Contextuality in infinite one-dimensional translation-invariant local Hamiltonians

Kaiyan Yang1,2, Xiao Zeng1,3, Yujing Luo1, Guowu Yang3, Lan Shu2, Miguel Navascués4 and Zizhu Wang1,*

In recent years there has been a growing interest in treating many-body systems as Bell scenarios, where lattice sites play the role of distant parties and only near-neighbor statistics are accessible. We investigate contextuality arising from three Bell scenarios in infinite, translation-invariant 1D models: nearest-neighbor with two dichotomic observables per site; nearest- and next-to-nearest neighbor with two dichotomic observables per site, and nearest-neighbor with three dichotomic observables per site. For the first scenario, we give strong evidence that it cannot exhibit contextuality, not even in non-signaling physical theories beyond quantum mechanics. For the second one, we identify several low-dimensional models that reach the ultimate quantum limits, paving the way for self-testing ground states of quantum many-body systems. For the last scenario, which generalizes the Heisenberg model, we give strong evidence that, in order to exhibit contextuality, the dimension of the local quantum system must be at least 3.

npj Quantum Information (2022) 8:89; https://doi.org/10.1038/s41534-022-00598-0

INTRODUCTION

In a many-body quantum system, correlations appear as one of the most common manifestations of the quantum nature of the system Fig. 1. Different types of correlations, such as entanglement, EPR steering, and nonlocality, were identified over the years and found applications in various quantum information processing tasks. Out of these types of correlations, nonlocality is the strongest and most difficult to test1,2. While experiments exploiting entanglement to teleport photons date back to the 1990s3, nonlocality passed the most stringent experimental tests only in 2015–2016. One of the key assumptions in any nonlocality experiment is keeping the different parties space-like separated. In a many-body quantum system, however, this assumption may be too formidable to be overcome.

In recent years, the exploration of contextuality in quantum many-body systems has been a fruitful endeavor. Contextuality witnesses adapted from Bell inequalities have been tested in Bose–Einstein condensates7,8. Translation and permutation symmetry allowed the full characterization of contextuality witnesses in many-body systems through bipartite correlators only5–6. One of the key assumptions in any nonlocality experiment is keeping the different parties space-like separated. In a many-body quantum system, however, this assumption may be too formidable to be overcome.

In this work, building on earlier characterizations of classical local behavior in many-body systems9, we investigate under which conditions the n-nearest neighbor statistics of a translation-invariant 1D quantum system evidence that the latter is contextual, by exploiting the connection between contextuality and Bell nonlocality. We focus on three different Bell scenarios, which differ in the number of measurement settings available to each party and the size of the near-neighbor marginals considered.

Our results show that some a priori promising Bell scenarios are unlikely to show any form of contextuality, even if we allow greater-than-quantum correlations. In other scenarios, we give evidence that some Bell inequalities require quantum systems of high enough local dimension to be violated. More interestingly, for several Bell inequalities, we find the maximum violation compatible with the laws of quantum mechanics, and identify the Hamiltonians achieving it. The ground states of contextual Hamiltonians are entangled, even though locally they may appear separable. As shown in ref. 9, it is possible to estimate the size at which the reduced density matrix of a quantum state becomes entangled, just by computing the difference between its average energy and the classical bound. Since the former can be easily estimated in essentially any noisy intermediate-scale quantum (NISQ) device, one can think of our contextuality witnesses as robust entanglement benchmarks for future quantum simulators. From a more fundamental perspective, identifying the maximum quantum violation of a k-local Bell functional opens the possibility to falsify quantum theory in the many-body regime. Indeed, given access to a NISQ device, we can represent the local measurements and the state preparation of the corresponding Bell test through a vector of lab controls θ. By estimating the gradient of the Bell functional with respect to the variables θ, we can sequentially update the latter so as to minimize the observed value of the Bell functional in the device (effectively mimicking the working principle of the variational quantum eigensolver10). If it so happened that the final value of the Bell functional was below the quantum limit, then we would have disproven the universal validity of the quantum theory, despite the lack of an alternative theoretical model.

