Energy as a Detector of Nonlocality of Many-Body Spin Systems

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We present a method to show that low-energy states of quantum many-body interacting systems in one spatial dimension are nonlocal. We assign a Bell inequality to the Hamiltonian of the system in a natural way and we efficiently find its classical bound using dynamic programing. The Bell inequality is such that its quantum value for a given state, and for appropriate observables, corresponds to the energy of the state. Thus, the presence of nonlocal correlations can be certified for states of low enough energy. The method can also be used to optimize certain Bell inequalities: in the translationally invariant (TI) case, we provide an exponentially faster computation of the classical bound and analytically closed expressions of the quantum value for appropriate observables and Hamiltonians. The power and generality of our method is illustrated through four representative examples: a tight TI inequality for eight parties, a quasi-TI uniparametric inequality for any even number of parties, ground states of spin-glass systems, and a nonintegrable interacting *XXZ*-like Hamiltonian. Our work opens the possibility for the use of low-energy states of commonly studied Hamiltonians as multipartite resources for quantum information protocols that require nonlocality.

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I. INTRODUCTION

Nonlocality is a fundamental property of nature in which the statistics obtained by performing some local measurements on some composite quantum systems cannot be reproduced by any local hidden variable model [1]. These so-called nonlocal correlations cannot be mimicked by any local deterministic strategy, even if assisted by shared randomness [2]. Nonlocality is detected by the violation of a Bell inequality [3] and it has recently been demonstrated in three loophole-free Bell experiments [4–6]. Detection of nonlocality is a sufficient condition to demonstrate, in a device-independent (DI) way, that the state producing such correlations is entangled. From an operational point of view, nonlocality is a resource that enables the implementation of DI quantum information protocols, such as DI quantum key distribution [7,8], DI randomness expansion [9] or amplification [10,11], or DI self-testing [12,13].

The study of quantum many-body systems has benefited during the past decades from insights of the field of

quantum information, in particular concerning the understanding of their correlations [14,15]. This has, however, mostly focused on the study and experimental detection of entanglement [16–18], while the role of nonlocal correlations, which are stronger, remains rather unexplored. There are at least three reasons for that. First, the known Bell inequalities for multipartite systems involve correlations among many particles [19–23], thus rendering their measurement a formidably challenging task. Second, the mathematical characterization of nonlocal correlations is an NP-hard problem [24]. Third, the size of the description of multipartite quantum states grows, in general, exponentially with the system size, posing a strong barrier to the analysis of the quantum correlations in large systems. However, recent advances [25,26] have shown that, by measuring only one- and two-body correlation functions, nonlocality can be revealed in some multipartite quantum systems, opening the way to its detection in many-body systems [27] (see also Ref. [28]).

In this work, we show that the ground states of some quantum spin Hamiltonians in one spatial dimension are nonlocal. We assign a Bell inequality to the given Hamiltonian in a natural way and we calculate its classical bound using dynamic programing. The Bell inequality is constructed in such a way that, for appropriate quantum observables, the Bell operator coincides with the

Hamiltonian. The idea is that if the ground state energy is beyond the classical bound, this signals the presence of nonlocal correlations in the ground state. The ground state energy is computed by exact diagonalization using the Jordan-Wigner (JW) transformation, which maps the system of spins to a quadratic system of fermions. The method just presented can also be seen from the opposite point of view, namely, as a way to optimize certain classes of Bell inequalities for many-body systems under some quantum observables. We also study the translationally invariant (TI) setting, in which we provide an exponentially faster algorithm to find the classical bound and we obtain analytical results for the quantum value. [In this work, we refer to the *quantum value* as the expectation value of the ground state of the Bell operator under appropriate quantum observables (such that it matches the Hamiltonian). This should not be confused with the *quantum bound* of a Bell inequality, which is the infimum over all quantum states and observables.] Then we illustrate our framework by applying it to four representative examples: first, a tight TI Bell inequality for eight parties; second, a quasi-TI Bell inequality for any even number of parties; third, we show that the ground state of an *XY* spin glass has nonlocal correlations in some parameter region; and finally, a non-integrable interacting *XXZ*-like Hamiltonian to which we assign a variation of Gisin's elegant Bell inequality [29] and we find its quantum value numerically using matrix product states and the density matrix renormalization group [30]. This shows that our method is not limited to Hamiltonians that can be mapped to a system of free fermions via the JW transformation, but it can be applied to any spin Hamiltonian with short-range interactions in one spatial dimension.

The paper is organized as follows. In Sec. II, we present our method. In Sec. III, we show how to optimize certain classes of many-body Bell inequalities. In Sec. IV, we particularize our results to the TI case. In Sec. V, we illustrate our methods with four examples. Finally, in Sec. VI, we conclude and explore future lines of research.

II. METHOD

In this section, we present a method to analyze when the ground state of some spin Hamiltonians is nonlocal, namely, when the quantum value is beyond the classical bound. We first present the setting (Sec. II A). We then construct a Bell inequality from the given Hamiltonian (Sec. II B) and we compute its classical bound using dynamic programing (Sec. II B 1). Then we find the quantum value of the inequality (Sec. II C). To this end, we first review the exact diagonalization of quadratic fermionic Hamiltonians (Sec. II C 1) and then we relate the spin Hamiltonian and the fermionic Hamiltonian via the Jordan-Wigner transformation (Sec. II C 2).

A. Setting

We consider quantum spin-1/2 Hamiltonians of n particles in one spatial dimension (henceforth, one-dimensional)

with periodic boundary conditions, with short-range interactions, up to R neighbors:

$$\mathcal{H} = \sum_{i=0}^{n-1} \left(t^{(i)}\sigma_z^{(i)} + \sum_{r=1}^{R}\sum_{\alpha,\beta=0}^{1} t_{\alpha,\beta}^{(i,r)} \mathrm{Str}_{\alpha,\beta}^{(i,r)} \right), \qquad (1)$$

where $t^{(i)}$ and $t_{\alpha,\beta}^{(i,r)}$ are real parameters,

$$\mathrm{Str}_{\alpha,\beta}^{(i,r)} := \sigma_{x+\alpha}^{(i)}\sigma_z^{(i+1)}\ldots\sigma_z^{(i+r-1)}\sigma_{x+\beta}^{(i+r)} \qquad (2)$$

are the so-called string operators, $\sigma_x^{(i)}$, $\sigma_y^{(i)}$, and $\sigma_z^{(i)}$ are the Pauli matrices acting on the ith site, and the indices of the sites are taken modulo n. We denote $x + 1 := y$ for short.

On one hand, as we explain it in detail in Sec. II C, this choice of Hamiltonians is convenient from a purely mathematical perspective, as they can be exactly diagonalized via the JW transformation. On the other hand, Hamiltonians of the form Eq. (1) are general enough to include many cases of interest. For instance, the case $R = 1$ corresponds to a one-dimensional spin-1/2 Hamiltonian with nearest-neighbors interactions, under a transverse magnetic field:

$$\mathcal{H} = \sum_{i=0}^{n-1} \left(t^{(i)}\sigma_z^{(i)} + \sum_{\alpha,\beta=0}^{1} t_{\alpha,\beta}^{(i,1)} \sigma_{x+\alpha}^{(i)}\sigma_{x+\beta}^{(i+1)} \right). \qquad (3)$$

Nevertheless, our method can also be applied to Hamiltonians with local interactions that do not rely on the string operator structure, at the price of having to compute their ground state energy numerically, as we illustrate in the example in Sec. V D.

B. Construction of a Bell inequality

In this section, we study the classes of Bell inequalities that are relevant for our work. We construct Bell inequalities such that, for some quantum observables, the corresponding Bell operator $\mathcal{B}$ satisfies

$$\mathcal{B} = \beta_C \mathbb{1} + \mathcal{H}, \qquad (4)$$

where $\beta_C \in \mathbb{R}$ is the so-called classical bound and $\mathcal{H}$ is defined as in Eq. (1). We use the following convention in writing down Bell inequalities. We want to obtain Bell inequalities of the form $I + \beta_C \geq 0$. The part of the Bell operator that corresponds to I will be the Hamiltonian $\mathcal{H}$, and thus, states with low enough energy, lower than $-\beta_C$, will give a violation of the Bell inequality. The classical bound β_C is defined as

$$\beta_C = -\min_{\mathrm{LHVM}} I, \qquad (5)$$

where the minimum is taken over all local hidden variable models (LHVM) (cf. Eq. [3]). Observe that the quantum

state that minimizes the expectation value of $\mathcal{B}$ is the ground state of $\mathcal{H}$.

This motivates the study of Bell inequalities in the following scenario: We have n parties with m dichotomic observables with outcomes ± 1 at their disposal. We denote the choices of measurements by $\mathbf{k} = (k_0, ..., k_{n-1})$, with $0 \le k_i < m$, and the outcomes they produce by $\mathbf{a} = (a_0, ..., a_{n-1})$, with $a_i = \pm 1$. We denote by $P(\mathbf{a}|\mathbf{k})$ the vector of conditional probabilities collected when they perform the Bell experiment. Because of the no-signaling principle, the marginals observed by any subset of parties do not depend on the choices of measurements performed by the rest; thus, $P(\{a_i\}_{i \in S}|\{k_i\}_{i \in S})$ is well defined on any subset S. In the case of dichotomic measurements, one normally works with the *correlators* $M_{\mathbf{k}}^{(i,r)}$,

$$M_{\mathbf{k}}^{(i,r)} := \sum_{\mathbf{a}} \left(\prod_{j=0}^{r} a_{i+j} \right) P(\mathbf{a}|\mathbf{k}), \qquad (6)$$

where, abusing notation, we are now denoting $\mathbf{k} = (k_i, ..., k_{i+r})$ and $\mathbf{a} = (a_i, ..., a_{i+r})$.

If $R > 1$, we will consider $m + 1$ measurements, due to the σ_z in between [cf. Eq. (2)]. The Bell inequalities that are naturally tailored to a Bell operator of the form of Eq. (4) can be written as $I + \beta_C \ge 0$, where

$$I := \sum_{i=0}^{n-1} \left(\gamma^{(i)} M_m^{(i,0)} + \sum_{r=1}^{R} \sum_{k,l=0}^{m-1} \gamma_{k,l}^{(i,r)} M_{(k,m,...,m,l)}^{(i,r)} \right), \quad (7)$$

and $\gamma^{(i)}$, $\gamma_{k,l}^{(i,r)}$ are real parameters that depend on the $t^{(i)}$ and $t_{\alpha,\beta}^{(i,r)}$ of Eq. (1). Despite the fact that I contains up to $(R+1)$-body terms, its coefficients $\gamma^{(i)}$ and $\gamma_{k,l}^{(i,r)}$ show that it is essentially a two-body Bell inequality, since the measurement choice of the parties in the middle of the string is fixed to be m, in the sense that the number of coefficients $\gamma^{(i)}$ and $\gamma_{k,l}^{(i,r)}$ is the same as in a two-body Bell inequality. Note that the number of measurements m performed on the x-y plane will not affect the form of Eq. (1). The only measurement that is not performed in this plane is in the z direction; therefore, we treat it as a special case and we say we have $m + 1$ measurements.

1. Classical optimization

We now describe how to efficiently compute the classical bound β_C of the Bell inequalities introduced in Eq. (7). It is well known that for a generic Bell inequality for n parties, m measurements, and d outcomes the classical bound cannot be found efficiently, as it requires solving a linear program with d^{mn} constraints [3]. The particular form of the Bell inequalities we are considering, however, allows us to find an algorithm that, in the many-body regime (i.e., for fixed d, m and R) has $O(n)$ complexity. For simplicity, we

consider a Bell inequality I of a slightly more general form than those of Eq. (7) and with $d = 2$ outcomes:

$$I := \sum_{i=0}^{n-1} \sum_{r=0}^{R} \sum_{\mathbf{k}=0}^{m^{r+1}-1} \gamma_{\mathbf{k}}^{(i,r)} M_{\mathbf{k}}^{(i,r)}, \qquad (8)$$

where $\mathbf{k} = (k_i, ..., k_{i+r})$ and $0 \le k_j < m$. After we present our method, it will become clear that there is no loss of generality in considering dichotomic measurements, as the result can be straightforwardly generalized to an arbitrary d.

To find β_C, we need to optimize I over all local hidden variable models. By Fine's theorem [2], it suffices to optimize I over all deterministic local strategies, in which the correlators $M_{\mathbf{k}}^{(i,r)}$ factorize as

$$M_{\mathbf{k}}^{(i,r)} = \prod_{j=0}^{r+1} M_{k_j}^{(i+j)}, \qquad (9)$$

where $M_{k_i}^{(i)}$ can be ± 1. Thus,

$$\beta_C = - \min_{M_{k_i}^{(i)} = \pm 1} I, \qquad (10)$$

where the minimum is taken over all possible assignments of $M_{k_i}^{(i)}$ to ± 1 for all i and k.

Let us first solve the case with open boundary conditions (OBC), i.e., the case where $\gamma_{\mathbf{k}}^{(i,r)} = 0$ when $i + r \ge n$. We follow a dynamic programing procedure [31] that splits the minimization Eq. (10) into nested parts.

To this end, we represent a local deterministic strategy as a matrix $\mathbf{M}$ whose rows index the measurement choices and whose columns index the party, and the entry (k, i) is the value assigned in the deterministic strategy to the kth observable of the ith party. Thus, $\mathbf{M}$ is a $(m \times n)$ matrix whose entries take integer values $+1$ or -1. Let $\mathbf{M}^{(i,R)}$ denote the submatrix of $\mathbf{M}$ consisting of columns i to $i + R - 1$. The goal of the dynamic programing is to find an optimal $\mathbf{M}$, which will give β_C. This will be obtained recursively.

