (9)$$

under the measurement assignment in Eqs. (5) and (6). Starting from this fixed operator, we obtain improved classical bounds (cf. Fig. 3): from -6 to -5.58 in the $(3,2,3,2)$ scenario and from -6 to -5.17 in the $(4,2,3,2)$ scenario.

B. Analytical results

In the numerical result of the $(4,2,3,2)$ scenario [cf. Eq. (8)], the optimized coefficients appear as floating-point values close to integers, and their arrangement reveals a highly regular symmetry. In particular, the measurement directions identified in Fig. 2(b) suggest that the four settings of party A exhibit a regular geometric structure, while the three settings of party B are mutually orthogonal. Motivated by this geometric structure, we reprocessed the numerical inequality by neglecting the small numerical deviations, aligning the coefficients to ± 1 , and rescaling by an overall constant factor. This procedure yields a compact analytical expression that is equivalent to the optimized inequality but highlights its underlying symmetry more clearly. The resulting inequality reads

$$\begin{aligned} \mathcal{I}_{\text{opt}} = & A_0B_1 - A_0B_2 - A_1B_0 + A_1B_2 \\ & + A_2B_0 + A_2B_2 - A_3B_1 - A_3B_2 \geq -4. \end{aligned} \quad (10)$$

Up to a constant factor, the four optimized measurement settings of party A are chosen as $\frac{1}{\sqrt{2}}(\sigma_y + \sigma_z)$, $\frac{1}{\sqrt{2}}(-\sigma_x - \sigma_z)$, $\frac{1}{\sqrt{2}}(\sigma_x - \sigma_z)$, and $\frac{1}{\sqrt{2}}(-\sigma_y + \sigma_z)$, while the three settings of

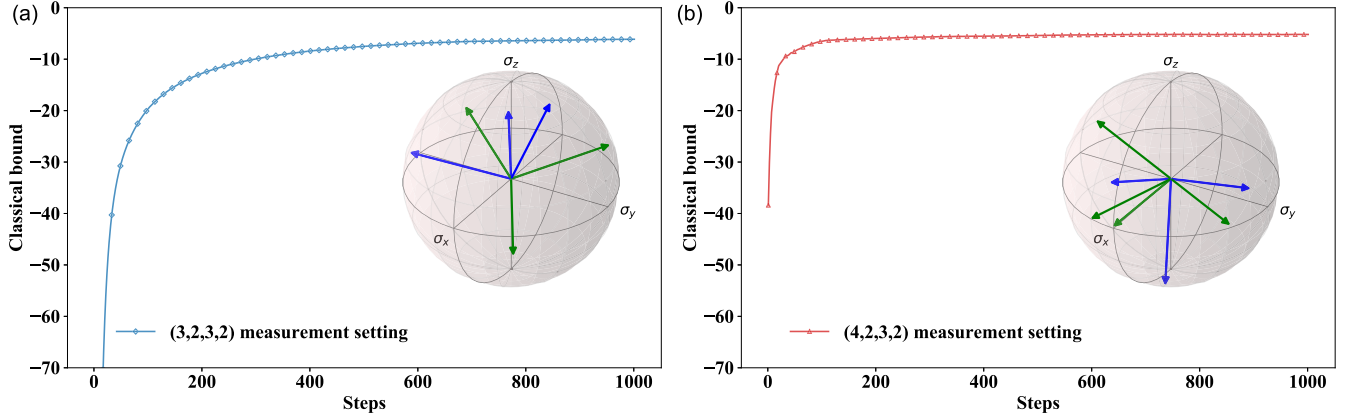


FIG. 3. Mappings from Hamiltonians to Bell inequalities. We present optimized classical bounds as a function of training steps, as well as Bloch spheres denoting the measurement settings corresponding to the highest classical bound. Green and blue arrows denote measurement observables of parties A and B , respectively. (a) Parties A and B with three dichotomic measurements with outputs ± 1 , i.e., the (3,2,3,2) scenario. (b) Parties A and B with four and three dichotomic measurements with outputs ± 1 , respectively, i.e., the (4,2,3,2) scenario.