One-dimensional quantum systems are the simplest many-body ensembles one can control in the lab. They can be found in natural condensed matter systems, as well as implemented via optical lattices or ion traps. For some such systems, the only experimentally available data are near-neighbor correlators averaged over the whole chain (the so-called structure factors). As shown in ref. 9, in the regime of large system size, structure factors correspond to the near-neighbor correlators of an infinite, translation-invariant chain. Comprehending Bell nonlocality in

1Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, 610054 Chengdu, China. 2School of Mathematical Sciences, University of Electronic Science and Technology of China, 611731 Chengdu, China. 3School of Computer Science and Engineering, University of Electronic Science and Technology of China, 611731 Chengdu, China. 4Institute for Quantum Optics and Quantum Information – IQOQI Vienna, Austrian Academy of Sciences, Boltzmanngasse 3, 1090 Vienna, Austria. 5Email: zizhu@uestc.edu.cn

Published in partnership with The University of New South Wales
large 1D systems hence requires us to characterize near-neighbor correlations in classical, quantum, and supra-quantum translation-invariant systems.

The correlations \( P(a_1, \ldots, a_n|x_1, \ldots, x_n) \) generated by \( n \) space-like separated classical systems with (classical) inputs \( x_i, i \in 1, \ldots, n \) and outputs \( a_i \) \( i \in 1, \ldots, n \) admit a decomposition of the form:

\[
P(a_1, \ldots, a_n|x_1, \ldots, x_n) = \int P(a_i|x_i, \lambda) \ldots P(a_n|x_n, \lambda) P(\lambda) \, d\lambda,
\]

where \( \lambda \) is a set of hidden variables with probability distribution \( P(\lambda) \). The distributions \( P(\lambda) \) and \( \{ P(a_i|x_i, \lambda) \}_{\lambda} \) are hence a local hidden variable model for the observed correlations \( P(a_1, \ldots, a_n|x_1, \ldots, x_n) \). In Bell tests, different parties are required to be space-like separated, which can be seen as the physical realization of the independence of probabilities in Eq. (1).

However, in a many-body quantum system, such a requirement is too formidable to overcome. As a result, when we assume that Eq. (1) holds in a quantum many-body system, what we are actually testing is contextuality\(^{15,16}\). The connection between contextuality and Bell nonlocality had been known since the 1970s. Every Bell inequality can be regarded as a contextuality witness; the other direction is less systematic\(^7\). The role of contextuality, especially of the Kochen–Specker type, in quantum computation has been actively investigated in recent years (for a review see ref. \(^{16}\)). It can be shown to be the source of the quantum advantage in several scenarios in quantum computation\(^{18–21}\). Most of these scenarios are constructed from the stabilizer formalism with magic states. While a hidden variable model for this formalism has been found recently\(^{22}\), the model itself is contextual\(^2\).

Our starting point is thus a Bell scenario with infinitely many parties in a chain, labeled by the integer numbers. At site \( i \in \mathbb{Z} \), the corresponding party can conduct a measurement \( x_i \in [1, \ldots, X] \), obtaining the result \( a_i \in A \). Since we assume translation invariance, the measurement statistics observed by any \( m \) consecutive parties equal those of parties \( 1, \ldots, m \), that is, \( \{ P(\lambda) \}_{\lambda} \) and \( \{ P(a_i|x_i, \lambda) \}_{\lambda} \) are the same. Any Bell scenario in the translation-invariant chain can therefore be fully specified by the three natural numbers \( m, X, |A| \).

Consequently, in this paper, a Bell scenario where only nearest-neighbor correlations are available and each party can conduct two dichotomic observables will be called the 222-scenario. Extending the interaction distance to next-to-nearest neighbors gives us the 322-scenario. Heisenberg-like Bell scenarios, with nearest-neighbor interactions but three dichotomic observables per site correspond to the 232-scenario.

We say that an \( m \)-partite distribution \( P_{1 \ldots m}(a_1, \ldots, a_m|x_1, \ldots, x_m) \) is no-signalling\(^{23}\) if, for all \( i \in \{1, \ldots, m\} \),

\[
\sum_{a_i} P_{1 \ldots m}(a_1, \ldots, a_i|x_i, \ldots, x_i', \ldots, x_m) = \sum_{a_i} P_{1 \ldots m}(a_1, \ldots, a_i|x_i, \ldots, x_i', \ldots, x_m),
\]

for all pairs of measurement settings \( x_i, x_i' \in X \). Intuitively, this condition signifies that the statistics of the remaining \( m-1 \) parties are not affected by the choice of measurement setting of party \( i \). Hence, party \( i \) cannot instantaneously transmit information to others.