Let h_i be the function defined for $i > 0$ as

$$h_i(\mathbf{M}^{(i-1,R+1)}) := \sum_{r=0}^{R} \sum_{\mathbf{k}=0}^{m^{r+1}-1} \gamma_{\mathbf{k}}^{(i-1,r)} M_{\mathbf{k}}^{(i-1,r)}. \qquad (11)$$

Note that because of Eq. (9), $h_i(\mathbf{M}^{(i-1,R+1)})$ is a real number. Now we define a recursive function E_i, which contains the optimization up to the $(i-1)$th site. Explicitly, $E_0(\mathbf{M}^{(0,R)}) := 0$ and

$$E_i(\mathbf{M}^{(i,R)}) := \min_{M_k^{(i-1)}} \{ E_{i-1}(\mathbf{M}^{(i-1,R)}) + h_i(\mathbf{M}^{(i-1,R+1)}) \},$$
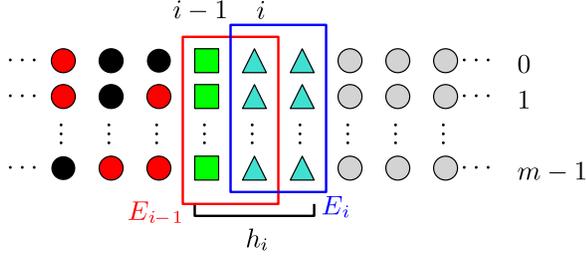
$$\qquad (12)$$

FIG. 1. The representation of the matrix $\mathbf{M}$ at the step where we compute E_i for an inequality with dichotomic measurements with $R = 2$. The color (red or black) corresponds to the outcome assigned to that observable. At the ith step, an optimal local deterministic strategy for parties 0 to $i - 2$ is already set, and we are minimizing the local deterministic strategy at the $(i - 1)$th site (green squares). In order to perform the minimization, we need the values of the ith and $(i + 1)$th parties to be fixed (blue triangles); i.e., we need to give a value to $\mathbf{M}^{(i,2)}$. We check the 2^m possible values for the observables at site $i - 1$ and we find an optimal assignment for them.

for $i > 0$. Note that E_i optimizes the local deterministic strategy on the $(i - 1)$th party, which amounts to choosing the optimal values of the $(i - 1)$th column of $\mathbf{M}$. This naturally depends on the next R columns, which we need to consider as variables and calculate E_i for all their possible values. Therefore, to efficiently evaluate $E_i(\mathbf{M}^{(i,R)})$, we only need to access the stored values of E_{i-1} on $\mathbf{M}^{(i-1,R)}$ and not E_{i-2} and so on. The computation of $E_i(\mathbf{M}^{(i,R)})$ thus requires evaluation of the 2^m different deterministic local strategies corresponding to the values $M_k^{(i-1)}$ (see Fig. 1).

The classical bound Eq. (10) is obtained as the end product of this minimization procedure; namely,

$$\beta_C = -E_n(\mathbf{M}^{(n,R)}). \tag{13}$$

Note that E_n is actually independent of $\mathbf{M}^{(n,R)}$ because we are in the OBC case, so all the $\gamma_{\mathbf{k}}$'s that would extend beyond the nth party are zero.

This procedure can be easily generalized if the Bell inequality has $d > 2$ outcomes. In this case, one has to take into account that the notion of correlators introduced in Eq. (6) is no longer well defined (as the one-to-one correspondence between probabilities $P(\mathbf{a}|\mathbf{k})$ and correlators $M_{\mathbf{k}}^{(i,r)}$ no longer holds). Thus, one needs to express the Bell inequality in terms of probabilities:

$$I = \sum_{i=0}^{n-1} \sum_{r=0}^{R} \sum_{\mathbf{k}=0}^{m^{r+1}-1} \sum_{\mathbf{a}=0}^{d^{r+1}-1} \gamma_{\mathbf{k},\mathbf{a}}^{(i,r)} P(\mathbf{a}|\mathbf{k}), \tag{14}$$

where $\mathbf{a} = (a_i, \ldots, a_{i+r})$ and $\mathbf{k}$ has the same structure. Note that $P(\mathbf{a}|\mathbf{k})$ implicitly depends on i and r [cf. Eq. (6)], thus being a marginal $(r + 1)$-body probability distribution. Again, like in the $d = 2$ case, by virtue

of Fine's theorem [2], it suffices to consider those probability distributions in which $P(\mathbf{a}|\mathbf{k})$ factorizes; i.e.,

$$P(\mathbf{a}|\mathbf{k}) = \prod_{j=0}^{r} P(a_{i+j}|k_{i+j}). \tag{15}$$

Since each $P(a_i|k_i)$ can now take d different deterministic values, the minimization in Eq. (12) is carried over variables that can take up to d different values. For instance, in Fig. 1, instead of only red and black, one would have d different possible colors.

In summary, the overall minimization is performed in $O(nd^{m(R+1)})$ time. Since d, m, and R are fixed, the overall scaling is $O(n)$, although in practice it is advisable to bear in mind the prefactor. This algorithm gives not only the classical bound β_C [for which it requires $O(d^{mR}) = O(1)$ memory], but it also constructs a deterministic local strategy achieving it [requiring $O(mn) = O(n)$ memory].

Let us now consider the periodic boundary conditions (PBC) case. This can be reduced to the OBC case by splitting the Bell inequality with PBC at an arbitrary position i while fixing a value of $\mathbf{M}^{(i,R)}$. The correlators that contain parties in the set $\{i, \ldots i + R\}$ can be effectively moved to the left or right of the cut by updating the coefficients of I: If all the parties on the correlator belong to the set $\{i, \ldots, i + R\}$, then this correlator has a definite value that becomes a constant in the optimization; if just one party lies outside, then the one-body weights at sites $i - 1$ or $i + R + 1$ can be updated accordingly, and so on. In Appendix B, we explain this procedure in detail.

Since the amount of $\mathbf{M}^{(i,R)}$'s for which the actual minimum of I is achieved is finite, the PBC case is solved by considering d^{mR} OBC cases. This does not change the overall complexity, but it increases the prefactor. The classical bound of I is in the PBC case found in $O(nd^{m(2R+1)}) = O(n)$ time and $O(1)$ memory for β_C and $O(n)$ memory for the deterministic local strategy.

Note that it is crucial for our method that R is constant. If R were comparable to n, the dynamic programing procedure would no longer be efficient. In fact, optimizing one-dimensional Bell inequalities with full-range correlators is equivalent to optimizing general Bell inequalities, where results in computer science indicate that this is an extremely hard problem [3,24]. Note that, even in the bipartite case, deciding whether a probability distribution for m dichotomic measurements is local is NP-complete [32].

C. Quantum value

In this section, we show how to find the ground state energy of the Hamiltonian $\mathcal{H}$ introduced in Eq. (1). To do that, we first review the exact diagonalization of quadratic Hamiltonians in fermionic operators (Sec. II C 1). Then, we transform the spin operator $\mathcal{H}$ to a quadratic fermionic

operator $\hat{\mathcal{H}}$ via the JW transformation [33]; see also Refs. [34,35] (Sec. II C 2).

Throughout this paper, we denote fermionic operators with a hat and spin operators without. Note that the JW transformation is a global operation that breaks the sense of locality in a Bell experiment, but we use it merely as a mathematical tool to find the ground state energy of $\mathcal{H}$.

Recall that a quadratic Hamiltonian in fermionic operators has the form

$$\hat{\mathcal{H}} = \sum_{0 \leq i \neq j < n} A_{ij} \hat{a}_i^\dagger \hat{a}_j + B_{ij} \hat{a}_i \hat{a}_j + \text{H.c.}, \qquad (16)$$

where A_{ij} and B_{ij} are complex numbers and H.c. stands for Hermitian conjugate. The $\hat{a}_i$ ($\hat{a}_i^\dagger$) are annihilation (creation) operators of a fermionic system of n Dirac modes, indexed by i, with $0 \leq i < n$. The ith mode is assigned an annihilation operator $\hat{a}_i$ and a creation operator $\hat{a}_i^\dagger$. The creation operator $\hat{a}_i^\dagger$, acting on the vacuum state $|\Omega\rangle$, populates it with a single excitation, $|1_i\rangle := \hat{a}_i^\dagger |\Omega\rangle$, whereas the annihilation operator satisfies $\hat{a}_i |\Omega\rangle = 0 \ \forall i$. Such operators satisfy the following canonical anticommutation relations (CARs):

$$\{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{i,j} \hat{\mathbb{1}}, \qquad \{\hat{a}_i, \hat{a}_j\} = 0 \quad \forall i, j. \qquad (17)$$

The CARs [Eq. (17)] imply that, without loss of generality, the matrices A and B in Eq. (16) can be taken to be Hermitian and antisymmetric, respectively.

1. Exact diagonalization

In this section, we compute the ground state energy of a Hamiltonian of the form Eq. (16). The operator $\hat{\mathcal{H}}$ of Eq. (16) can be written in terms of Majorana fermions as

$$\hat{\mathcal{H}} = \frac{\mathbb{i}}{2} \sum_{i,j=0}^{n-1} \sum_{\alpha,\beta=0}^{1} H_{i,\alpha;j,\beta} \hat{c}_{i,\alpha} \hat{c}_{j,\beta}, \qquad (18)$$

where the $2n$ Majorana fermions $\hat{c}_{i,\alpha}$ are defined as

$$\hat{c}_{i,\alpha} := \mathbb{i}^\alpha (\hat{a}_i + (-1)^\alpha \hat{a}_i^\dagger), \qquad \alpha \in \{0,1\}, \qquad 0 \leq i < n, \qquad (19)$$

where $\mathbb{i}^2 + 1 = 0$. Note that $\hat{c}_{i,\alpha}$ are Hermitian operators, and they satisfy the CARs

$$\{\hat{c}_{i,\alpha}, \hat{c}_{j,\beta}\} = 2\delta_{i,j} \delta_{\alpha,\beta} \hat{\mathbb{1}}. \qquad (20)$$

It follows that the matrix H in Eq. (18) can be taken real antisymmetric due to Eq. (20) without loss of generality. Since every real antisymmetric matrix H admits a Williamson decomposition $H = OJO^T$ [36], where O is an orthogonal transformation and

$$J = \bigoplus_{k=0}^{n-1} \begin{pmatrix} 0 & \varepsilon_k \\ -\varepsilon_k & 0 \end{pmatrix}, \qquad (21)$$

the operator $\hat{\mathcal{H}}$ is diagonalized by introducing a new set of Majorana operators $\hat{d}_{k,a}$:

$$\hat{\mathcal{H}} = \mathbb{i} \sum_{k=0}^{n-1} \varepsilon_k \hat{d}_{k,0} \hat{d}_{k,1}, \qquad (22)$$

where $\{\mathbb{i} \hat{d}_{k,0} \hat{d}_{k,1}\}$ mutually commute and the new Majorana operators are defined as

$$\hat{d}_{k,a} := \sum_{i,\alpha} O_{i,\alpha;k,a} \hat{c}_{i,\alpha}, \qquad (23)$$

satisfying the same CARs as in Eq. (20). Note that every orthogonal transformation $O \in \mathcal{O}(2n)$ [the set of orthogonal matrices of size n is denoted $\mathcal{O}(n)$] takes a set of Majorana fermions $\{\hat{c}_{i,\alpha}\}$ into a new set $\{\hat{d}_{k,a}\}$ obeying the same CARs as Majorana fermions. In Appendix E, we discuss details on how to obtain an O for which Eq. (21) holds.

The minimal eigenvalue E_0 of $\hat{\mathcal{H}}$ is then given by

$$E_0 = \sum_{k=0}^{n-1} s_k \varepsilon_k, \qquad (24)$$

achieved on a simultaneous eigenstate of the operators $\{\mathbb{i} \hat{d}_{k,0} \hat{d}_{k,1}\}$, with respective eigenvalue $s_k := -\text{sgn}(\varepsilon_k)$.

2. From spins to fermions

In this section, we review the JW transformation and we show that the spin Hamiltonians that can be diagonalized with the method we describe in Sec. II C 1 are precisely those of the form of Eq. (1).

The JW transformation establishes an isomorphism between the Fock space of n Majorana modes and the n-qubit Hilbert space $(\mathbb{C}^2)^{\otimes n}$. For Majorana fermions, the JW transformation can be expressed as

$$\hat{c}_{i,\alpha} \leftrightarrow (-1)^\alpha \left(\prod_{j=0}^{i-1} \sigma_z^{(j)} \right) \sigma_{x+\alpha}^{(i)}, \qquad \alpha \in \{0,1\}. \qquad (25)$$

It follows that for every fermionic operator we obtain an operator acting on $(\mathbb{C}^2)^{\otimes n}$ and vice versa. The operator $\hat{\mathcal{H}}$ as in Eq. (18) consists of the terms $\mathbb{i} \hat{c}_{i,0} \hat{c}_{i,1}$, which correspond to $\sigma_z^{(i)}$, and

$$\mathbb{i} (-1)^\beta \hat{c}_{i,1-\alpha} \hat{c}_{i+r,\beta}, \qquad \alpha, \beta \in \{0,1\}, \qquad r \geq 1, \qquad (26)$$

which correspond to the string operators $\text{Str}_{\alpha,\beta}^{i,r}$ [cf. Eq. (2)] if $i + r < n$. If $i + r \geq n$, we need to define a global parity operator

$$\hat{\mathbb{P}} := \prod_{i=0}^{n-1} \mathrm{i} \hat{c}_{i,0} \hat{c}_{i,1} \leftrightarrow \prod_{i=0}^{n-1} \sigma_z^{(i)} =: \mathbb{P}. \qquad (27)$$

In this case, the string operator takes the form

$$(-1)^{1+\alpha+\beta} \mathrm{Str}_{1-\beta,1-\alpha}^{i+r-n,n-r} = \mathrm{Str}_{\alpha,\beta}^{i,r} \mathbb{P}. \qquad (28)$$

Note that, since $\mathcal{H}$ commutes with $\mathbb{P}$, its ground state has a well-defined eigenvalue $p = \pm 1$ of the parity. This fact becomes relevant in Sec. III.

III. NEW METHOD TO OPTIMIZE BELL INEQUALITIES

The method described so far can also be seen from the opposite perspective: One considers Bell inequalities of the form of Eq. (7) with given coefficients $\gamma_{\mathbf{k}}^{(i,r)}$'s, and one calculates its β_C with dynamic programing. On the other hand, we optimize the quantum value over a restricted set of measurements, namely, single qubit σ_z measurements, and for the r-body correlators, qubit measurements in the x-y plane for parties i and $i + r$ and σ_z measurements in the intermediate ones [cf. Eq. (7)]. The resulting Bell operator can be mapped to a system of fermions as in Eq. (18), whose diagonalization allows us to find the minimal quantum value.

The latter process is carried out as follows. Let us denote the kth observable of the ith party by $\mathcal{M}_k^{(i)}$, with k ranging from 0 to $m - 1$ (or m if $R > 1$). We pick qubit observables parametrized as $\mathcal{M}_m^{(i)} = \sigma_z^{(i)}$ and $\mathcal{M}_k^{(i)} = \cos\varphi_k^{(i)}\sigma_x^{(i)} + \sin\varphi_k^{(i)}\sigma_y^{(i)}$ $(k < m)$ and construct the Bell operator $\mathcal{B}$, which is of the form Eq. (4). Note that to build the Bell operator, one simply needs to substitute the correlators in Eq. (7) by the corresponding quantum observables:

$$M_{\mathbf{k}}^{(i,r)} \to \overset{r+1}{\underset{j=0}{\otimes}} \mathcal{M}_{k_j}^{(i+j)}. \qquad (29)$$

If there exists a quantum state ρ for which $\mathrm{Tr}(\mathcal{B}\rho) < 0$, then ρ is nonlocal. If this is the case, we shall denote the quantum violation observed by $QV := \mathrm{Tr}(\mathcal{B}\rho)$. Note that ρ can be taken, without loss of generality, as a projector onto a ground state of $\mathcal{H}$. We look for the optimal measurement settings $\varphi_k^{(i)*}$, such that $\mathcal{B}$ has the minimal eigenvalue.