party B are simply σ_x , σ_y , and $-\sigma_z$. Substitution into Eq. (10) gives $\sqrt{2}(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + 2\sigma_z \otimes \sigma_z)$. Multiplication by $4/\sqrt{6}$ recovers the target operator in Eq. (7) and rescales the local bound to $-16/\sqrt{6} \simeq -6.53$. According to this formulation, this result can be regarded as playing two CHSH games for $\{A_0, A_3; B_1, B_2\}$ and $\{A_1, A_2; B_0, B_2\}$ together and taking a summation. This inequality is the combination of two tight Bell inequalities $A_0B_1 - A_0B_2 - A_3B_1 - A_3B_2 \geq -2$ and $-A_1B_0 + A_1B_2 + A_2B_0 + A_2B_2 \geq -2$. It is not tight for the (4,2,3,2) Bell scenario without considering the single-body terms A_i and B_j . Geometrically, the corresponding face of this inequality has dimension 10, whereas the facets defined by genuinely tight inequalities should have dimension 11.

C. Noise robustness and iterative optimization

Assessing the robustness of Bell inequality violations requires accounting for noise, an inherent feature of near-term quantum devices. Analyzing its effect is essential for developing noise-resilient inequalities and measurement protocols. We now present results for noisy conditions obtained from numerical simulations. We choose the inequality in Eq. (4) and Hamiltonian in Eq. (7) and carry out simulations of such mappings for the case of depolarizing quantum noise, i.e., in each operation for preparing the target state, we attach a noise channel

$$\mathcal{N}_p(\rho) = (1 - 3p)\rho + p(\sigma_x\rho\sigma_x + \sigma_y\rho\sigma_y + \sigma_z\rho\sigma_z) \quad (11)$$

for the state ρ , where p denotes the noise strength. We apply the channel after each gate of the state-preparation circuit. For each noise strength p , we compute the two-body Pauli correlators of the simulated noisy state. We then optimize the measurement parameters θ using these simulated correlators (see Appendix B). As shown in Fig. 4(a), the violation obtained with the original Hamiltonian disappears at $p = 0.008$, whereas the optimized Hamiltonian remains below the same classical bound up to $p = 0.012$.

With optimizable mappings for both directions established, we can iteratively apply the optimization to both sides. The starting point we consider is the above model with depolarizing noise $p = 0.010$, where the original inequality

fails to be violated due to the effect of noise as shown in Fig. 4(a). The procedure begins with optimizing the measurement settings to compile a new Hamiltonian with lower energy. Then for this Hamiltonian, we optimize the Bell inequality for higher classical bounds while keeping the Hamiltonian fixed. These two steps form a loop which we repeatedly execute several times until converging to a stable point [cf. Fig. 4(b)]. After two loops, the classical bound and

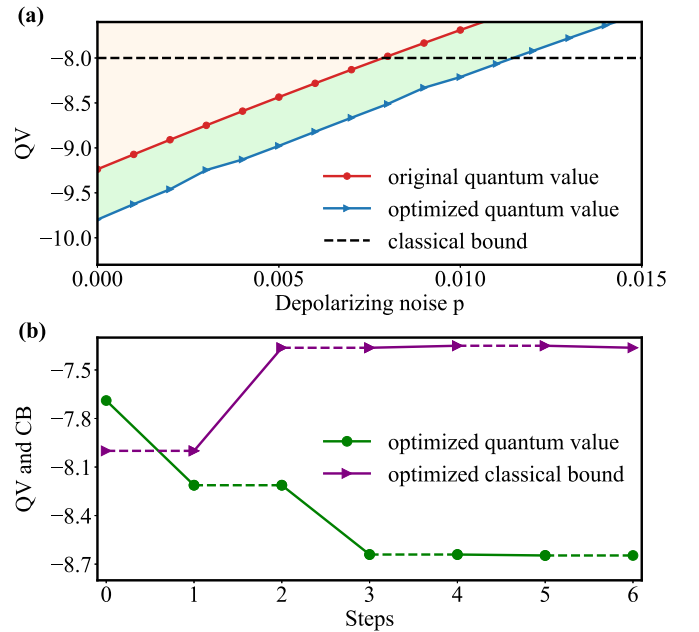


FIG. 4. (a) Original quantum values (QV) and optimized quantum values considering different depolarizing noise strengths, where the black dashed line denotes the classical bound. (b) Iterative optimization of both the Bell inequality and the Hamiltonian to maximize the gap between the classical bound (CB) and quantum value. The dashed line with triangle markers denotes that the Bell inequality remains fixed at this step while optimizing the measurement settings. Similarly, the dashed line with circular markers denotes that the Hamiltonian is fixed at this step during which the inequality is optimized.

quantum value converge, and the larger gap between them enables better certification of Bell-operator correlations.