Some no-signalling distributions \( P_{1 \ldots m}(a_1, \ldots, a_m|x_1, \ldots, x_m) \) can be shown not to arise out of an infinite no-signalling Ti system. This idea is formalized in the following definition: we say that \( P_{1 \ldots m}(a_1, \ldots, a_m|x_1, \ldots, x_m) \) admits a Ti no-signalling extension if there exists a mapping \( Q \) from finite sets \( B \subset \mathbb{Z} \) to no-signalling \( |B| \)-partite measurement statistics \( Q_B(a_B|x_B) \) with the following properties:

\[
\sum_{a_B} Q_B(a_B|C, a_C|x_B|C) = \sum_{a_B} Q_B(a_B|C, a_C|x_B|C),
\]

\[
\sum_{a_B} Q_B(a_B|C, a_C|x_B|C),
\]

for all finite sets \( B, C, D \subset \mathbb{Z} \) with \( C \subset B, D \) (compatibility).

We call Ti-NS the set of all distributions \( P_{1 \ldots m}(a_1, \ldots, a_m|x_1, \ldots, x_m) \) admitting a no-signalling, translation-invariant extension.

The existence of a no-signalling extension is just a pre-requisite for the existence of an overall infinite translation-invariant state. Whether such an entity exists at all depends also on the physics generating the observed correlations. We say that \( P_{1 \ldots m}(a_1, \ldots, a_m|x_1, \ldots, x_m) \) admits an NS extension \( Q \) and there exist distributions \( P(\lambda), \{ P_i(a_i|x_i) \} : i \in \mathbb{Z} \) such that, for all \( N \),

\[
Q_{N \ldots N}(a_{N \ldots N}, \ldots, a_N|x_{N \ldots N}, \ldots, x_N) = \sum_\lambda P(\lambda) \prod_{i=N}^N P_i(a_i|x_i).
\]

We call Ti-LHV the set of all distributions \( P_{1 \ldots m}(a_1, \ldots, a_m|x_1, \ldots, x_m) \) admitting a Ti classical extension.

Analogously, \( P_{1 \ldots m}(a_1, \ldots, a_m|x_1, \ldots, x_m) \) admits a Ti quantum extension if it admits a NS extension \( Q \) and there exist a Hilbert space \( \mathcal{H} \), measurement operators \( E_{x_i}: \mathcal{H} \rightarrow \mathcal{H} \), with \( \sum_{x_i} E_{x_i} = I \), and a translation-invariant quantum state \( \rho \) on the infinite chain with local Hilbert space \( \mathcal{H} \) such that, for all \( N \),

\[
Q_{N \ldots N}(a_{N \ldots N}, \ldots, a_N|x_{N \ldots N}, \ldots, x_N) = \sum_\lambda \rho \bigotimes_{i=N}^N E_{x_i}|a_i\rangle \langle a_i| \bigotimes_{i=N}^N |a_i\rangle \langle a_i|.
\]

We call Ti-Q the set of all distributions \( P_{1 \ldots m}(a_1, \ldots, a_m|x_1, \ldots, x_m) \) admitting a Ti quantum extension.

In ref. \(^9\), two of us provided a full characterization of the set of \( m \)-nearest-neighbor correlations admitting a Ti classical extension. This set happens to be a polytope, i.e., a convex set defined by a finite number of linear inequalities or facets. When all local measurements are dichotomic (\(|A| = 2\)), one can regard any measurement \( x \) by party \( i \) as an observable \( \sigma_i \) with possible values \( \pm 1 \), and specify any no-signaling \( m \)-nearest-neighbor distribution \( P_{1 \ldots m}(a_1, \ldots, a_m|x_1, \ldots, x_m) \) through the averages of the different products of the observables \( \sigma_i^x, \ldots, \sigma_m^x \). For \( m = 2 \), in this 'observable representation' a facet would take the form

\[
\sum_{x=1 \ldots X} J_x \langle \sigma_i^x \rangle + \sum_{y=1 \ldots X} J_y \langle \sigma_i^y \sigma_i^y \rangle \geq 1.
\]

Should the observed one-particle averages \( \langle \sigma_i^x \rangle \) be of a Ti quantum system, we obtain the quantum limit \( Q \) of the Bell functional \( J \).