The spin Hamiltonian $\mathcal{H}$ is again diagonalized by applying the JW transformation [cf. Eq. (25)], and Eq. (1) is almost transformed into Eq. (18) up to the string operators that cross the origin, which carry a parity operator $\hat{\mathbb{P}}$. Since the eigenstate with the lowest eigenvalue of $\hat{\mathcal{H}}$ has a well-defined parity $p = \pm 1$ (because $[\hat{\mathcal{H}}, \hat{\mathbb{P}}] = 0$), we can change $\mathbb{P}$ by p in Eq. (28) so that $\hat{\mathcal{H}}$ is now quadratic. One has to make sure, though, that the superselection rule imposed by initially choosing p is obeyed. That is, the ground state of $\hat{\mathcal{H}}$ needs to satisfy

$$p = (\det O) \prod_{k=0}^{n-1} s_k. \qquad (30)$$

Equation (30) stems from the fact that, under the transformations of Eq. (23), $\hat{\mathbb{P}}$ is transformed as (see Appendix A for a proof)

$$\hat{\mathbb{P}} = (\det O) \prod_{i=0}^{n-1} \mathrm{i} \hat{d}_{i,0} \hat{d}_{i,1}. \qquad (31)$$

If Eq. (30) does not hold, one has to modify Eq. (24) accordingly by picking

$$E_0 \to E_0 + 2\min_k |\varepsilon_k|. \qquad (32)$$

The minimal E_0 for $p = 1$ or $p = -1$ is the minimal eigenvalue of $\mathcal{B}$.

Finally, note that if $R = 1$ and $m = 2$, the minimal eigenvalue of $\mathcal{B}(\varphi_k^{(i)*})$ yields the minimal value of I achievable within quantum theory, denoted $-\beta_Q$, because the optimal quantum violation of Bell inequalities with n parties and two dichotomic observables is obtained with qubits and traceless observables on a plane [37]. However, if $R > 1$ or $m > 2$, this result does not hold in general, as higher-dimensional systems and more general observables can produce more nonlocal correlations.

IV. TRANSLATIONALLY INVARIANT CASE

In this section, we consider the case in which $\mathcal{H}$ in Eq. (1) is translationally invariant. In the spirit of Sec. III, the following procedure can be seen as an optimization of a TI Bell inequality with the same set of observables at each site. We first present an algorithm to compute the classical bound of a TI Bell inequality with short-range correlators, which is exponentially faster in the number of parties than the one of Sec. II B 1 (Sec. IV A). We then find the ground state energy of a TI Hamiltonian of the form of Eq. (1) analytically (Sec. IV B).

A. Exponentially faster solution of the classical bound

In this section, we present a method that is exponentially faster in the number of particles than the one in Sec. II B 1 to compute the classical bound of TI Bell inequalities of the form of Eq. (8), i.e., where $\gamma_{\mathbf{k}}^{(i,r)}$ are independent of i. For the sake of simplicity, we first present this problem in a more abstract setting. Then we adapt it to TI Bell inequalities.

Consider a function $f^{(0)}: S \times S \to \mathbb{R}$, where S is a finite set. We describe how to compute

$$F := \min_{x_0,\dots,x_w} \sum_{j=0}^{w-1} f^{(0)}(x_j, x_{j+1}) \qquad (33)$$

in $O(\log_2 w)$ steps. To this end, let us define

$$f^{(t+1)}(x, y) := \min_z [f^{(t)}(x, z) + f^{(t)}(z, y)] \qquad (34)$$

for $t > 0$. Note that the superscript t indicates the iteration step. The idea is to successively rewrite F in terms of $f^{(t+1)}$ instead of $f^{(t)}$, thus eliminating at each step approximately half of the variables in the minimization. For instance, by writing F in terms of $f^{(1)}$, one has already carried out the minimization over all the variables with odd index (except the last one if w is odd). Note that any function $f^{(t)}$ is defined by specifying $|S|^2$ numbers, where $|S|$ is the number of elements of S. Computing Eq. (34) requires $O(|S|^3)$ operations. Note that when w is a power of 2, then F is given by

$$F = \min_{x_0, x_w} f^{(\log_2 w)}(x_0, x_w). \qquad (35)$$

In the general case, however, we cannot assume w to be a power of 2. Nevertheless, every positive integer w can be uniquely expressed as a sum of different powers of 2. The idea is to apply the procedure described above to each of these powers of 2 and then optimize over the remaining $O(\log_2 w)$ variables. To this end, recall that the binary expression for w is

$$w = \sum_{i=0}^{\lfloor \log_2 w \rfloor} a_i 2^i = \sum_{j=0}^{|w|-1} 2^{b_j}, \qquad (36)$$

where $\lfloor \cdot \rfloor$ is the floor function, $a_i \in \{0, 1\}$ correspond to the digits of w in binary, $|w| := \sum_i a_i$ is the Hamming weight of w, and the b_j's enumerate the indices i for which $a_i = 1$, sorted in decreasing order. For instance, if $w = 11$, $(a_3, a_2, a_1, a_0) = (1, 0, 1, 1)$ and $(b_0, b_1, b_2) = (3, 1, 0)$, and if $w = 15$, then $(a_3, a_2, a_1, a_0) = (1, 1, 1, 1)$ and $(b_0, b_1, b_2, b_3) = (3, 2, 1, 0)$.

Note that F can now be rewritten as

$$F = \min_{y_0 \cdots y_{|w|}} \sum_{j=0}^{|w|-1} f^{(b_j)}(y_j, y_{j+1}), \qquad (37)$$

which is a minimization over $1 + |w| \le 1 + \lceil \log_2(w) \rceil$ variables y_j, where $\lceil \cdot \rceil$ is the ceiling function. Note that the $f^{(b_j)}$ need no longer be the same function for different j, so the expression for F given in Eq. (37) is not TI in general. Note that at the $\lfloor \log_2 w \rfloor$th step of the optimization we have the x_0 variable on the left (see Fig. 2) and several remaining variables x_j for $j \ge \lfloor \log_2 w \rfloor$. Since these remaining variables highly depend on the binary expression of w, we denote them by y_j [cf. Eq. (37)]. To minimize over y_j, we proceed in a similar fashion, now defining $g^{(0)} := f^{(b_0)}$ and
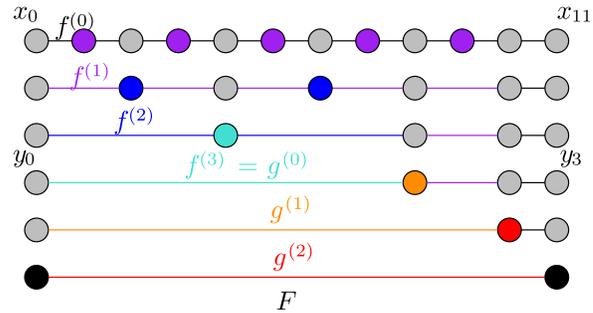

FIG. 2. Here, we find F for $w = 11$. We represent the variables x_i with circles and the functions f or g with lines. Each line with the same color corresponds to the same function. The variables that are not in gray are eliminated at the next step. At the zeroth iteration, there are 10 functions $f^{(0)}$ depending on 11 variables. We compute $f^{(1)}$ and we substitute it as many times as possible, so that at the first iteration we eliminate the variables in purple. Then we eliminate the variables in blue by computing $f^{(2)}$ and the variables in turquoise by computing $f^{(3)}$. We then compute the functions g by joining them with the remaining f's, thus eliminating the orange and the red variables. Finally, we minimize on the ends, where we can impose conditions on the boundary if needed.

$$g^{(t+1)}(x, y) := \min_z [g^{(t)}(x, z) + f^{(b_{t+1})}(z, y)] \qquad (38)$$

for $t > 0$. Observe that now the optimization is linear, similar to the dynamic programing we present in Sec. II B 1. It follows that F can now be computed as

$$F = \min_{x_0, x_w} g^{(|w|-1)}(x_0, x_w). \qquad (39)$$

In Fig. 2, we describe this procedure with an example.

To adapt this algorithm to the minimization of I, we start by noting that I can be written as

$$I = \sum_{i=0}^{n-1} h(\mathbf{M}^{(i,R+1)}), \qquad (40)$$

where h is defined as

$$h(\mathbf{M}^{(i,R+1)}) := \sum_{r=0}^{R} \sum_{\mathbf{k}=0}^{m^{r+1}-1} \gamma_{\mathbf{k}}^{(r)} M_{\mathbf{k}}^{(i,r)}, \qquad (41)$$

and the indices of the parties are taken modulo n in the $M_{\mathbf{k}}^{(i,r)}$ defined in Eq. (9). Observe that every ith and $(i + R + 1)$th parties share R parties via h. In particular, by picking $i = j(R + 1) - 1$, we denote their local deterministic strategy as

$$x_j := \mathbf{M}^{[j(R+1),R]}. \qquad (42)$$

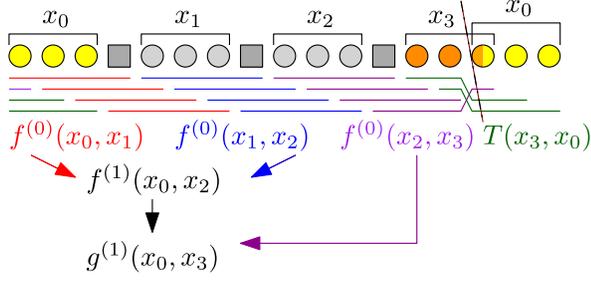We now rewrite the optimization of I over $\mathbf{M}$ in terms of x_j. To this end, let us define

FIG. 3. An example with $n = 14$ and $R = 3$ (this corresponds to $w = 3$). Each circle or square corresponds to a party, starting at $i = 0$ on the left. The dash-dotted line represents crossing the origin and each line below the parties represents a function h (note that h has a range of $R + 1$ parties). The lines corresponding to the h's are arranged in groups of $R + 1$ (except for the T corresponding to the tail), which we represent with the same color. Each full group contains a single gray square. By minimizing the local deterministic strategy at the square, we can define $f^{(0)}$, which depends on the local deterministic strategy chosen at the R neighbors of each side. These groups of R parties correspond to the x_j in Fig. 2. They encode the possible d^{mR} local deterministic strategies for each x_j. Now, in $O(\log n)$ steps we find $g^{|w|-1}(x_0, x_w)$. Finally, we find the classical bound by minimizing the sum of $g^{|w|-1}$ and T restricted to the x_0 and x_w that have a compatible overlap.

$$f^{(0)}(x_j, x_{j+1}) := \min_{M_k^{(jR+j+R)}} \sum_{i=0}^{R} h[\mathbf{M}^{(j(R+1)+i,R+1)}]. \quad (43)$$

Since we cannot assume that n is a multiple of $R + 1$, we take $w := \lfloor n/(R+1) \rfloor$. Then,

$$\min_{\mathbf{M}} I = \widetilde{\min}_{x_0,x_w} g^{(|w|-1)}(x_0, x_w) + T(x_w, x_0), \quad (44)$$

where the tail $T(x_w, x_0)$ is defined as

$$T(x_w, x_0) := \sum_{i=(R+1)w}^{n-1} h(\mathbf{M}^{(i,R)}), \quad (45)$$

with the indices of the parties taken modulo n and $\widetilde{\min}$ is the minimum taken on those x_0, x_w that are compatible with PBC [for instance, if $w = n(R + 1)$, then $T = 0$ and $\widetilde{\min}$ is taken over $x_0 = x_w$]. In Fig. 3, we illustrate the procedure we describe with an example.

B. Analytical solution of the quantum value

Here we consider Eq. (1) in the TI case, which corresponds to $t^{(i)}$ and $t_{\alpha,\beta}^{(i,r)}$ being independent of i. In terms of Bell inequalities, this corresponds to the optimization of TI Bell inequalities with the same set of observables being performed at each site. We give analytically closed expressions in this case. As we prove in

Appendix C, the Williamson eigenvalues for a TI Bell operator of the form of Eq. (4) are given by

$$\varepsilon_{k,\pm} := a_k + c_k \pm \sqrt{(a_k - c_k)^2 + 4(b_k^2 + x_k^2)}, \quad (46)$$

with k ranging from 1 to $\lfloor (n - (p - 1)/2)/2 \rfloor$, where

$$x_k := H_{00;01} + \sum_{r=1}^{R} \cos(v_{k,r})(H_{00;r1} - H_{01;r0}), \quad (47)$$

$$a_k := -2 \sum_{r=1}^{R} \sin(v_{k,r}) H_{00;r0}, \quad (48)$$

$$b_k := -\sum_{r=1}^{R} \sin(v_{k,r})(H_{00;r1} + H_{01;r0}), \quad (49)$$

$$c_k := -2 \sum_{r=1}^{R} \sin(v_{k,r}) H_{01;r1}, \quad (50)$$

with $v_{k,r} := r\pi[2k - (p + 1)/2]/n$. Depending on the parity of n, the following eigenvalues also appear:

$$\varepsilon_{0,\pm} := \sum_{q=0}^{n-1} (\pm 1)^q H_{00;q1}. \quad (51)$$

If $p = -1$, then $\varepsilon_{0,+}$ always appears and $\varepsilon_{0,-}$ appears only if n is even. If $p = 1$, then $\varepsilon_{0,-}$ appears only if n is odd and $\varepsilon_{0,+}$ does not appear (see Appendix C).

The superselection rule Eq. (30) to be fulfilled in this case reads

$$p = (-1)^{\lfloor [n+(p-1)/2]/2 \rfloor} \prod_{k=0}^{n-1} s_k. \quad (52)$$

Note that if we just want to find the ground state energy of a TI fermionic Hamiltonian Eq. (16), then the matrices A and B are circulant, which means that the previous analysis can be done assuming that $p = -1$ and no superselection rule needs to be obeyed in this case, as Eq. (52) appears from the transformation of spins to fermions. This result is applied to the example of Sec. V A.

V. EXAMPLES

In this section, we present three different examples in which we illustrate the tools we present throughout the paper. In Sec. V A, we optimize a tight TI inequality for $n = 8$ parties with $R = 2$ and PBC, showing that it has quantum violation when the same set of qubit measurements are performed at each site. Interestingly, such optimal measurements are $\mathcal{M}_0 = \sigma_x$, $\mathcal{M}_1 = \sigma_y$, and $\mathcal{M}_2 = \sigma_z$. In Sec. V B, we construct a quasi-TI Bell

inequality for any even number of parties and any number of measurements, which depends on one parameter. We find its classical bound analytically with dynamic programing. The Bell operator corresponds to a spin XY model, which we also solve analytically. Finally, in Sec. V C, we show that the ground state of a spin glass is nonlocal in some parameter region.