We remark that the experimental data need to be obtained only once, assuming the data allow for the estimation of any two-body correlator, e.g., via randomized Pauli strings. Otherwise, we would have to supplement existing data with new measurements for the freshly chosen measurement settings.

V. MANY-BODY EXPERIMENTS

We now implement the Hamiltonian-to-inequality optimization in a many-body setting and demonstrate its feasibility with a superconducting quantum processor. To apply our method in practice, we build a quantum spin model in a honeycomb grid as shown in Fig. 2(c), which is implemented by 73 superconducting qubits arranged on an 11×11 square lattice. These selected qubits feature median fidelities of simultaneous single- and two-qubit gates around 99.95% and 99.4%, respectively (see Appendix C for detailed device information). Regarding the complexity of our implemented quantum circuits, each qubit undergoes six single-qubit rotation gates, and each pair of connected qubits is involved in two controlled-NOT (CNOT) gates. In total, for our 73-qubit honeycomb lattice configuration, the circuit contains 438 single-qubit gates and 184 CNOT gates. The entire circuit consists of 12 layers. The median coherence times of the quantum processor are $T_1 = 81.4 \mu\text{s}$ and $T_2 = 23.5 \mu\text{s}$, which are sufficient to support the circuit depth and ensure high-fidelity quantum state preparation and measurement.

The Hamiltonian is a generalized version of Eq. (7) by assigning the two-body Hamiltonian at nearest-neighbor sites with coupling strengths $J_k(\epsilon)$ to the lattice model shown in Fig. 2(c),

$$\mathcal{H} = \sum_{\kappa \text{ link}} \frac{4}{\sqrt{3}} J_{\kappa}(\epsilon) (\sigma_x^{(m)} \sigma_x^{(n)} + \sigma_y^{(m)} \sigma_y^{(n)} + 2\sigma_z^{(m)} \sigma_z^{(n)})_{\kappa},$$

where the local observables act on the two linked qubits indexed m and n . For the red links in Fig. 2(c), the coupling strength is $J_{\kappa}(\epsilon) = 1 + \epsilon$, while it is $(1 - \epsilon)/2$ for green and blue links. The Bell inequality is designed by summing over the edges of the honeycomb lattice, which has a similar structure to the Hamiltonian. We set $\epsilon = 0.94$ in our experiment. Since the honeycomb graph is bipartite, a deterministic assignment minimizing the common oriented two-party Bell expression can be repeated across the two sublattices. For $J_{\kappa} \geq 0$, it minimizes all edge terms simultaneously, so the global classical bound is the weighted sum of the two-party bounds in this setting.

To certify the experimental violation of Bell-operator correlations, we prepare low-energy states with parametrized quantum circuits. Starting with a fixed product state, we variationally optimize the parameters of the quantum circuit on the device to obtain ground-state approximations. The parametrized quantum circuit we utilized has the same structure as that in Ref. [31]. We set the energy $\langle \mathcal{H} \rangle_{\eta}$ as the cost function to be minimized, where η denotes the circuit parameters. The gradients are directly computed through quantum measurements according to the parameter shift rule [40,41], and we use the Adam optimizer to update the parameters [cf. Fig. 2(c)].

The two Bell inequalities used for certification, together with their measurement settings θ , were obtained from the fixed-Hamiltonian optimization in Sec. IV A without using the experimental correlators. Their classical bounds were then evaluated over local deterministic strategies. Each measurement configuration is sampled with 1000 shots, and the error bars denote the standard deviation over repeated estimates of the Bell-operator expectation value. For the original Bell inequality in Eq. (4), the energy of experimentally prepared states, even with corrections for readout errors, does not exhibit a violation of the classical bound beyond the statistical uncertainty (black line 1). To address this, we apply the two previously found Bell inequalities and extend them to the many-body system. As exhibited by dashed line 2 in Fig. 2(c), by considering the Bell inequality from Fig. 2(a), the classical bound can be notably increased, which allows the experimentally prepared states to violate the inequality without readout correction methods. When switching to the inequality adapted from Fig. 2(b), the experimental Bell-operator value lies at least three standard deviations below the classical bound. We note that the experimental Bell test reported here is not loophole-free, and thus does not provide a fully device-independent demonstration in practice, while the underlying inequalities remain formally valid.