In the following, we describe a method that, for any \( d \in \mathbb{N} \), carries such a minimization variationally over Ti quantum systems of local dimension \( d \), thus obtaining an upper bound \( Q_d \) on \( Q \). The method also returns a concrete Ti quantum system, with \( \dim(\mathcal{H}) = d \), achieving the Bell value \( Q_d \) with measurement operators \( \{ E_{a|x} \} \). Most statistical models studied in the literature use projective measurements, i.e., \( E_{a|x} \). Projectors are for most of our results, we only consider projective measurements, with one notable exception. When we need to verify that no 232-type Hamiltonian can violate the classical bound when \( d = 2 \), only considering projective measurements is too restrictive. Therefore for these Hamiltonians we allow fully general complex positive
operator-valued measurements (POVMs) as their local observables, using a modified version of the algorithm presented in the following section to perform the optimization.

RESULTS

Upper bounding the ground state energy density

To minimize the left-hand side expressions of the form (5), we start from the following observation: let \( \{ \sigma_i : C^d \to C^d : x \in X \} \) be a set of \( d \)-dimensional Hermitian operators with spectrum contained in \([−1, 1]\). Then, the minimum value of Eq. (5) over all TI quantum states corresponds to the minimum energy-per-site of the TI Hamiltonian

\[
\mathcal{H}_{222}(\sigma_1, \ldots, \sigma_m) = \sum_{i \in \mathbb{Z}} \sum_{x=1}^X \sigma_x^i + \sum_{x,y=1}^X \sigma_x^i \sigma_y^{i+1}.
\]

(6)

Tools from condensed matter physics such as uniform matrix product states (uMPS) allow us to compute the desired energy efficiency. In order to minimize (5) for a given local dimension \( d \), all we have to do is suitably explore the manifold of the set of local observables, e.g. via gradient descent.

Our first step consists of finding a parametrization of all the local observables. Consider observables \( \sigma_{\alpha} | \alpha \in X \), each of which can be diagonalized by a unitary matrix \( u_\alpha \) as

\[
\sigma_\alpha = U_\alpha A_\alpha U_\alpha^\dagger,
\]

(7)

where \( A_\alpha \) is a diagonal matrix with entries \( \pm 1 \). To make this more explicit, we use the vector \( [n_x, n_y] \) to describe a number of \( -1 \) in the eigenvalues of \( \sigma_\alpha \) and \( \sigma_\beta \).

We can then use the space of skew-Hermitian matrices to effectively parameterize each \( U_\alpha \) as

\[
U_\alpha = e^{\sigma_\alpha},
\]

(8)

where \( S_\alpha \) is skew-Hermitian. Let \( \{ B_1, B_2, \ldots, B_n \} \) be a basis of the vector space of skew-Hermitian matrices. Here \( n = d^2 - d \) denotes the dimension of the space. Expanding \( S_\alpha \) in this basis gives

\[
S_{\alpha}(W) = \sum_{k=1}^n w_{\alpha k} B_k,
\]

(9)

where \( w_{\alpha k} \in \{ w_{\alpha k} | \alpha \in X; k = 1, \ldots, n \} \) are scalars. Our optimization parameters are therefore \( w_{\alpha k} \). As \( \sum_{k=1}^n w_{\alpha k} \) is skew-Hermitian, it can be parameterized as

\[
\sigma_\alpha(W) = \left( e^{\sum_{k=1}^n w_{\alpha k} B_k} \right) A_\alpha \left( e^{\sum_{k=1}^n w_{\alpha k} B_k} \right)^\dagger.
\]

(10)

Consequently, \( \mathcal{H}_{222} \) is parameterized as \( \mathcal{H}_{222}(W_x, W_y) \).