A. Translationally invariant Bell inequality for eight parties

The general form of a translationally invariant Bell inequality $I + \beta_C \geq 0$, with $m = d = R = 2$, is [cf. Eq. (7)]

$$I := \gamma \mathcal{T}_2 + \sum_{k,l \in \{0,1\}} (\gamma_{k,l} \mathcal{T}_{k,l} + \gamma_{k,2,l} \mathcal{T}_{k,2,l}), \quad (53)$$

where the translationally invariant correlators $\mathcal{T}$ are defined as

$$\mathcal{T}_{k_1,\ldots,k_r} := \sum_{i=0}^{n-1} M^{(i,r)}_{(k_1,\ldots,k_r)}. \quad (54)$$

In Table I (in Appendix D), we show the optimal (tight) Bell inequalities of these kind for $n \leq 8$ and the quantum violation we can observe. Let us remark that finding all Bell inequalities for a given scenario is a computationally very expensive task and one typically manages to do it only for very small values of n, m, d, and R, even if symmetries are imposed [38]. When looking for Bell inequalities of the form Eq. (53), $n = 8$ is the maximum number of parties for which this task could be carried out in a reasonable time. Here, we present a particular case as an example.

If one takes the following coefficients, $\gamma = 0$, $\gamma_{00} = \gamma_{10} = -\gamma_{01} = -\gamma_{11} = 2$, $-\gamma_{020} = -\gamma_{021} = \gamma_{120} = \gamma_{121} = 1$, then the dynamic programing gives $\beta_C = 32$ and the measurement settings $\mathcal{M}_0 = \sigma_x$, $\mathcal{M}_1 = \sigma_y$, $\mathcal{M}_2 = \sigma_z$ produce a quantum violation of $QV = \langle I \rangle + \beta_C \simeq -0.2187$.

The latter is proven by applying Eq. (46) to the example. More specifically, we observe that the chosen coefficients and measurements yield an H matrix [cf. Eq. (18) and Appendix C] with upperdiagonal blocks h_1 and h_2,

$$h_1 = \begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix}, \qquad h_2 = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad (55)$$

and the rest of the h_r blocks are zero. This greatly simplifies the expression for ε_k as $x_k = 0$ and $a_k = c_k$ imply $\varepsilon_k = 2(a_k \pm |b_k|)$ (note that in the range of interest, $b_k \leq 0$, so that $\varepsilon_k = 2(a_k \mp b_k)$]. If we take the plus sign, we have

$$\varepsilon_{k,+} = -8 \cos \left(\pi \frac{4k + 3 - p}{8} \right), \quad (56)$$

and if we take the minus sign, we obtain

$$\varepsilon_{k,-} = 16 \cos \left(\pi \frac{4k + 11 - p}{16} \right). \quad (57)$$

Thus, we can now calculate the ground state energy consistent with each p, which is given by

$$E_0 = -16 - 8\sqrt{2},$$

if $p = -1$, and

$$E_0 = -8[\sqrt{2} + 2\cos(\pi/8) + 2\sin(\pi/8)],$$

if $p = 1$. One does not need to check the superselection rule Eq. (52) for $p = -1$ as some of the ε_k are zero. However, we do need to check it for $p = 1$. There, we take an even (2) number of sign flips to the ε_k and the determinant of O is 1 (cf. Appendix C). It follows that Eq. (30) holds. The case for $p = -1$ gives $E_0 \simeq -27.3137$, whereas for $p = 1$, it gives $E_0 = -32.2187$. Hence, $\langle I \rangle + \beta_C = -0.2187 < 0$, signaling the presence of nonlocality.

B. Quasi-translationally-invariant Bell inequality

Let us consider the chained Bell inequality [39] between two parties labeled A and B:

$$I^{(A,B)}_{\text{chain}} \geq -2(m-1), \quad (58)$$

where $I^{(A,B)}_{\text{chain}}$ is given by

$$I^{(A,B)}_{\text{chain}} := \sum_{i=0}^{m-1} (A_{m-i-2}B_i + A_{m-i-1}B_i), \quad (59)$$

where it is assumed that $A_{-1} := -A_{m-1}$. Note that the Clauser-Horne-Shimony-Holt (CHSH) inequality [40], $I^{(A,B)}_{\text{CHSH}} := A_0B_0 + A_0B_1 + A_1B_0 - A_1B_1$, is a particular case of Eq. (59) for $m = 2$. Inequality Eq. (58) is violated maximally with the following settings,

$$A_i = \sin(\phi_i)\sigma_x - \cos(\phi_i)\sigma_y \quad (60)$$

and $B_i = A_i$, where the angles are given by $\phi_i := (i+1)\pi/m$, and with the state

$$|\psi_m\rangle := \frac{1}{\sqrt{2}} (e^{-i\pi/2m}|00\rangle - |11\rangle), \quad (61)$$

giving $\beta_Q = \langle I^{(A,B)}_{\text{chain}} \rangle = -2m\cos(\pi/2m)$. Notice that the maximal violation relative to the classical bound is $\beta^r_Q := \beta_Q/\beta_C = [m/(m-1)]\cos(\pi/2m)$.

The bipartite Bell operator corresponding to the chained Bell inequality with the above measurements can be written as

$$\mathcal{B} = \alpha_m(\sigma_x \otimes \sigma_x - \sigma_y \otimes \sigma_y) + \beta_m(\sigma_x \otimes \sigma_y + \sigma_y \otimes \sigma_x),$$

$$(62)$$

where $\alpha_m := m\cos^2(\pi/2m)$ and $\beta_m := (m/2)\sin(\pi/m)$. By defining $\sigma_{\pi/2m} := \cos(\pi/2m)\sigma_x + \sin(\pi/2m)\sigma_y$, this operator can be further reexpressed in a formally similar manner to the XY Hamiltonian as

$$\mathcal{B} = m(\sigma_{\pi/2m}^{(A)}\sigma_{\pi/2m}^{(B)} - \sigma_y^{(A)}\sigma_y^{(B)}). \qquad (63)$$

Let us now consider the following Hamiltonian:

$$\mathcal{H} = m\sum_{i=0}^{2n-1} f_i(\epsilon)(\sigma_{\pi/2m}^{(i)}\sigma_{\pi/2m}^{(i+1)} - \sigma_y^{(i)}\sigma_y^{(i+1)}), \qquad (64)$$

where the weights $f_i(\epsilon)$ alternate from even to odd sites as $f_i(\epsilon) := 1 + (-1)^i\epsilon$ and ϵ is an arbitrary real parameter. We note that the Hamiltonian Eq. (64) is a particular case of the one-dimensional Bell inequality,

$$I_{\text{chain}}^{(2n)}(\epsilon) := \sum_{i=0}^{2n-1} f_i(\epsilon)I_{\text{chain}}^{(i,i+1)}, \qquad (65)$$

when the same measurements Eq. (60) are taken at each site.

Let us now determine the classical bound of $I_{\text{chain}}^{(2n)}(\epsilon)$. For even n (for odd n and $n < m$, the classical bound is slightly different; however, for the purposes of the present example, it is enough to consider the classical bound for even n), the dynamic programing gives $\beta_C = 4n(m-1)\max\{1, |\epsilon|\}$. The explanation for this result is that, whenever $\epsilon > 1$, it is better to use a classical strategy that would give $-2(m-1)$ on every $I_{\text{chain}}^{(2i,2i+1)}$ inequality and $2(m-1)$ on every $I_{\text{chain}}^{(2i+1,2(i+1))}$ inequality. An exemplary local strategy achieving this bound is given by

k	$4i$	$4i+1$	$4i+2$	$4i+3$
$M_0^{(k)}$	$+$	$-$	$+$	$+$
$M_1^{(k)}$	$+$	$-$	$-$	$+$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$M_{m-2}^{(k)}$	$+$	$-$	$-$	$+$
$M_{m-1}^{(k)}$	$+$	$+$	$-$	$-$

periodically repeated every four sites. On the other hand, if $0 \le \epsilon \le 1$, the optimal strategy consists in producing $-2(m-1)$ for every link, for instance, by picking $(M_0^{(2i)}, \ldots, M_{m-1}^{(2i)}) = (+, \cdots, +)$ and $(M_0^{(2i+1)}, \ldots, M_{m-1}^{(2i+1)}) = (-, \cdots, -)$. The analysis for $\epsilon < 0$ is analogous.

It is worth highlighting two limiting cases.

(i) $\epsilon = 1$. This corresponds to a sum of disjoint chained Bell inequalities between pairs $(2i, 2i+1)$.

$$I_{\text{chain}}^{(2n)}(1) = 2\sum_{i=0}^{n-1} I_{\text{chain}}^{(2i,2i+1)}, \qquad (66)$$

which is maximally violated by the state $|\psi_m\rangle_{AB} \otimes |\psi_m\rangle_{CD} \otimes \ldots$. The quantum value is then $\beta_Q = 2nm\cos(\pi/2m)$. Hence, there is a $O(1)$ violation

relative to the classical bound that holds for every n:

$$\beta_Q/\beta_C = \frac{m}{m-1}\cos\left(\frac{\pi}{2m}\right) > 1. \qquad (67)$$

(ii) $\epsilon = 0$. This case corresponds to a sum of the chained Bell inequalities with the same weights between neighbors:

$$I_{\text{chain}}^{(2n)}(0) = \sum_{i=0}^{2n-1} I_{\text{chain}}^{(i,i+1)}. \qquad (68)$$

This inequality cannot be violated, as quantum correlations are monogamous with respect to the chained Bell inequality [37,41]. Loosely speaking, if party B violates I_{chain} with A, it cannot violate it simultaneously with C. For some types of monogamy relations, this result holds for various generalizations of the CHSH inequality to more measurements, outcomes, and parties [42].

It is then clear that there is some critical value of ϵ for which correlations stop being nonlocal and one is able to simulate them locally.

Let us now notice that the $4n \times 4n$ matrix H appearing in Eq. (18) and corresponding to the Hamiltonian Eq. (64) has the form $H = H_0 \otimes H_1$, where

$$H_0 := m\begin{pmatrix} 0 & f_0 & 0 & \cdots & 0 & pf_1 \\ -f_0 & 0 & f_1 & 0 & \cdots & 0 \\ 0 & -f_1 & 0 & f_0 & 0 & \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & -f_1 & 0 & f_0 \\ -pf_1 & 0 & \cdots & 0 & -f_0 & 0 \end{pmatrix}, \qquad (69)$$

with $f_0 := 1 + \epsilon$ and $f_1 = 1 - \epsilon$ for short, and

$$H_1 = \begin{pmatrix} \frac{1}{2}\sin(\frac{\pi}{m}) & \cos^2(\frac{\pi}{2m}) \\ \cos^2(\frac{\pi}{2m}) & -\frac{1}{2}\sin(\frac{\pi}{m}) \end{pmatrix}$$
$$= \alpha_m\sigma_x + \beta_m\sigma_z. \qquad (70)$$

This is seen by applying the JW transformation to Eq. (62).

In this case, to find the Williamson eigenvalues of H it is sufficient to find those of H_0, which will appear with both signs, as H_1 has eigenvalues $\pm\cos(\pi/2m)$.

A similar analysis as the previous example shows that H can also be block diagonalized with a real discrete Fourier transform (DFT) into 4×4 blocks. The Williamson eigenvalues of H_0 are

$$\varepsilon_k = m\sqrt{2[1 + \epsilon^2 + (\epsilon^2 - 1)\cos(\nu_k)]}, \qquad 0 \le k < n, \tag{71}$$

where $\nu_k := \pi[2k + (p + 1)/2]/n$.

Hence, the quantum bound will be

$$\beta_Q(\epsilon) = 2\cos\left(\frac{\pi}{2m}\right) \sum_{k=0}^{n-1} \varepsilon_k. \tag{72}$$

Although one should check the superselection rule Eq. (30), it is not necessary for large n, as the difference between β_Q for $p = 1$ and β_Q for $p = -1$ vanishes as n grows.

Let us analyze the behavior of $\beta_Q(\epsilon)$ in the thermodynamic limit. The contribution per particle to $\beta_Q(\epsilon)$, denoted $\tilde{\beta}_Q(\epsilon)$, is

$$\tilde{\beta}_Q(\epsilon) := 2\cos\left(\frac{\pi}{2m}\right) \lim_{n\to\infty} \sum_{k=0}^{n-1} \frac{1}{2n}\varepsilon_k,$$

which is a Riemann sum, so it is by definition

$$\tilde{\beta}_Q(\epsilon) = \sqrt{2}m\cos\left(\frac{\pi}{2m}\right)$$
$$\times \int_0^1 \sqrt{1 + \epsilon^2 + (\epsilon^2 - 1)\cos(2\pi x)}dx. \tag{73}$$

This can be expressed more compactly as

$$\tilde{\beta}_Q(\epsilon) = \frac{4}{\pi}m\cos\left(\frac{\pi}{2m}\right)E(1 - \epsilon^2), \tag{74}$$

where $E(t)$ is the complete elliptic integral of the second kind. [The complete elliptic integral of the second kind is defined as $E(t) := \int_0^{\pi/2} \sqrt{1 - t\sin^2(\theta)}d\theta$, with the parameter t obeying $0 < t < 1$.]

In Fig. 4, we see such behavior compared to the contribution per particle to the classical bound, $\tilde{\beta}_C(\epsilon) = 2(m - 1)\max\{1, |\epsilon|\}$. In Fig. 5, we compare the length of the detected nonlocal parameter region with the number of measurement settings m.