VI. DISCUSSION AND OUTLOOK

The connection between Bell inequalities and Hamiltonians provides a useful tool for studying Bell-operator correlations in quantum systems. We introduced an iterative framework that alternates between (i) improving the classical threshold by searching for a fixed target Hamiltonian or equivalent inequalities with larger classical bounds and (ii) improving the observed quantum value by optimizing measurement settings for a fixed inequality. By enlarging the classical-quantum separation, the procedure yields more noise-resilient certification criteria. We demonstrated this advantage experimentally in a 73-qubit superconducting implementation of a honeycomb-lattice model, where an optimized inequality certifies Bell-operator correlations using the same correlator data for which the original inequality did not yield a violation of the classical bound.

The optimization framework presented in this work opens up several avenues for future research. A challenge encountered in optimizing more complex scenarios is the accumulation of local minima in the θ parameter space. This could possibly be mitigated by applying cutting-edge machine-learning techniques from deep reinforcement learning [42] or large language models. For Bell inequalities or quantum systems featuring certain symmetries, group equivariant machine learning models may be utilized to explore the solution in the symmetry-restricted space [43]. Finally, in this work we apply classical optimization techniques for nonlocality problems. With the advances in variational quantum algorithms [44], it is also appealing to develop hybrid quantum-classical optimization algorithms to probe the interplay between Bell inequalities and quantum systems. Beyond the bipartite case, scalability depends not only on the measurement optimization but also on the cost of evaluating the classical bound. For projective measurements, the number

of continuous measurement parameters grows linearly with the total number of local settings, whereas direct evaluation of the exact classical bound involves exponentially many deterministic assignments. Complete facet lists provide useful benchmarks in the small scenarios considered here, while partial lists of tight inequalities remain useful when complete classifications are unavailable [45,46].

While we have addressed the optimization of many-body systems by focusing only on relatively small subsystems, it would be highly desirable to apply this framework to increasingly larger systems and investigate the scaling behaviors [46]. This includes correlators involving more parties and a larger number of measurements for an individual party. We have exemplified the usefulness of our framework in turning experimental data that are quantum, but could not be certified so, into certifiably violating Bell-operator correlations, simply as a postprocessing step that does not require extra experimental work.

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DATA AVAILABILITY

The code and data that support the findings of this article are openly available at [47].

APPENDIX A: ENERGY AS A WITNESS OF NONLOCALITY AND OPTIMIZABLE MAPPINGS

The connection between Bell inequalities and Hamiltonians provides an avenue to test nonlocality through certain engineered quantum systems [28–30,48–50]. For a given Bell inequality, we can construct a Hamiltonian by replacing the measurements in the inequality with certain measurement settings. If the ground-state energy of this Hamiltonian falls below the classical bound β_C , the observed energy can be a nonlocality witness [29]. Conversely, for a specified spin Hamiltonian, there might be numerous corresponding Bell inequalities with certain measurement settings. In this work we aim to find desirable Bell inequalities and measurement settings such that the gap between β_Q and β_C is maximal by searching the coefficient space of Bell inequalities and parameters of measurement settings. We explain the optimization scheme from two directions in the following two sections.

1. Bell inequality to Hamiltonian

As introduced in Sec. II, we can construct a Hamiltonian that coincides with the Bell operator associated with a given Bell inequality $\mathcal{I} - \beta_C \geq 0$. As an example, consider the CHSH inequality $\mathcal{I} = A_0B_0 + A_0B_1 + A_1B_0 - A_1B_1$. By letting $A_0 = B_0 = \sigma_x$ and $A_1 = B_1 = \sigma_y$, the Bell operator is

$$\begin{aligned}\mathcal{B}_{\text{CHSH}} &= \sigma_x^{(1)}\sigma_x^{(2)} + \sigma_x^{(1)}\sigma_y^{(2)} + \sigma_y^{(1)}\sigma_x^{(2)} - \sigma_y^{(1)}\sigma_y^{(2)} \\ &= 2\left[\frac{1}{2}(\sigma_x + \sigma_y)^{(1)}(\sigma_x + \sigma_y)^{(2)} - \sigma_y^{(1)}\sigma_y^{(2)}\right].\end{aligned}$$