Using Jordan’s lemma 2, the number of real parameters can be reduced when \( |X| = 2 \). For example, applying Jordan’s lemma to \( \mathcal{H}_{222} \) when \( d = 4 \) yields a basis in which both \( \sigma_x \) and \( \sigma_y \) are block-diagonal:

\[
\sigma_x = \begin{bmatrix} 
\sigma_{x1} & 0 \\
0 & \sigma_{x2} 
\end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 
\sigma_{y1} & 0 \\
0 & \sigma_{y2} 
\end{bmatrix},
\]

(11)

where \( \sigma_{x1}, \sigma_{x2}, \sigma_{y1}, \sigma_{y2} \) are 2 \( \times \) 2 Hermitian matrices.

We are now ready to present our uMPS-based gradient descent method. The method is iterative. For \( x \neq y \), let \( W_{\alpha}(k) \) denote the parameterization of observable \( \sigma_\alpha \) at the \( k \)-th iteration. We will refer to the parameterization \( \{ W_{\alpha}(k), W_{\beta}(k) \} \) of both observables as \( W(k) \). At each iteration \( k \), the parameters \( W(k) \) are updated to \( W(k+1) \) through the following procedure.

First, we minimize the energy-per-site of the Hamiltonian

\[
\mathcal{H}_{222}(k) = \mathcal{H}_{222}(\sigma_x(k), \sigma_y(k)) \text{ over the manifold of } u\text{MPS.}
\]

The result \( e(k) \) can be computed using, e.g., the time-dependent variational principle (TDVP) algorithm 24-26 or the variational uniform matrix product state (VUMPS) algorithm 24,27. We mainly use the TDVP algorithm for its good numerical stability and reasonable speed of convergence.

Following the TDVP algorithm, \( e(k) \) can be expressed as

\[
e(k) = \sum_{x \neq y} h(x,y) \left| \sigma_x^a(k) \sigma_y^b(k) \right| \left( \sigma_x^a(k) \sigma_y^b(k) \right)^\dagger,
\]

(12)

where \( \sum_{x \neq y} h(x,y) \left| \sigma_x^a(k) \right| \left( \sigma_y^b(k) \right)^\dagger \) is the local term of \( \mathcal{H}_{222}(k) \); \( \left| \sigma_x^a(k) \right| \in \mathbb{C}^{d \times d} \) is the tensor defining the optimal uMPS, and \( \left( \sigma_y^b(k) \right)^\dagger \) are the left and right leading eigenvectors of the transfer matrix \( T(k) = \sum_{x \neq y} \sigma_x^a(k) \sigma_y^b(k) \).

Next, we seek to find observables leading to a Hamiltonian with a smaller energy-per-site, when evaluated over the uMPS with tensor \( \left( \sigma_x^a(k) \right)^\dagger \) just identified. Hence, with \( \left( \sigma_x^a(k) \right)^\dagger \) fixed, we replace the local term \( h(x,y) \) by \( h(x,y) \left( \sigma_x^a(W), \sigma_y(W) \right) \) in Eq. (12). This leads to a function \( e(W;k) \) of the parameters \( W \) defining the observables. To update the parameters \( W(k) \), we move away from \( W(k) \) in the direction of maximum function decrease at point \( W(k) \). That is, we move against the gradient of \( e(W;k) \):

\[
W(k+1) = W(k) - e(W;k) \cdot \nabla e(W;k).
\]

(13)

Here \( e(W;k) \) is a scaling parameter, which we take to be of the form \( e(W;k) = \max(y(a,k), y(b,k)) \), where \( a \in \{0,1\} \) and \( q(k) \) is linear with respect to the iteration number \( k \).

Starting from an initial seed \( W(0) \), we iterate the two steps above, hence generating a sequence of parameter values \( \{ W(0), W(1), \ldots \} \). At every iteration \( k \), we check the condition \( \| e(W;k) \|_2 < \varepsilon \), for some desired convergence threshold \( \varepsilon \). If the condition holds, we stop the algorithm and return the optimal parameters \( W = W(k) \).