C. Spin glass

Finally, we consider a Hamiltonian similar to Eq. (64) for $m = 2$, where all the couplings are random, generated from a Gaussian probability distribution with mean μ and standard deviation σ, like a spin glass:

$$H = \sum_{i=0}^{n-1} J_{\mu,\sigma}^{(i)}[\sigma_{\pi/4}^{(i)}\sigma_{\pi/4}^{(i+1)} - \sigma_y^{(i)}\sigma_y^{(i+1)}]. \tag{75}$$

We can efficiently compute the ground state of Eq. (75) and the classical bound of the CHSH-like Bell inequality associated to it with the methods we present, although numerically. We expect that, when $|\mu|/\sigma \gg 1$, we do not
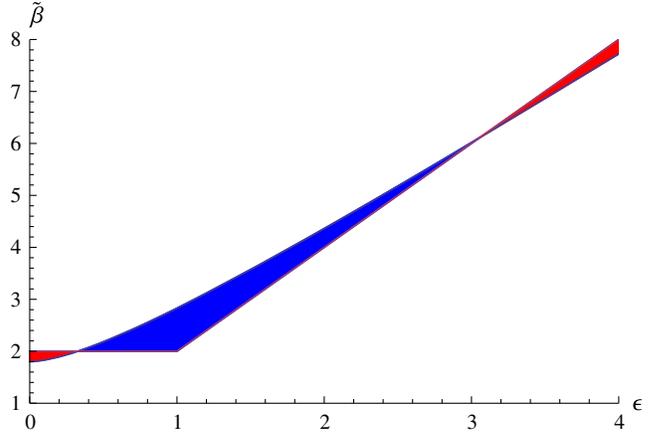

FIG. 4. For $m = 2$, the curves $\tilde{\beta}_Q(\epsilon)$ [cf. Eq. (74)] and $\tilde{\beta}_C(\epsilon) = 2\max\{1, |\epsilon|\}$. These capture the behavior of the nonlocality of the ground state of Eq. (64) in the limit of large n. Whenever $\tilde{\beta}_Q(\epsilon)$ is above $\tilde{\beta}_C(\epsilon)$ (blue region), nonlocality is detected. Otherwise (red region) a more stringent test is needed or the state admits a local hidden variable model. The intersection points between the two curves are $\epsilon_* \approx 0.327618$ and $\epsilon^* \approx 3.05234$.

detect nonlocality, as the resulting inequality is close to the monogamous limit $\epsilon = 0$ of the example in Sec. V B. However, if σ is big enough, one expects to have links with high weight surrounded with links with smaller weight; then, it may compensate to violate those links with higher weight. In Fig. 6, we show the result, for $n = 10^2$ spins, averaged over 10^3 realizations. There is clearly a transition for which the complexity of the ground state allows or does not allow for the statistics that one obtains when performing measurements on it to be simulable locally.
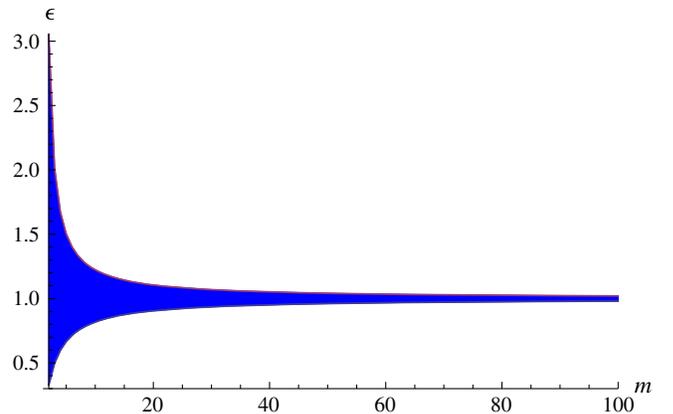

FIG. 5. For different values of m, the intervals $[\epsilon_*, \epsilon^*]$ for which we detect that the ground state of Eq. (64) is nonlocal. Observe that, for $m = 2$, which corresponds to the case where the chained Bell inequality is the CHSH Bell inequality, we detect nonlocality in the largest parameter region (cf. Fig. 4). For $\epsilon = 1$, nonlocality is always detected, since $\tilde{\beta}_Q(1)/\tilde{\beta}_C(1) = m\cos(\pi/2m)/(m-1) > 1$ for all $m > 1$, as it is shown in Eq. (67).
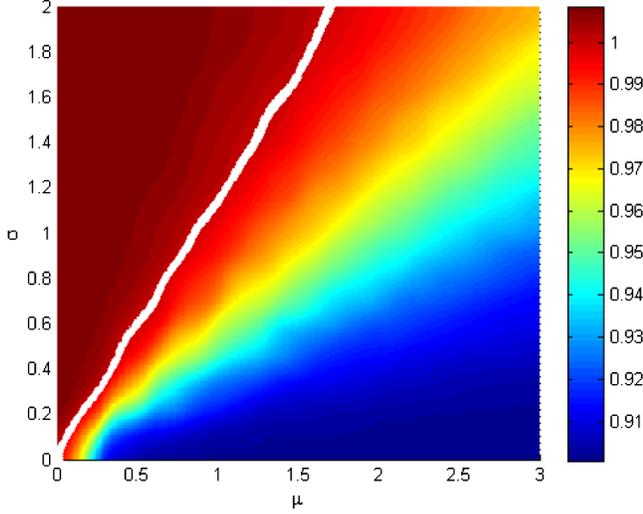
FIG. 6. Ratio of the quantum value over the classical bound of the ground state of Eq. (75) and the Bell inequality we associate to it. The plot corresponds to a spin glass of $n = 100$ spins with PBC, averaged over 1000 realizations. The horizontal axis corresponds to the mean μ of the Gaussian distribution and the vertical axis corresponds to its standard deviation σ. If $\mu = 0$, the value is constant for all $\sigma > 0$, as both the expected value of the ground state and the classical bound grow at the same rate with σ. The white line represents the level curve for $\beta_C = \beta_Q$. The top left part of the plot corresponds to the region of parameters in which we detect nonlocality ($\beta_C < \beta_Q$). Note that in the bottom right region one finds values for which $\beta_Q/\beta_C < 1$ due to the fact that there is no simultaneous eigenvalue of $\sigma_{\pi/4}$ and σ_y (the classical bound cannot be saturated using $\sigma_{\pi/4}$ and σ_y as observables).

D. *XXZ*-like spin model based on Gisin's elegant Bell inequality

In this last example, we present an *XXZ*-like Hamiltonian, which is not solvable via the JW transformation. We find its ground state energy numerically, using tensor networks and density matrix renormalization group (DMRG) [30]. In this case, we find a much richer structure than in Sec. V B. The Bell inequality that we associate to this Hamiltonian is a modification of Gisin's elegant Bell inequality [29]. Gisin's original inequality is defined in a bipartite scenario with four dichotomic measurements with outcomes ± 1 on Alice and three dichotomic measurements with outcomes ± 1 on Bob:

$$I = (\,A_0 \quad A_1 \quad A_2 \quad A_3\,) \begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix} \begin{pmatrix} B_0 \\ B_1 \\ B_2 \end{pmatrix},$$

(76)

and it reads $|I| \leq 6$. We observe that with the following observables,

$$A_0 = \frac{\sigma_x + \sigma_y + \sigma_z}{\sqrt{3}}, \qquad A_1 = \frac{\sigma_x - \sigma_y - \sigma_z}{\sqrt{3}},$$

$$A_2 = \frac{-\sigma_x + \sigma_y - \sigma_z}{\sqrt{3}}, \qquad A_3 = \frac{-\sigma_x - \sigma_y + \sigma_z}{\sqrt{3}},$$

$$B_0 = \sigma_x, \qquad B_1 = \sigma_y, \qquad B_2 = \sigma_z, \tag{77}$$

the corresponding Bell operator becomes

$$\mathcal{B} = \frac{4}{\sqrt{3}}(\sigma_x\sigma_x + \sigma_y\sigma_y + \sigma_z\sigma_z), \tag{78}$$

and its ground state is $|\psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$, yielding an expectation value $\langle \psi^- |\mathcal{B}|\psi^-\rangle = -4\sqrt{3} \simeq -6.9282$.

Let us now introduce the following modification, where Δ is a real parameter,

$$J_{\text{even}} = (\,A_0 \quad A_1 \quad A_2 \quad A_3\,)S_\Delta \begin{pmatrix} B_0 \\ B_1 \\ B_2 \end{pmatrix}, \tag{79}$$

$$J_{\text{odd}} = (\,B_0 \quad B_1 \quad B_2\,)S_\Delta^T \begin{pmatrix} A_0 \\ A_1 \\ A_2 \\ A_3 \end{pmatrix}, \tag{80}$$

where S_Δ is a 4×3 matrix defined as

$$S_\Delta = \begin{pmatrix} 1 & 1 & \Delta \\ 1 & -1 & -\Delta \\ -1 & 1 & -\Delta \\ -1 & -1 & \Delta \end{pmatrix}. \tag{81}$$

The classical bound becomes

$$J_{\text{even/odd}} \geq \begin{cases} 4\Delta & \text{if} & \Delta \leq -2 \\ -4 + 2\Delta & \text{if} & -2 < \Delta \leq 0 \\ -4 - 2\Delta & \text{if} & 0 < \Delta \leq 2 \\ -4\Delta & \text{if} & 2 < \Delta. \end{cases} \tag{82}$$

Now we have that the Bell operator has become

$$\mathcal{B} = \frac{4}{\sqrt{3}}(\sigma_x\sigma_x + \sigma_y\sigma_y + \Delta\sigma_z\sigma_z) \tag{83}$$

in either case. Its ground state energy is

$$\langle \psi_{\text{gnd}}|\mathcal{B}|\psi_{\text{gnd}}\rangle = \begin{cases} \frac{4\Delta}{\sqrt{3}} & \text{if } \Delta \leq -1 \\ \frac{-4(2+\Delta)}{\sqrt{3}} & \text{if } \Delta > -1. \end{cases} \tag{84}$$
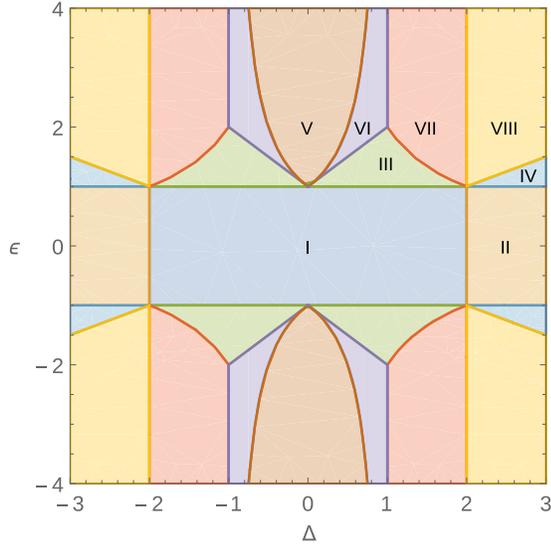
FIG. 7. The classical bound of Eq. (85). Each region [cf. Eq. (86)] has a different expression for the classical bound [cf. Eqs. (87), (88)]. The classical bound of Eq. (85) depends only on the absolute values of ϵ and Δ.
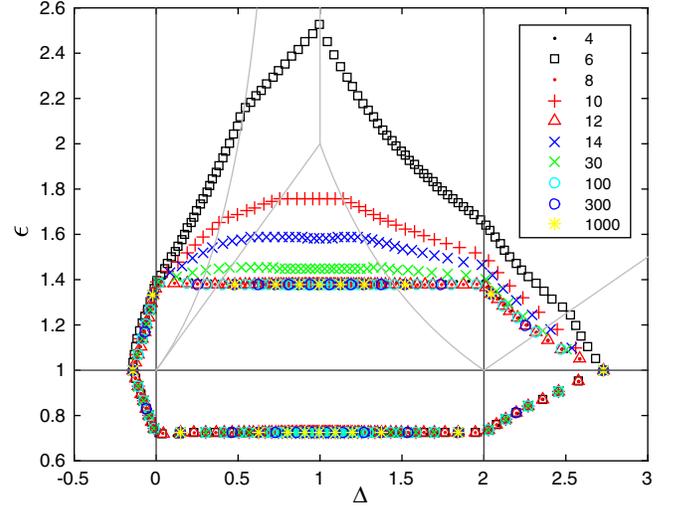

FIG. 8. Level curves for which the quantum value equals the classical bound. Note the different behavior depending on the parity of $n/2$ and the effect of the different regions plotted in Fig. 7, also sketched here in gray (for odd $n/2$) and black (even $n/2$) for clarity. The region for which there is quantum violation is the bounded set [i.e., containing the point $(\Delta, \epsilon) = (1, 1)$]. The plot is symmetric with respect to the line $\epsilon = 0$.

The ground state is $|\psi^-\rangle$ if $\Delta > -1$ and it lies in the subspace spanned by $|00\rangle$ and $|11\rangle$ if $\Delta \le -1$.

We can now construct the many-body Bell inequality in a similar fashion as in Sec. V B:

$$J = \sum_{i=0}^{n/2-1} (1 + \epsilon) J_{\text{even}}^{(2i,2i+1)} + (1 - \epsilon) J_{\text{odd}}^{(2i+1,2i+2)}. \quad (85)$$

Note that the Bell inequality J has four binary measurements with outcomes ± 1 on the even sites and three binary measurements with outcomes ± 1 on the odd sites.

The dynamic programing procedure yields the following classical bound in terms of ϵ and Δ, which is a $\mathcal{C}^0$ piecewise continuous function. Because of all the cases that appear, and the complexity of the inequality, we omit the description of the local deterministic strategy. The regions are defined as follows (see Fig. 7):

$$R_{\text{I}} = \{(\Delta, \epsilon) : |\Delta| \le 2, |\epsilon| \le 1\},$$
$$R_{\text{II}} = \{(\Delta, \epsilon) : |\Delta| > 2, |\epsilon| \le 1\},$$
$$R_{\text{III}} = \{(\Delta, \epsilon) : |\Delta| \cdot |\epsilon| \le 2, |\epsilon| \le |\Delta| + 1, |\epsilon| > 1\},$$
$$R_{\text{IV}} = \{(\Delta, \epsilon) : |\epsilon| \le |\Delta|/2, |\epsilon| > 1\},$$
$$R_{\text{V}} = \{(\Delta, \epsilon) : |\epsilon| > 1/(1 - |\Delta|)\},$$
$$R_{\text{VI}} = \{(\Delta, \epsilon) : |\epsilon| \le 1/(1 - |\Delta|), |\Delta| \le 1, |\epsilon| > |\Delta| + 1\},$$
$$R_{\text{VII}} = \{(\Delta, \epsilon) : |\epsilon| \cdot |\Delta| > 2, 1 < |\Delta| \le 2\},$$
$$R_{\text{VIII}} = \{(\Delta, \epsilon) : |\epsilon| > |\Delta|/2, |\Delta| > 2\}. \quad (86)$$

If $n \equiv 2 \mod 4$, $n > 2$, the classical bound is, on each region:

$$\beta_{C,\text{I}} = -n(4 + 2|\Delta|),$$
$$\beta_{C,\text{II}} = -4n|\Delta|,$$
$$\beta_{C,\text{III}} = -8 - 4|\Delta| - (4n - 8)|\epsilon| - (2n - 4)|\Delta||\epsilon|,$$
$$\beta_{C,\text{IV}} = -8|\Delta| - (4n - 8)|\epsilon||\Delta|,$$
$$\beta_{C,\text{V}} = -4n|\epsilon| - (2n - 8)|\epsilon||\Delta|,$$
$$\beta_{C,\text{VI}} = -4 - (4n - 4)|\epsilon| - (2n - 4)|\epsilon||\Delta|,$$
$$\beta_{C,\text{VII}} = -4|\Delta| - (4n - 8)|\epsilon| - 2n|\epsilon||\Delta|,$$
$$\beta_{C,\text{VIII}} = -8|\epsilon| - 4|\Delta| - (4n - 8)|\epsilon||\Delta|, \quad (87)$$

whereas if $n \equiv 0 \mod 4$, the classical bound simplifies to

$$\beta_{C,\text{I}} = -n(4 + 2|\Delta|),$$
$$\beta_{C,\text{II}} = -4n|\Delta|,$$
$$\beta_{C,\text{III}} = \beta_{C,\text{V}} = \beta_{C,\text{VI}} = \beta_{C,\text{VII}} = -n|\epsilon|(4 + 2|\Delta|),$$
$$\beta_{C,\text{IV}} = \beta_{C,\text{VIII}} = -4n|\epsilon||\Delta|. \quad (88)$$

Using the A_k measurements on the even sites and the B_l ones on the odd sites, this yields the following XXZ-type Hamiltonian:

$$\mathcal{H} = \sum_{i=0}^{n-1} \tilde{f}_i(\epsilon)(\sigma_x^{(i)}\sigma_x^{(i+1)} + \sigma_y^{(i)}\sigma_y^{(i+1)} + \Delta\sigma_z^{(i)}\sigma_z^{(i+1)}), \quad (89)$$

where $\tilde{f}_i(\epsilon) = 4[1 + (-1)^i\epsilon]/\sqrt{3}$. The ground state of Eq. (89) does not have an analytically closed form and has to be computed using DMRG. To do so, we use the ITensor library [30]. The results are plotted in Fig. 8, where

we observe quantum violations in a parameter region that does not seem to vanish as n grows. We also observe a different behavior depending on the parity of $n/2$, which we attribute to some sort of frustration arising in the classical optimization, especially for low values of n.