We can write $\mathcal{B}_{\text{CHSH}}$ in a way similar to the XY Hamiltonian by letting $\sigma_{\pi/4} = \frac{\sqrt{2}}{2}(\sigma_x + \sigma_y) = \cos\frac{\pi}{4}\sigma_x + \sin\frac{\pi}{4}\sigma_y$. In this way, we obtain the Hamiltonian in the form of [29]

$$\mathcal{H}_{\text{CHSH}} = \mathcal{B}_{\text{CHSH}} = 2(\sigma_{\pi/4}^{(1)}\sigma_{\pi/4}^{(2)} - \sigma_y^{(1)}\sigma_y^{(2)}).$$

2. Hamiltonian to Bell inequality

In this section we study the map from a Hamiltonian to Bell inequalities and use the model adapted in the main text as an illustrative example. We are given a Hamiltonian with two-body interactions at nearest-neighbor sites with coupling strengths $J_\kappa(\epsilon)$,

$$\mathcal{H}(\Delta) = \frac{4}{\sqrt{3}} \sum_{(m,n)_\kappa} J_\kappa(\epsilon) (\sigma_x^{(m)}\sigma_x^{(n)} + \sigma_y^{(m)}\sigma_y^{(n)} + \Delta\sigma_z^{(m)}\sigma_z^{(n)}),$$

where Δ is a real parameter and the κ link denotes the links between two connected qubits indexed m and n .

Our goal is to find a Bell inequality and a measurement setting such that the Bell operator $\mathcal{B}$ corresponds to this given Hamiltonian:

$$\mathcal{B} \equiv \mathcal{H}(\Delta).$$

If we restrict the study to the local part $\mathcal{H}_{\text{local}} = \frac{4}{\sqrt{3}}(\sigma_x^{(m)}\sigma_x^{(n)} + \sigma_y^{(m)}\sigma_y^{(n)} + \Delta\sigma_z^{(m)}\sigma_z^{(n)})$ of the Hamiltonian $\mathcal{H}(\Delta)$, the tensor-product structure involves two parties. We

choose dichotomic Pauli observables, whose outcomes are ± 1 , and therefore $d = 2$ for each party. Thus, for the local part $\mathcal{H}_{\text{local}}$, the scenario is $(m_1, 2, m_2, 2)$. To obtain nontrivial correlations, we set $m_i \geq 2$ for $i = 1, 2$.

According to the general form of Bell expression in the $(m_1, 2, m_2, 2)$ scenario, the Bell operator $\mathcal{B}_{\text{local}}$ without local terms associated with $\mathcal{H}_{\text{local}}$ can be written as

$$\mathcal{B}_{\text{local}} = \sum_{x_1, x_2=0}^{m_1-1, m_2-1} \alpha_{x_1, x_2} A_{x_1} B_{x_2}. \quad (\text{A1})$$

Note that $\mathcal{B} = \sum_{\kappa} J_{\kappa}(\epsilon)(\mathcal{B}_{\text{local}})_{\kappa}$.

The single-qubit operator we utilize can be written as

$$A_{x_1} = \vec{n} \cdot \vec{\sigma} = n_x \sigma_x + n_y \sigma_y + n_z \sigma_z,$$

where the coefficient vector $\vec{n} = (n_x, n_y, n_z)$ is normalized: $n_x^2 + n_y^2 + n_z^2 = 1$. Thus the parametrized measurements of parties A and B can be written as

$$\begin{aligned} A_{x_1} &= \cos \theta_{x_1} \sigma_x + \sin \theta_{x_1} \cos \phi_{x_1} \sigma_y + \sin \theta_{x_1} \sin \phi_{x_1} \sigma_z, \\ B_{x_2} &= \cos \gamma_{x_2} \sigma_x + \sin \gamma_{x_2} \cos \varphi_{x_2} \sigma_y + \sin \gamma_{x_2} \sin \varphi_{x_2} \sigma_z, \end{aligned} \quad (\text{A2})$$