In our experience, the quantity \( e(W;k) \) is typically a very good estimate of the lowest quantum value of the considered contextuality functional over TI quantum systems of local dimension \( d \). If \( e \) happens to be smaller than the classical bound of the corresponding facet inequality, then we can state that the found quantum system characterized by the TI Hamiltonian \( \mathcal{H}_{222}(W) \) exhibits contextuality.

To test the algorithm, we apply it to compute the minimum ground state energy densities \( Q_d \) \( (d = 2, 3, 4) \) of six \( 32^2 \)-type TI quantum systems. All the results are plotted in Fig. 2. We find that the initial ground state energy densities determined by random parameters typically do not violate the classical bound \( L_{322} \) (red line). As the iteration number increases, \( Q_2 \) and \( Q_3 \) decrease approximately linearly and begin to show contextuality. In Fig. 2e and f, \( Q_2 \) oscillates during the first several iterations. As the optimization process continues, \( Q_2 \) also begins to cross \( L_{322} \) after 20 iterations. The ground state energy densities of all six models converge to values below their classical bounds within 20 iterations.

Lower bounding the ground state energy density

Consider the scenario shown in Fig. 3: an infinite chain of elephants, each of which represents a physical system, be it quantum, classical, or else. Call \( \varepsilon \) the overall state of the chain. Depending on the context, \( \varepsilon \) will be a classical probability distribution, a quantum state, or a no-signaling box. Because \( \varepsilon \) is TI, the marginal distribution or the reduced state of each of the 5 marked elephants, taken from an arbitrary contiguous subset of the chain, should be equal: \( \varepsilon_1 = \ldots = \varepsilon_5 \). Moreover, the reduced state of any contiguous subset of elephants should also be equal: \( \varepsilon_1, \ldots, x + k = \varepsilon_{x+1}, \ldots, x + k \) \( \forall 1 \leq k \leq 3 \). When \( k = 3 \), the marginals/reduced...
states are shown in Fig. 3 as green and red rectangles. For any contiguous subset of $\varepsilon$ of length $l$, the marginals/reduced states are said to be locally translation-invariant (LTI) if

$$\varepsilon_1, \ldots, \varepsilon_{l-1} = \varepsilon_2, \ldots, \varepsilon_l.$$ 

(14)

Clearly, LTI is a necessary condition for $\varepsilon$ to be TI. For classical probability distributions in 1D, LTI is also sufficient: any LTI marginal can be extended to an infinite TI distribution\cite{28}. In fact, this property is the key to the characterization of the set TI-LHV presented in ref.\cite{9}.

Unfortunately, LTI is not enough to characterize the near-neighbor density matrices of TI quantum states or even the near-neighbor marginals of TI no-signaling systems. In those scenarios, LTI can be used to relax the set of such marginals, rather than to fully characterize it. Define thus $\text{LTI}_{l-\text{NS}}$ as the set of boxes admitting an
extension to an \( n \)-partite no-signaling box with local translation invariance. As shown in ref. \(^9\), the distance between any element of the set \( \text{LTI}_{n-\text{NS}} \) and its subset \( \text{TI-NS} \) is upper bounded by \( O(1) \).

A straightforward extension of bound \( \text{TI-Q} \) is impossible, as the approximate characterization of general multipartite quantum correlations is an undecidable problem\(^{29}\). One can, however, relax the existence of quantum states and observables reproducing the observed correlations to that of positive semidefinite moment matrices. Those are matrices \( \Gamma \) whose rows and columns are labeled by monomials of measurement operators with at most \( s \) (the order of the relaxation) measurement operators per party, and where each entry \( \Gamma_{ij} \) is supposed to represent the quantity \( \langle \sigma^i \sigma^j \rangle \) (see ref. \(^{30,31}\) for details). In order to bound \( \text{TI-Q} \), we demand the existence of a moment matrix for an \( n \)-partite Bell scenario and then impose \( \text{LTI} \) over the said moment matrix. Call \( \text{LTI}_{n-\text{NS}} \), the corresponding relaxation.

For any Bell functional, we can thus find a lower bound on its minimal value in \( \text{TI-NS} \) and \( \text{TI-Q} \) by, respectively, optimizing over \( \text{LTI}_{n-\text{NS}} \) (with linear programming techniques\(^{22}\)) and \( \text{LTI}_{n-\text{NS}} \) (with semidefinite programming techniques\(^{33}\)). Moreover, one can improve those lower bounds by increasing the values of \( n, s \).