VI. CONCLUSIONS AND OUTLOOK

In this work, we show, on the one hand, that the ground states of some spin Hamiltonians are nonlocal. We associate a Bell inequality to the Hamiltonian and we compute its classical bound. We exactly diagonalize the Hamiltonian and we compute the quantum value of the corresponding Bell inequality. We achieve this goal by combining two rather unexplored techniques in quantum information, which are dynamic programing and the Jordan-Wigner transformation. This allows us to detect the presence of nonlocal correlations. On the other hand, these tools provide us with a new way to determine the classical bound of certain classes of Bell inequalities, and look for their quantum violation under conveniently chosen observables. In the case of two dichotomic measurements, the optimization also yields the quantum bound (the maximal quantum violation) of the inequality. In the TI case, we provide an algorithm to find the classical bound that is exponentially faster in the system size and we obtain exact analytical solutions for the quantum value. Then, we apply these techniques to several examples in which we reveal nonlocality: a tight TI Bell inequality with a TI Bell operator for eight parties, a quasi-TI Bell inequality with a uniparametric quasi-TI XY Hamiltonian, and the ground state of a XY spin glass in some parameter region. We also see that, for interacting models such as XXZ-like spin Hamiltonians, our method can be applied. There, we find the ground state energy numerically and we map the Hamiltonian to a modified version of Gisin's elegant Bell inequality. These findings open the possibility to the implementation of multipartite quantum information protocols that use nonlocality as a key resource, by using ground states of Hamiltonians that appear naturally.

We remark that the Hamiltonians and the Bell inequalities we study have a finite interaction range, which in the TI case makes them particularly interesting from an experimentally friendly perspective. Note that previous Bell inequalities for quantum many-body systems with low-order correlators were specially designed for a permutationally invariant (PI) symmetry [25,26]; while being able to detect nonlocality in ground states of physical Hamiltonians, such as the Lipkin-Meshkov-Glick [43] or a spin-squeezed Bose-Einstein condensate [27], the information accessible to these inequalities is bound to a de Finetti theorem [44,45], thus becoming more compatible with that produced by a separable state as the system grows [26]. This requires to increase the number of measurements with the system size in order to close the finite-statistics loophole [27]. However, many systems of interest are not

PI, but TI, and we study the latter in this work. In this case, a de Finetti restriction does not apply, making the detection of nonlocality more robust to experimental imperfections. Interestingly, to study the Bell inequalities proposed in Refs. [25,26], in the classical and quantum many-body regime, one employs powerful mathematical tools (namely, convex hulls of semialgebraic sets [46] or the Schur-Weyl duality from representation theory [47], respectively), which no longer apply when the PI symmetry is broken. Here, we use other mathematical tools (dynamic programing for the classical bound and the JW transformation for the quantum value) that allow us to solve, even exactly, the two cases with this much weaker symmetry.

Let us finalize by pointing out possible future research directions that stem from our work. Throughout this paper, we restrict ourselves to the study of nonlocality in one-dimensional spin short-ranged Hamiltonians, as we can compute their ground state energy with exact diagonalization. One can eliminate this restriction and study short-ranged spin Hamiltonians by using a matrix product state description of the state, which is a good ansatz for these systems [48]. The Bell inequalities that we would naturally associate to them would still be of the form of Eq. (8), because the interaction range R would be fixed, so we could still efficiently find their classical bound. Conversely, we can eliminate the restriction on the subset of observables that we choose in Sec. III and the string of σ_z's in the middle of the string operators, thus studying purely two-body correlator inequalities like the classes derived in Ref. [38]. In such cases, powerful numerical algorithms such as DMRG [49] would be suitably tailored to perform the quantum optimization and check whether nonlocality is detected. Another interesting problem is related to the persistency of nonlocality [50]. While the tools to carry this kind of analysis in the PI case have been put forward [26], in the case of one spatial dimension, we do not know yet how robust the inequalities we present are to particle losses. One could also generalize our results towards other directions. Since Bell inequalities with more than two inputs or outputs per party are not, in general, maximally violated by measuring qubits [51], if one would like to increase the chance to detect nonlocality with these more general classes of Bell inequalities, increasing the physical dimension of the system would be a way to obtain better results. The tools we present here could be extended by using a generalized JW transformation [52] from qudits to parafermions, although the problem becomes algebraically more involved.

We also see through the examples we present that there is a strong relation between Hamiltonians of physical systems and Bell inequalities that we associate to them. Whereas we naturally establish this connection in the following direction, starting from the Hamiltonian of a physical system, we assign a Bell inequality to it, one can think of this relation in a more general way, since there are many Bell inequalities

that, with the appropriate observables, realize the same physical Hamiltonian. Moreover, in Sec. V D, we see that this correspondence can be nontrivial, as the inequality does not even have the same number of measurements at every site. With the tools we present here, it is now possible that, given a physical one-dimensional Hamiltonian with short-range interactions, we can tailor the best Bell inequality that reveals the nonlocality of its ground state, as such a Hamiltonian corresponds to the realization of a Bell operator of many different Bell inequalities, each with its own classical bound, which we can compute efficiently.

ACKNOWLEDGMENTS

APPENDIX A: PARITY OPERATOR

Here, we prove Eq. (31). Let $O \in \mathcal{O}(2n)$ be an orthogonal transformation relating the sets of Majorana fermions $\{\hat{c}_{i,\alpha}\}$ and $\{\hat{d}_{k,a}\}$, as in Eq. (23). Recall that the Cartan-Dieudonné theorem [53] states that every orthogonal transformation $O \in \mathcal{O}(2n)$ decomposes as a product of a number of reflections (at most, $2n$). Hence, it suffices to show that a reflection flips the parity operator; i.e., our aim is to show that

$$\prod_{i=0}^{n-1} \mathbb{i}\hat{c}_{i,0}\hat{c}_{i,1} = -\prod_{i=0}^{n-1} \mathbb{i}\hat{d}_{i,0}\hat{d}_{i,1}, \qquad (A1)$$

whenever O is a reflection. Recall that any reflection with respect to a hyperplane with normal vector $\vec{u}$ can be written as $\mathbb{1} - 2\vec{u}\vec{u}^T$. We denote the lhs of Eq. (A1) $\hat{\mathbb{P}}_c$ and the rhs of Eq. (A1) $-\hat{\mathbb{P}}_d$.

The CARs [Eq. (20)] ensure that

$$[\mathbb{i}\hat{c}_{i,0}\hat{c}_{i,1}, \mathbb{i}\hat{c}_{j,0}\hat{c}_{j,1}] = [\mathbb{i}\hat{d}_{k,0}\hat{d}_{k,1}, \mathbb{i}\hat{d}_{l,0}\hat{d}_{l,1}] = 0 \quad (A2)$$

and

$$(\mathbb{i}\hat{c}_{i,0}\hat{c}_{i,1})^2 = (\mathbb{i}\hat{d}_{k,0}\hat{d}_{k,1})^2 = \hat{\mathbb{1}}. \qquad (A3)$$

Hence, the operators $\{\mathbb{i}\hat{c}_{i,0}\hat{c}_{i,1}\}$ and $\{\mathbb{i}\hat{d}_{k,0}\hat{d}_{k,1}\}$, respectively, share an eigenbasis and split the Fock space into even and odd subspaces with respect to the parity operator $\hat{\mathbb{P}}$ defined in Eq. (27).

We prove in Theorem 1 that this partition of the Fock space does not change under orthogonal transformations. Moreover, if $\det O = -1$, the subspaces are just swapped. Theorem 1 is supported on Lemma 2, which proves that reflections swap the eigenspaces, and Lemma 1 contains the technical steps to prove Lemma 2. Hence, Eq. (A1) follows and, because every orthogonal transformation is a product of a number of reflections, we obtain Eq. (31).

Lemma 1.—Consider a reflection $O = \mathbb{1} - \vec{u}\vec{u}^T$, where $\vec{u}$ is a normalized vector. Let us define the following quantities:

$$S_0 := u_{k,0}\sum_{i,\alpha}u_{i,\alpha}\hat{c}_{i,\alpha}\hat{c}_{k,1},$$

$$S_1 := u_{k,1}\sum_{i,\alpha}u_{i,\alpha}\hat{c}_{k,0}\hat{c}_{i,\alpha},$$

$$S_{01} := u_{k,0}u_{k,1}\sum_{i,\alpha,j,\beta}u_{i,\alpha}u_{j,\beta}\hat{c}_{i,\alpha}\hat{c}_{j,\beta}. \qquad (A4)$$

Then, the identities

$$S_{01} = u_{k,0}u_{k,1}\mathbb{1} \qquad (A5)$$

and

$$\mathbb{i}\sum_{k=0}^{n-1}(S_0 + S_1)|\Omega\rangle = |\Omega\rangle + 2\mathbb{i}\sum_{k=0}^{n-1}u_{k,0}u_{k,1}|\Omega\rangle. \qquad (A6)$$

hold.

Proof.—To prove Eq. (A5), we can split the sum into the indices for which $(i,\alpha) = (j,\beta)$ and the indices for which $(i,\alpha) \neq (j,\beta)$.

In the first case, since the CARs Eq. (20) imply that $(\hat{c}_{i,\alpha})^2 = \mathbb{1}$, we have a term $u_{k,0}u_{k,1}\sum_{i,\alpha}u_{i,\alpha}^2(\hat{c}_{i,\alpha})^2$ that contributes $u_{k,0}u_{k,1}\mathbb{1}$, because $\vec{u}$ is normalized.

In the second case, we note that we can rewrite the sum as

$$u_{k,0}u_{k,1}\sum_{(i,\alpha)<(j,\beta)}u_{i,\alpha}u_{j,\beta}\{\hat{c}_{i,\alpha},\hat{c}_{j,\beta}\} = 0, \qquad (A7)$$

because of the CARs Eq. (20).

In order to prove Eq. (A6), we begin by noting that

$$\hat{c}_{i,\alpha}\hat{c}_{k,\beta}|\Omega\rangle = \begin{cases} \mathbb{i}^{\alpha+\beta}(-1)^{\beta}|\Omega\rangle & \text{if } i = k \\ \mathbb{i}^{\alpha+\beta}(-1)^{\alpha+\beta}\hat{a}_i^{\dagger}\hat{a}_k^{\dagger}|\Omega\rangle & \text{if } i \neq k. \end{cases} \qquad (A8)$$

We can now split the sum Eq. (A6) into the parts where $i = k$ and $i \neq k$.

For the first part, we have a contribution in Eq. (A6) that amounts to

$$\mathfrak{i}\sum_{k=0}^{n-1}[(u_{k,0}^2 + u_{k,1}^2)\hat{c}_{k,0}\hat{c}_{k,1} + 2u_{k,0}u_{k,1}\mathbb{1}]|\Omega\rangle,$$

which, using Eq. (A8), simplifies to

$$|\Omega\rangle + 2\mathfrak{i}\sum_{k=0}^{n-1}u_{k,0}u_{k,1}|\Omega\rangle. \qquad (A9)$$

For the second part, the contribution to Eq. (A6) is

$$\mathfrak{i}\sum_{i\neq k}\sum_{\alpha}[u_{k,0}u_{i,\alpha}\mathfrak{i}^{\alpha+1}(-1)^{\alpha+1} - u_{k,1}u_{i,\alpha}\mathfrak{i}^{\alpha}(-1)^{\alpha}]\hat{a}_i^\dagger\hat{a}_k^\dagger|\Omega\rangle;$$

expanding the sum over α, we have

$$\sum_{i\neq k}[(u_{k,0}u_{i,0} - u_{k,1}u_{i,1}) - \mathfrak{i}(u_{k,1}u_{i,0} + u_{k,0}u_{i,1})]\hat{a}_i^\dagger\hat{a}_k^\dagger|\Omega\rangle.$$

Splitting the sum between those indices for which $i < k$ and those for which $i > k$, we have that it can be rewritten into an expression involving the CARs (17):

$$\sum_{i<k}[(u_{k,0}u_{i,0} - u_{k,1}u_{i,1}) - \mathfrak{i}(u_{k,1}u_{i,0} + u_{k,0}u_{i,1})]\{a_i^\dagger, a_k^\dagger\}|\Omega\rangle.$$

Because $\{a_i^\dagger, a_k^\dagger\} = 0$, this last expression is zero ∎

Lemma 2.—Let O be a reflection. Then,

$$\sum_{k=0}^{n-1}\frac{\mathfrak{i}\hat{d}_{k,0}\hat{d}_{k,1} + \mathbb{1}}{2}|\Omega\rangle = \left(\sum_{k=0}^{n-1}\frac{\mathfrak{i}\hat{c}_{k,0}\hat{c}_{k,1} + \mathbb{1}}{2} - \mathbb{1}\right)|\Omega\rangle. \qquad (A10)$$

Proof.—By hypothesis, $O_{i,\alpha;j,\beta} = \delta_{i,j}\delta_{\alpha,\beta} - 2u_{i,\alpha}u_{j,\beta}$, where δ is the Kronecker delta function. Let us now see how the operator $\sum_{k=0}^{n-1}\mathfrak{i}\hat{d}_{k,0}\hat{d}_{k,1}$ relates to the $\{\hat{c}_{i,\alpha}\}$ Majorana fermions.

By definition [cf. Eq. (23)], we can write

$$\mathfrak{i}\hat{d}_{k,0}\hat{d}_{k,1} = \mathfrak{i}\hat{c}_{k,0}\hat{c}_{k,1} - 2\mathfrak{i}(S_0 + S_1) + 4\mathfrak{i}S_{01}.$$

Lemma 1 allows us to conclude

$$\sum_{k=0}^{n-1}\mathfrak{i}\hat{d}_{k,0}\hat{d}_{k,1}|\Omega\rangle = \sum_{k=0}^{n-1}\mathfrak{i}\hat{c}_{k,0}\hat{c}_{k,1}|\Omega\rangle - 2|\Omega\rangle, \qquad (A11)$$

showing that a reflection flips the parity of the vacuum: The occupation number operator, in terms of the $\{\hat{d}_{k,a}\}$ operators has opposite parity than the occupation number operator in terms of the $\{\hat{c}_{i,\alpha}\}$ operators:

$$\sum_{k=0}^{n-1}\frac{\mathfrak{i}\hat{d}_{k,0}\hat{d}_{k,1} + \mathbb{1}}{2}|\Omega\rangle = \left(\sum_{k=0}^{n-1}\frac{\mathfrak{i}\hat{c}_{k,0}\hat{c}_{k,1} + \mathbb{1}}{2} - \mathbb{1}\right)|\Omega\rangle. \qquad (A12)$$

∎

Theorem 1.—Let $O \in \mathcal{O}(2n)$. Let $\mathcal{F}$ be the Fock space of n Dirac fermions. The operator $\hat{\mathbb{P}}_c$ splits $\mathcal{F}$ into even and odd subspaces: $\mathcal{F} = \mathcal{F}_e \oplus \mathcal{F}_o$. Similarly, $\hat{\mathbb{P}}_d$ splits $\mathcal{F}$ as $\mathcal{F} = \mathcal{F}_e' \oplus \mathcal{F}_o'$. Then, either $\mathcal{F}_e = \mathcal{F}_e'$ (if $\det O = 1$) or $\mathcal{F}_e = \mathcal{F}_o'$ (if $\det O = -1$).