where $\theta_{x_1}, \gamma_{x_2} \in [0, \pi]$ and $\phi_{x_1}, \varphi_{x_2} \in [0, 2\pi)$ are variational real parameters and $x_1 \in [m_1]$ and $x_2 \in [m_2]$. In this case, by inserting Eq. (A2) into the general form of Bell inequality of the $(m_1, 2, m_2, 2)$ scenario as Eq. (A1), the Bell operator $\mathcal{B}_{\text{local}}$ is

$$\begin{aligned} \mathcal{B}_{\text{local}} &= \sum_{x_1, x_2=0}^{m_1-1, m_2-1} \alpha_{x_1, x_2} A_{x_1} B_{x_2} \\ &= \sum_{x_1, x_2=0}^{m_1-1, m_2-1} \alpha_{x_1, x_2} (\cos \theta_{x_1} \sigma_x + \sin \theta_{x_1} \cos \phi_{x_1} \sigma_y + \sin \theta_{x_1} \sin \phi_{x_1} \sigma_z) \\ &\quad \otimes (\cos \gamma_{x_2} \sigma_x + \sin \gamma_{x_2} \cos \varphi_{x_2} \sigma_y + \sin \gamma_{x_2} \sin \varphi_{x_2} \sigma_z), \end{aligned} \quad (\text{A3})$$

where α_{x_1, x_2} are the coefficients of correlators $A_{x_1} B_{x_2}$. To find the coefficients α_{x_1, x_2} of the Bell expression $\mathcal{I}$ of the Bell inequality $\mathcal{I} - \beta_C \geq 0$, we write the above Bell operator as a system of linear equations by projecting into the basis $\{\sigma_i \otimes \sigma_j \mid i, j \in \{x, y, z\}\}$. With the unnormalized Pauli basis used here, the corresponding expansion coefficient of $\mathcal{H}_{\text{local}}$ is $\frac{1}{4} \text{Tr}[(\sigma_i \otimes \sigma_j) \mathcal{H}_{\text{local}}]$ for $i, j \in \{x, y, z\}$. In this way, we obtain a system of linear equations

$$\mathbf{T}(\theta) \cdot \vec{\alpha} = \vec{h}, \quad (\text{A4})$$

where

$$\mathbf{T}(\theta) = \begin{pmatrix} \cos \theta_0 \cos \gamma_0 & \cdots & \cos \theta_{x_1} \cos \gamma_{x_2} & \cdots & \cos \theta_{m_1-1} \cos \gamma_{m_2-1} \\ \cos \theta_0 \sin \gamma_0 \cos \varphi_0 & \cdots & \cos \theta_{x_1} \sin \gamma_{x_2} \cos \varphi_{x_2} & \cdots & \cos \theta_{m_1-1} \sin \gamma_{m_2-1} \cos \varphi_{m_2-1} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \sin \theta_0 \sin \phi_0 \sin \gamma_0 \sin \varphi_0 & \cdots & \sin \theta_{x_1} \sin \phi_{x_1} \sin \gamma_{x_2} \sin \varphi_{x_2} & \cdots & \sin \theta_{m_1-1} \sin \phi_{m_1-1} \sin \gamma_{m_2-1} \sin \varphi_{m_2-1} \end{pmatrix}$$

is a $9 \times m_1 m_2$ matrix,

$$\vec{\alpha} = (\alpha_{0,0}, \alpha_{0,1}, \dots, \alpha_{x_1, x_2}, \dots, \alpha_{m_1-1, m_2-1})^T,$$

and

$$\vec{h} = \frac{1}{4} (\text{Tr}[(\sigma_x \otimes \sigma_x) \mathcal{H}_{\text{local}}], \dots, \text{Tr}[(\sigma_i \otimes \sigma_j) \mathcal{H}_{\text{local}}], \dots, \text{Tr}[(\sigma_z \otimes \sigma_z) \mathcal{H}_{\text{local}}])^T, \quad i, j \in \{x, y, z\}.$$

The matrix $\mathbf{T}(\theta)$ is fully determined by choosing

$$\theta = (\theta_0, \dots, \theta_{m_1-1}, \phi_0, \dots, \phi_{m_1-1}, \gamma_0, \dots, \gamma_{m_2-1}, \varphi_0, \dots, \varphi_{m_2-1}).$$

Since $\text{rank}[\mathbf{T}(\theta)] \leq \min\{9, m_1 m_2\}$, the existence and multiplicity of solutions must be distinguished.

(i) If $\mathbf{T}(\theta)$ is invertible ($m_1 = m_2 = 3$ and $\text{rank}[\mathbf{T}(\theta)] = 9$), there is a unique solution for $\vec{\alpha} = \mathbf{T}(\theta)^{-1} \vec{h}$. In this case, the solution $\vec{\alpha}$ is unique, so the Bell expression corresponding to $\mathcal{H}_{\text{local}}$ with operators given by Eq. (A3) is also unique.

(ii) In general, Eq. (A4) is solvable if and only if $\vec{h} \in \text{im } \mathbf{T}(\theta)$, or equivalently $\text{rank } \mathbf{T} = \text{rank}[\mathbf{T} \mid \vec{h}]$. When it is solvable, all solutions have the form $\vec{\alpha} = \vec{\alpha}_0 + \vec{u}$ with $\vec{u} \in \ker \mathbf{T}$. The solution is nonunique precisely when $\ker \mathbf{T} \neq \{0\}$; incompatibility instead gives no solution. For a full-row-rank

9×12 system, a compatible $\vec{h}$ has a three-dimensional affine solution space.

APPENDIX B: DETAILS FOR THE NUMERICS

Both optimizations, the minimization of the quantum value and the maximization of the classical bound by adapting the measurements, are nonconvex. Thus, their convergence depends on the choice of parameters in the numerical algorithms. Here we give detailed settings of the hyperparameters used in the numerical simulations.

1. Variant of Gisin's elegant Bell inequality

We provide the details of a variant of Gisin's elegant inequality introduced in the main text. In this setting, A has four dichotomic measurements and B has three, both with outcomes ± 1 . The inequality is expressed as

$$\begin{aligned}\mathcal{I}_G(\Delta) &= (A_0 + A_1 - A_2 - A_3)B_0 \\ &\quad + (A_0 - A_1 + A_2 - A_3)B_1 \\ &\quad + \Delta(A_0 - A_1 - A_2 + A_3)B_2 \\ &\geq -2|\Delta| - |\Delta + 2| - |\Delta - 2|.\end{aligned}$$

By assigning four measurements

$$\begin{aligned}A_0 &= \frac{\sigma_x + \sigma_y + \sigma_z}{\sqrt{3}}, & A_1 &= \frac{\sigma_x - \sigma_y - \sigma_z}{\sqrt{3}}, \\ A_2 &= \frac{-\sigma_x + \sigma_y - \sigma_z}{\sqrt{3}}, & A_3 &= \frac{-\sigma_x - \sigma_y + \sigma_z}{\sqrt{3}}\end{aligned}$$

to party A and three measurements

$$B_0 = \sigma_x, \quad B_1 = \sigma_y, \quad B_2 = \sigma_z$$

to party B , we obtain the Bell operator in the main text when $\Delta = 2$.

2. Hamiltonian to Bell inequality

To map a fixed XXZ-like Hamiltonian to Bell inequalities (cf. Fig. 2 in the main text), we start with a random initialization of measurement settings θ to provide the initial $\mathbf{T}(\theta)$. For the case $(m_1, 2, m_2, 2) = (3, 2, 3, 2)$, $\mathbf{T}(\theta)$ is a 9×9 matrix. Whenever $\text{rank } \mathbf{T}(\theta) = 9$, it is invertible and $\tilde{\alpha} = \mathbf{T}(\theta)^{-1}\tilde{h}$ is the unique solution of Eq. (A4); singular choices instead require the compatibility test above. For a full-rank choice, this solution determines the Bell inequality and its classical bound. Thus, we use $\mathcal{C}(\mathbf{T}(\theta))$ to represent the resulting classical bound. The classical bound can be alternatively computed using tensor-network contraction in tropical algebra [37,51,52].