Proof.—Recall that the expectation value of the operator $\hat{a}_i^\dagger\hat{a}_i$ is the occupation number of the ith mode, denoted n_i. Then, a basis of the Fock space of n fermionic Dirac modes can be defined as

$$|\mathbf{N}\rangle := |n_0, \ldots, n_{n-1}\rangle := \prod_{k=0}^{n-1}(\hat{a}_k^\dagger)^{n_k}|\Omega\rangle, \qquad (A13)$$

where the product is written from left to right. Note that n_k can only be 0 or 1, due to Eq. (17). The CARs Eq. (17) further imply that $\hat{a}_i|\mathbf{N}\rangle = (-1)^{\sum_{j=0}^{i-1}n_j}|\mathbf{N}'\rangle$ whenever $n_i = 1$ ($\mathbf{N}'$ and $\mathbf{N}$ differ only in its ith index) and $\hat{a}_i|\mathbf{N}\rangle = 0$ whenever $n_i = 0$.

Let $|\psi\rangle$ be an eigenvector of $\hat{\mathbb{P}}_c$ of eigenvalue 1. We can assume, without loss of generality, that $|\psi\rangle$ is a basis element $|\mathbf{N}\rangle$ of the Fock space, with $\sum_{i=0}^{n-1}n_i \equiv 0$ mod 2. By noting that $\mathfrak{i}\hat{d}_{k,0}\hat{d}_{k,1}$ can be expressed as

$$\mathfrak{i}\sum_{i,\alpha,j,\beta}\mathfrak{i}^{\alpha+\beta}O_{i,\alpha;k,0}O_{j,\beta;k,1}[\hat{a}_i + (-1)^\alpha\hat{a}_i^\dagger)(\hat{a}_j + (-1)^\beta\hat{a}_j^\dagger],$$

we see that the only operators that appear are products of $\hat{a}_i$ or $\hat{a}_i^\dagger$ with $\hat{a}_j$ or $\hat{a}_j^\dagger$. Hence, they either annihilate $|\mathbf{N}\rangle$ or they add -2, 0, or 2 to its particle number, always conserving its parity. This leaves us with a linear combination of vectors that live in the same subspace $\mathcal{F}_e$, so it remains on $\mathcal{F}_e$. The same argument applies to $\mathcal{F}_o$.

Hence, the subspaces $\mathcal{F}_e$ and $\mathcal{F}_o$ of the operator $\hat{\mathbb{P}}_c$ are invariant under orthogonal transformations of the Majorana fermions. However, under $\hat{\mathbb{P}}_d$, they might change its parity. Because of linearity and Eq. (A13), it suffices to prove that $|\Omega\rangle$ is an eigenstate of $\hat{\mathbb{P}}_d$, as it stems from Lemma 2. If its eigenvalue is 1, then $\mathcal{F}_e = \mathcal{F}_e'$; if it is -1, then $\mathcal{F}_e = \mathcal{F}_o'$. ∎

APPENDIX B: PBC TO OBC REDUCTION

Here, we describe the reduction of the optimization problem of finding the classical bound in a Bell inequality with PBC to the optimization problem of finding the classical bound for a Bell inequality with OBC in one dimension.
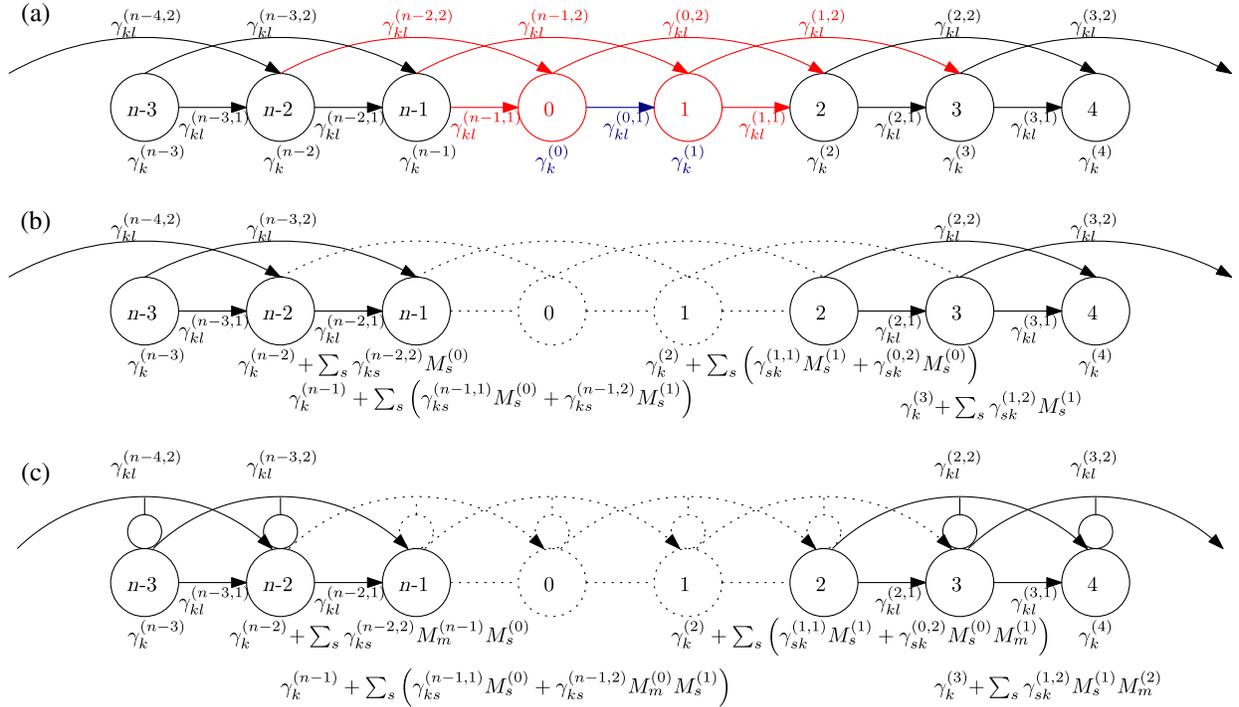
FIG. 9.   In (a), we have a two-body Bell inequality with $R = 2$ and PBC. The coefficients below the circles correspond to the weights of the one-body correlators associated to those parties, and the coefficients next to the arrows correspond to the weights of the correlators between the parties they join. In (b), we consider the intermediate case in which there are no observables $M_m^{(i)}$ in the middle of the string operators, whereas in (c) we include them [the big circles represent the set of observables labeled from 0 to $m-1$ and the smaller circle represents the mth one [cf. Eq. (7)]. In order to transform it to an OBC case, we choose a deterministic local strategy for the parties labeled by 0 and 1. and we choose a deterministic local strategy for parties labeled by 0 and 1, represented in red in (a). Thus, the values of the one-body correlators from zeroth and first parties have a fixed value, as well as the two-body correlators between them. These are marked in blue. These terms' contribution represents an offset on the classical bound. The two-body correlators starting at $n-2$ and ending at 0 are updated to the one-body terms of the $(n-2)$th party. The correlators starting at $n-1$ and ending either at 0 or 1 are updated to the one-body terms of the $(n-1)$th party. Similarly, we update the one-body terms of parties 2 and 3. These terms are marked in red. The rest of the inequality remains untouched and such terms are marked in black. This process is the transformation from (a) to (b). Note that if the local deterministic strategy chosen in parties 0 and 1 is the optimal one, then the classical bound for the PBC problem is given by the offset generated by parties 0 and 1 (blue) plus the classical bound of the OBC problem between parties 2 and $n-1$. Since there is a finite number of deterministic local strategies that parties 0 and 1 can have, eventually we find the optimal bound for the PBC problem. Finally, in (c) we depict the same procedure, but some more assignments $M_m^{(i)}$ have to be fixed in advance to update the one-body terms accordingly.

For the sake of clarity, we first describe the procedure for inequalities with an arbitrary interaction range R, but without the chain of $M_m^{(j)}$ observables in the middle of the string operators [cf. Eq. (7)], so that the inequalities strictly contain one- or two-body correlators. We pick R consecutive parties. Without loss of generality, we can assume them to be labeled from 0 to $R - 1$. To these parties we assign one of the $d^{m \cdot R}$ possible deterministic local strategies. Let (i, j) be a pair of parties. There are three cases to consider.

(i) If i and j are between 0 and $R - 1$, any correlator between parties i and j now has a definite value.

(ii) If either i or j but not both are between 0 and $R - 1$, only one side of the correlator has a definite value. Because the classical bound is computed on a deterministic local strategy, the value of the correlator factorizes as the product

of the local values assigned by the strategy we are considering. Hence, these correlators can be effectively moved outside of the interval $0, \ldots, R - 1$ by updating the one-body term of the party outside that interval.

(iii) In any other case, the correlator remains the same.

In Figs. 9(a) and 9(b) we illustrate this procedure for an example with $R = 2$. The first case is illustrated in blue, the second is illustrated in red, and the last one is illustrated in black.

Finally, if we have an inequality of the form of Eq. (7), the intermediate $M_m^{(j)}$ terms should also be taken into account when performing this procedure. In order to move to the one-body terms the R-body terms, now an extra number of $M_m^{(j)}$ observables should also be chosen in advance for those parties at distance $R - 1$ to the set $\{0, \ldots, R - 1\}$ (but only the mth observable; it is not

necessary to fix the rest). For instance, in the example of Fig. [9(c)], one would have to specify the value of $M_m^{(n-1)}$ and $M_m^{(2)}$. Observe that if $R > 2$, then in the OBC problem, some of the $M_m^{(j)}$ values closest to the boundary become fixed [$2(R-2)$ of them]. This has to be taken into account when performing the dynamical programing, as one should explore only those configurations compatible with the boundary conditions imposed by the PBC problem with the deterministic local strategy that we have chosen to make the reduction.

APPENDIX C: QUANTUM OPTIMIZATION OF TRANSLATIONALLY INVARIANT BELL INEQUALITIES

Here, we discuss the quantum optimization for the translationally invariant case (i.e., when the Bell inequality is TI and the same set of measurements is performed at each site, thus leading to a TI Bell operator). We begin by observing that there are two cases to consider, depending on the choice of the parity p of the fermion number. If $p = -1$, the matrix H [cf. Eq. [(18)] is block circulant: $H_{i,\alpha;j,\beta} = H_{i+1,\alpha;j+1,\beta}$, where the party indices are taken modulo n. We can then define h_r to be the 2×2 block of H whose entries are given by $(h_r)_{\alpha;\beta} := H_{0,\alpha;r,\beta}$. If $p = 1$, the matrix H is no longer block circulant because the blocks of H that correspond to interactions that cross the origin carry a minus sign (these blocks are located on the R top right diagonals and R bottom left diagonals of H). In this latter case, it is convenient to construct

$$\tilde{H} := |-\rangle\langle-| \otimes H, \tag{C1}$$

where $|-\rangle := (|0\rangle - |1\rangle)/\sqrt{2}$, which is now circulant. Note that half of the spectrum of $\tilde{H}$ is zeros and the other half coincides with the spectrum of H. For instance, for the case of nearest-neighbor interactions ($R = 1$), $n = 3$ parties and $p = 1$, H takes the block form

$$H = \begin{pmatrix} h_0 & h_1 & h_1^T \\ -h_1^T & h_0 & h_1 \\ -h_1 & -h_1^T & h_0 \end{pmatrix}. \tag{C2}$$

It is then clear that $\tilde{H}$ is block circulant.

Circulant matrices can be diagonalized via a discrete Fourier transform (DFT). The DFT matrix is unitary in general, but we want to use an orthogonal transformation instead, so that we can transform Majorana fermions into Majorana fermions and obtain Eq. [(21)]. Let us consider the following real DFT matrix of order n:

$$(\mathcal{R}_n)_{kl} := \sqrt{\frac{2}{n}} \cos\left(\frac{2\pi kl}{n} - \frac{\pi}{4}\right), \qquad 0 \le k, l < n. \tag{C3}$$

It is easy to see that $\mathcal{R}_n = \mathcal{R}_n^T$ and $\mathcal{R}_n^2 = \mathbb{1}$, so $\mathcal{R}_n$ is orthogonal. In the following, we are going to use the fact that for any n, $\det(\mathcal{R}_n \otimes \mathbb{1}_2) = (\det \mathcal{R}_n)^2 = 1$.

Let us now, with the aid of the orthogonal transformation $\mathcal{R}_n$, study which invariant subspaces H acts upon. If $p = -1$, then we compute $(\mathcal{R}_n \otimes \mathbb{1}_2)H(\mathcal{R}_n \otimes \mathbb{1}_2)$; if $p = 1$, then we calculate $(\mathcal{R}_{2n} \otimes \mathbb{1}_2)\tilde{H}(\mathcal{R}_{2n} \otimes \mathbb{1}_2)$. Note that $\mathbb{1}_2$ acts on the two Majorana modes associated to one site.

On the one hand, if $p = -1$, a direct calculation of $H' := (\mathcal{R}_n \otimes \mathbb{1}_2)H(\mathcal{R}_n \otimes \mathbb{1}_2)$ shows that

$$H' = \left(\bigoplus_{k=1}^{\lfloor(n-1)/2\rfloor} J_k\right) \oplus \left[\sum_{q=0}^{n-1} h_q\right] \oplus \left[\sum_{q=0}^{n-1}(-1)^q h_q\right], \tag{C4}$$

where the last subspace appears only if n is even and each J_k is a 4×4 block defined as

$$J_k := \sum_{q=0}^{n-1} \begin{pmatrix} \cos(2\pi kq/n) & -\sin(2\pi kq/n) \\ \sin(2\pi kq/n) & \cos(2\pi kq/n) \end{pmatrix} \otimes h_q. \tag{C5}$$

On the other hand, if $p = 1$, one similarly proves that $H'' := (\mathcal{R}_{2n} \otimes \mathbb{1}_2)\tilde{H}(\mathcal{R}_{2n} \otimes \mathbb{1}_2)$:

$$H'' = \left(\bigoplus_{k=1}^{\lfloor n/2\rfloor} J_k'\right) \oplus \left[\sum_{q=0}^{n-1}(-1)^q h_q\right], \tag{C6}$$

where the last subspace appears only if n is odd, and each J_k' is a 4×4 block defined as

$$J_k' := \sum_{q=0}^{n-1} \begin{pmatrix} \cos\left(\pi q \frac{2k-1}{n}\right) & -\sin\left(\pi q \frac{2k-1}{n}\right) \\ \sin\left(\pi q \frac{2k-1}{n}\right) & \cos\left(\pi q \frac{2k-1}{n}\right) \end{pmatrix} \otimes h_q. \tag{C7}$$

We can further simplify these expressions by noting that $H = -H^T$ is blockwise equivalent to $h_q = -h_{n-q}^T$. This implies that the 2×2 blocks in Eqs. [(C4)] and [(C6)] are already brought to the Williamson form:

$$\sum_{q=0}^{n-1} h_q = \sum_{q=0}^{n-1} \begin{pmatrix} 0 & (h_q)_{0;1} \\ -(h_q)_{0;1} & 0 \end{pmatrix} \tag{C8}$$

and

$$\sum_{q=0}^{n-1}(-1)^q h_q = \sum_{q=0}^{n-1}(-1)^q \begin{pmatrix} 0 & (h_q)_{0;1} \\ -(h_q)_{0;1} & 0 \end{pmatrix}. \tag{C9}$$

We then define the quantity

$$\varepsilon_{0,\pm} = \sum_{q=0}^{n-1}(\pm 1)^q (h_q)_{0;1}, \tag{C10}$$

which corresponds to the Williamson eigenvalue(s) for the 2×2 blocks.

To bring H to a Williamson form, it remains to bring the 4×4 blocks J_k and J'_k to a Williamson form. To this end, let us start by defining $v_{k,q} := q\pi[2k - (p+1)/2]/n$ and

$$x_k := \sum_{q=0}^{n-1} \cos(v_{k,q})(h_q)_{0;1}, \qquad (C11)$$

$$a_k := -\sum_{q=0}^{n-1} \sin(v_{k,q})(h_q)_{0;0}, \qquad (C12)$$

$$b_k := -\sum_{q=0}^{n-1} \sin(v_{k,q})(h_q)_{0;1}, \qquad (C13)$$

$$c_k := -\sum_{q=0}^{n-1} \sin(v_{k,q})(h_q)_{1;1}. \qquad (C14)$$

Let us note that the blocks J_k (or J'_k) take the following form:

$$\begin{pmatrix} 0 & x & a & b \\ -x & 0 & b & c \\ -a & -b & 0 & x \\ -b & -c & -x & 0 \end{pmatrix}_k. \qquad (C15)$$

Now we are ready to find an orthogonal transformation that brings J_k or J'_k to a Williamson form, which we state in the following lemma.

Lemma 3.—For every J_k (or J'_k) of the form Eq. (C15), there exists an orthogonal transformation O_k that brings it to a Williamson form:

$$O_k^T J_k O_k = \begin{pmatrix} 0 & \varepsilon_{k,+} & 0 & 0 \\ -\varepsilon_{k,+} & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_{k,-} \\ 0 & 0 & -\varepsilon_{k,-} & 0 \end{pmatrix}. \qquad (C16)$$

Its two Williamson eigenvalues $\varepsilon_{k,\pm}$ are given by

$$\varepsilon_{k,\pm} = a_k + c_k \pm \sqrt{\Delta_k}, \qquad (C17)$$

where $\Delta_k := (a_k - c_k)^2 + 4(b_k^2 + x_k^2)$ and k ranges from 1 to $\lfloor n/2 + (p-1)/4 \rfloor$. Furthermore, this orthogonal transformation always satisfies $\det O_k = -1$.

Proof.—The choice of O_k is not unique in general. Here, we construct O_k as the product of three matrices. Since k is fixed, we skip explicitly stating the subindex throughout the proof. We construct O as $O := LMR$, where L and R are diagonal matrices whose entries are defined by

$$L^{-1} = \frac{1}{4}\text{diag}\{a - c - \sqrt{\Delta}, 2, a - c + \sqrt{\Delta}, 2\} \qquad (C18)$$

and

$$R^{-1} = \sqrt{\frac{2}{b^2 + x^2}}\text{diag}\{r_-, r_-, r_+, r_+\}, \qquad (C19)$$

where $r_\pm := \sqrt{\Delta \pm (a - c)\sqrt{\Delta}}$. The matrix M in the middle is not diagonal, and in its most general form can depend on two real parameters, which we denote ϕ and θ. We have that the entries of M are given by

$$\begin{pmatrix} f_{b,-x}(\phi)g_+ & f_{-x,b}(\phi)g_+ & f_{-b,x}(\theta) & f_{x,b}(\theta) \\ \cos\phi & -\sin\phi & \cos\theta & -\sin\theta \\ -f_{x,b}(\phi) & f_{-b,x}(\phi) & f_{x,b}(\theta)g_- & f_{b,-x}(\theta)g_- \\ \sin\phi & \cos\phi & \sin\theta & \cos\theta \end{pmatrix}, \qquad (C20)$$

where

$$f_{y,z}(\alpha) := y\cos\alpha + z\sin\alpha$$

and

$$g_\pm := (c - a \pm \sqrt{\Delta})^2/4(b^2 + x^2).$$

We can now show that O is indeed an orthogonal transformation with determinant -1, since $\det L = -16/(b^2 + x^2)$, $\det R = (b^2 + x^2)/16\Delta$, and the determinant of M is independent of both φ and θ, and it is $\det M = \Delta$. The multiplication of these three terms gives the result $\det O = -1$. Hence, one can pick convenient values for ϕ and θ in order to show that $O^T J O$ already has a Williamson form Eq. (C16) simply by matrix multiplication. ∎

Tracking all the transformations we have made, i.e., counting the parity flips imposed by the choice of all the orthogonal transformations we have made, the superselection rule Eq. (30) that must be obeyed takes the form of Eq. (52).

If, in addition, we impose a finite interaction range R, then we can further simplify the expressions for x_k, a_k, b_k, and c_k thanks to the property $h_r = -h_{n-r}^T$ and arrive at Eqs. (47), (48), (49), (50).

APPENDIX D: TIGHT TRANSLATIONALLY INVARIANT INEQUALITIES

Here, we provide a list of tight optimal TI Bell inequalities Eq. (53) for $R = 2$ that are violated when performing the same set of measurements on each party, which are of the form

TABLE I. Number of tight Bell inequalities (facets) and number of extremal points (vertices) of the local polytope projected onto the space of TI, n party, up to R-range correlators [cf. Eq. (53)].

n	Number of facets	Number of vertices
3	166	72
4	5628	204
5	46 804	1148
6	20 268	1816
7	175 444	6064
8	29 290	4044

$$\mathcal{M}_0 = \cos\varphi\sigma_x + \sin\varphi\sigma_y,$$
$$\mathcal{M}_1 = \cos\theta\sigma_x + \sin\theta\sigma_y,$$
$$\mathcal{M}_2 = \sigma_z.$$

Note that, since

$$\text{Tr}(\mathcal{B}\rho) = \text{Tr}[(\mathcal{U}\mathcal{B}\mathcal{U}^\dagger)(\mathcal{U}\rho\mathcal{U}^\dagger)], \qquad (\text{D1})$$

where $\mathcal{U}$ is a unitary transformation of the form $U^{\otimes n}$, the maximal quantum violation of a TI Bell inequality with the above measurements depends only on $\theta - \varphi$, as there always exists a unitary U that brings $\mathcal{M}_0$ to σ_x by performing a rotation in the $x - y$ plane [26]. Hence, there is no loss of generality in assuming $\varphi = 0$.

For $n \leq 8$, it is still computationally feasible to find all the facets of the polytope of local correlations projected onto the space of the correlators appearing in Eq. (53). To achieve this goal, we construct all the vertices of the local polytope of correlations for n parties, three measurements, and two outcomes, which are 2^{3n} in total, and we project them to the space of translationally invariant correlators that

appear in Eq. (53), following the same procedure of Ref. [38]. With linear programing, we can remove all the projected vertices that are a convex combination of other projected vertices. Then, we can use an algorithm such as CDD [54] to compute the convex hull of the extremal projected vertices and obtain a minimal description of it in terms of facets. We call these facets *tight* Bell inequalities. We summarize these findings in Table I.

Following the same procedure as in Sec. V A, we find the inequalities that are violated, which we classify in Table II.

Note that, by renaming the outcomes of the measurements, the labels of the measurements, or the labels of the parties, one can obtain other inequalities that are not listed in Table II; however, these relabelings do not change the properties we are interested in, such as the classical bound or its quantum violation, so we consider them to be equivalent and we include only one representative for each equivalence class.

From the values of Table II, we see that QV/β_C approaches zero as n grows. Similar to what was found in Ref. [38], numerics suggest that, for translationally invariant Bell inequalities, there is a trade-off between n and R. In Ref. [38], the maximal n for $R = 1$ was 5, whereas here for $R = 2$ we did not find any violation beyond $n = 8$. Furthermore, for $n = 6$, 7 there are no translationally invariant Bell inequalities of the form Eq. (53) that are violated by performing the same qubit measurements at each site. One may still perform different qubit measurements on each site and be able to maximally violate the inequality, as it was proven in Ref. [37]; however, to achieve the same violation with the same set of measurements at each site, one may then need to increase the dimension of the state and use positive-operator valued measures [38].

TABLE II. Classes of inequalities of the form of Eq. (53) that are violated for different n with the same set of measurements at each site. We present one representative per class; the rest can be found by applying a suitable symmetry such as a renaming of the measurements, outcomes, and/or parties [38]. The γ's constitute the coefficients of the Bell inequality, β_C is the classical bound, QV is the quantum violation achieved with the measurement settings defined through φ_0 and φ_1. Note that due to Eq. (D1), this depends only on $\varphi_1 - \varphi_0$ (recall that the measurement settings we use parametrize the quantum observables as $\mathcal{M}_k^{(i)} = \cos\varphi_k^{(i)}\sigma_x^{(i)} + \sin\varphi_k^{(i)}\sigma_y^{(i)}$, and we omit the index i because we are in the TI case).

n	γ	γ_{00}	γ_{01}	γ_{10}	γ_{11}	γ_{020}	γ_{021}	γ_{120}	γ_{121}	β_C	QV	$\varphi_1 - \varphi_0$
3	-2	1	-1	1	1	-1	-1	1	-1	6	-2.9282032303	$\pi/2$
3	0	1	-1	3	-3	1	1	1	1	12	-2.5830052443	$\pi/2$
3	2	-1	1	1	1	-1	1	1	1	6	-2.5830052443	$\pi/2$
4	0	0	0	0	0	1	-2	0	-1	8	-3.313708499	$\pi/2$
4	-2	4	2	2	0	5	-3	1	-1	32	-0.5471047512	0.3254696365π
4	0	2	2	2	2	5	-5	1	-1	32	-0.5115214246	$\pi/2$
4	-1	2	5	5	6	-2	-10	2	11	72	-0.4999666746	0.3188572387π
4	-1	-2	-3	-3	-4	-7	7	-1	2	48	-0.4670552431	0.278787455π
4	2	0	-2	-2	-4	3	1	-3	-3	32	-0.218521874	0.2029607403π
5	0	1	1	-1	-1	1	-1	1	-1	12	-0.3107341487	$\pi/2$
8	0	2	-2	2	-2	-1	-1	1	1	32	-0.2187	$\pi/2$

Interestingly, we also note that the highest ratio QV/β_C is obtained for $n = 3$. This is not surprising, as for $n = 3$ our inequalities contain full-body correlators (see Table II). However, for $n = 4$, the first class achieves a much higher violation than the others. This is because the inequality consists of a sum of CHSH-like inequalities between parties 0 and 2 and between parties 1 and 3:

$$I = \sum_{i=0}^{3} M^{(i,2)}_{(0,2,0)} - 2M^{(i,2)}_{(0,2,1)} - M^{(i,2)}_{(1,2,1)}. \quad \text{(D2)}$$

The minimum over quantum values that can be achieved is $\beta_Q = -4(2\sqrt{2})$, so that $|\beta_Q|/\beta_C = \sqrt{2}$. This inequality can be generalized to any even number of parties at the price of increasing the interaction range R. By picking $R = n/2$ one can always pair party k with party $k + R$ into a CHSH-like link while maintaining $|\beta_Q|/\beta_C = \sqrt{2}$ for any even n. However, let us remark that for the scope of this work, we are interested in studying the nonlocality of ground states of local Hamiltonians (i.e., with a fixed R).

APPENDIX E: ORTHOGONAL TRANSFORMATION FOR MAJORANA FERMIONS

We consider an antisymmetric matrix H of size $2n$. If we want to decompose it as $H = OJO^T$, where O is a $2n \times 2n$ orthogonal matrix and J has the form Eq. (21), we can, in the majority of situations, use the spectral theorem to find O: The matrix H^2 is symmetric, so it diagonalizes as $H^2 = ODO^T$, with D a diagonal matrix with entries $-\varepsilon_k^2$, appearing with multiplicity 2 for each k, and the columns of O forming an orthonormal basis. If all the ε_k are different, then one can safely conclude that $H = OJO^T$, because if H is antisymmetric, then J has to be of the form Eq. (46). Hence, one can say that O is unique (up to permutations that determine the order and the signs of ε_k).

However, if ε_k has a multiplicity greater than 1, this need no longer be the case, as the O found via the spectral theorem is no longer unique (one can perform an arbitrary orthogonal transformation in each eigenspace). Note that this pathologic case is of interest to our problem, as for tight Bell inequalities with the optimal set of measurements, it is common to find ε_k's with the same value (for instance, in the example in Sec. VA). There are two ways to circumvent this problem. One way is to add some noise to H such that all the ε_k's can be considered different; however, we lose precision in the solution and add numerical instability. We describe the other way below.

Let ε be a nonzero Williamson eigenvalue of H with multiplicity m. Then, $O^T H O$ has a $2m \times 2m$ block, denoted J_ε, that satisfies

$$J_\varepsilon^2 = -\varepsilon^2 \mathbb{1}_{2m}. \quad \text{(E1)}$$

Thus, any orthogonal transformation acting on J_ε leaves J_ε^2 invariant, but not necessarily J_ε in the form Eq. (21). Let $|e_1\rangle$ be a unit vector in the J_ε eigenspace (picked from the corresponding columns of O) and let $|e_2\rangle := J_\varepsilon |e_1\rangle/\varepsilon$ be another unit vector. Then, we observe that $|e_1\rangle = -J_\varepsilon |e_2\rangle/\varepsilon$ because of Eq. (E1). Now, by picking another unit vector $|e_3\rangle$ from $\mathbb{1}_{2m} - |e_1\rangle\langle e_1| - |e_2\rangle\langle e_2|$, we find $|e_4\rangle$ with the same procedure. We repeat this process m times. By multiplying O by the orthogonal transformation given by the vectors $|e_1\rangle, |e_2\rangle, …, |e_{2m}\rangle$, we obtain the right transformation bringing H to the form Eq. (21).

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