For the optimization, we apply gradient-based methods to search for θ^* with the highest classical bound. With finite-difference methods, we calculate the gradient $\nabla_{\theta}\mathcal{C}(\mathbf{T}(\theta))$. To illustrate the basic idea, we can use direct gradient ascent to maximize the classical bound $\mathcal{C}(\mathbf{T}(\theta))$,

$$\theta_{n+1} = \theta_n + \epsilon \nabla_{\theta}\mathcal{C}(\theta_n),$$

where ϵ is the learning rate and θ_i denotes the parameters at training step i . For better training performance, in our work we instead feed the gradients into the Adam (0.9,0.999) optimizer with a learning rate of 0.02 to optimize the parameters during this procedure. Here 0.9 and 0.999 denote the hyperparameters determining the initial decay rates for the first- and second-moment estimates, respectively.

For the case $(m_1, 2, m_2, 2) = (4, 2, 3, 2)$, Eq. (A4) is underdetermined. When $\tilde{h} \in \text{im } \mathbf{T}(\theta)$, it has an affine solution space. Let $\mathcal{N}(\mathbf{T}(\theta))$ denote the null space of $\mathbf{T}(\theta)$. Given any solution $\tilde{\alpha}_0$, every vector $\tilde{\alpha} = \tilde{\alpha}_0 + \tilde{u}$ with $\tilde{u} \in \mathcal{N}(\mathbf{T}(\theta))$ is also a solution. When $\mathbf{T}$ has full row rank, this 9×12 system has a three-dimensional affine solution space. In the numerical results reported here, we use its unique minimum-norm representative for computational efficiency rather than optimizing over the full affine family.

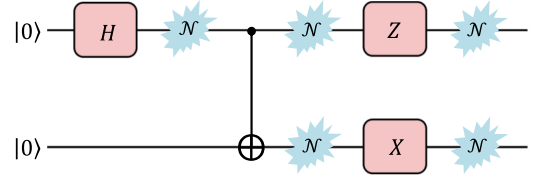


FIG. 5. Quantum circuit preparing the singlet state with the depolarizing noise introduced. We use $\mathcal{N}$ to represent the depolarizing noise $\mathcal{N}_p(\rho) = (1 - 3p)\rho + p(\sigma_x\rho\sigma_x + \sigma_y\rho\sigma_y + \sigma_z\rho\sigma_z)$ for a given noise strength p .

3. Bell inequality to Hamiltonian

For a given Bell inequality, we can optimize the measurement settings to search for lower quantum values. In the numerical explorations of mapping Bell inequalities to Hamiltonians, the basic setting has been introduced in the main text. Here we provide more detailed information about noisy quantum simulations and the optimization scheme.

We first carry out the preparation of target states considering depolarizing noise. For the XXZ-like two-qubit Hamiltonian in Eq. (7), the ground state is the singlet state $\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$. We apply the circuit in Fig. 5 to prepare this state and add noise during the procedure. By measuring the output states, we obtain the expectation values of all the two-body Pauli correlators and collect them as the simulated data.

In the main text we use a row vector $\vec{c}$ to represent the set of measured values of quantum correlators. The target is to minimize the energy $\mathcal{E}(\theta) = \vec{c} \cdot \mathbf{T}(\theta) \cdot \tilde{\alpha}$. We can similarly apply gradient descent to search for measurement configurations to minimize it. In practice, we feed the obtained gradients into the Adam (0.9,0.999) optimizer with a learning rate of 0.01.

APPENDIX C: DEVICE INFORMATION

The superconducting quantum processor used in this work consists of 121 qubits arranged in an 11×11 square lattice employed in Refs. [31,53,54]. This processor is capable of performing a universal quantum gate set formed by 30-ns arbitrary single-qubit gates and 40-ns two-qubit controlled-Z (CZ) gates. We chose and benchmarked 73 qubits to carry out the experiment; their properties are summarized in Table I. The optimization scheme follows the parameter-shift strategy from Refs. [31,40,41].

TABLE I. Performance of the 73 qubits. The single-qubit gate error and CZ gate error are calibrated through cross-entropy benchmarking. Note that the gate errors are average errors rather than Pauli errors. The readout error is the average readout error for the 0 state and the 1 state.

Parameter	Median value
T_1	81.4 μ s
T_2 spin echo	23.5 μ s
Single-qubit gate error	4.54×10^{-4}
CZ gate error	6.34×10^{-3}
Readout error	8.72×10^{-3}

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