### Contextuality in 222-type Hamiltonians

The \( \text{LTI-LHV} \) polytope for 2 dichotomic observables has 36 facets. Computing their \( \text{LTI}_{n-\text{NS}} \) lower bounds reveals that most of them coincide with the corresponding classical bounds. In fact, there is only one inequality, up to local relabeling, which can potentially show contextuality. In its 1D \( \text{TI} \) quantum Hamiltonian form, it reads

\[
H_{222} = \sum_{j=1}^{\infty} \left( 2a_j^2 + a_j^2 a_j^1 + a_j^1 a_j^1 - a_j^1 a_j^1 - a_j^1 a_j^1 \right), \tag{15}
\]

with classical bound \(-2\).

Lower bounding Eq. (15) with \( \text{LTI}_{n-\text{NS}} \) with increasing \( n \), we observed some curious phenomena. Because exact optimal solutions of linear programs are rational numbers, we obtain the solutions in Table 1.

The numerators and denominators in the table form two integer sequences: A027691\(^{34}\) and A152948\(^{35}\) in The On-Line Encyclopedia of Integer Sequences. Moreover, the displaced inverse of a quadratic function

\[
-2 - \frac{4}{n^2 - 3n + 6}, \quad n \in \mathbb{N}, \quad n \geq 3 \tag{16}
\]

perfectly fits the sequence of lower bounds in Table 1 (see Fig. 4).

In the limit \( n \to \infty \), this function converges to the classical bound \(-2\). In other words, if the solution of the optimization over \( \text{LTI}_{n-\text{NS}} \) satisfies (16) for all \( n \geq 3 \), then no Hamiltonian of the form (15), quantum or otherwise, can possibly violate the classical bound.

Proving that a series of rational numbers, the solutions of linear programs of exponentially increasing size, converges to a certain value is very hard. However, we do have additional numerical evidence to support our claim that the lowest possible ground state energy density of 1D \( \text{TI} \) quantum Hamiltonians of the form (15) is \(-2\). We used our algorithm to search for the quantum Hamiltonian with the lowest ground state energy density, for local observables of dimension \( 2 \leq d \leq 6 \). For each \( d \), \( \sigma_x \) and \( \sigma_y \) are parameterized by the method described below, and we find the lowest quantum value \( \mathcal{Q}_d \) among all possible systems is \(-2\). Moreover, the corresponding two-body reduced density matrix of the quantum system for the ground state is a rank 1 projector, which shows that the ground state is in fact a product state. We present these ground states and the parameters for observables in Table 2.

To make sense of Table 2, we next explicitly write the parametrization of the \( d \)-dimensional observables achieving the classical bound. Two \( 2 \times 2 \) matrices having eigenvalues one \( 1 \) and one \(-1\) will repeatedly appear below: \( \Lambda \) is the diagonal matrix with diagonal entries \( \pm 1 \), \( B(w) \) is a matrix governed by one parameter \( \{w\} \):

\[
\Lambda = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad B(w) = \begin{bmatrix} \cos(2w) & -\sin(2w) \\ \sin(2w) & \cos(2w) \end{bmatrix}. \tag{17}
\]

When \( d = 2 \) is assigned to local observables in \( \mathcal{H}_{222} \), \( \sigma_x \) is a diagonal matrix with diagonal entries \( 1 \) and \(-1\), i.e., \( \sigma_x = \Lambda \) and \( \sigma_y \), determined by one parameter \( \{w\} \), has the same parameterized form as \( B(w) \), i.e., \( \sigma_y(w) = B(w) \). In this case, \( \{n_x, n_y\} = \{1, 1\} \) and \( \sigma_x, \sigma_y \) are of the form

\[
\sigma_x = \Lambda, \quad \sigma_y(w) = B(w). \tag{18}
\]

When \( d = 3 \) is assigned to local observables in \( \mathcal{H}_{222} \), \( \sigma_x \) is a diagonal matrix with diagonal entries \( (1,-1,-1) \). \( \sigma_y \) is a block diagonal matrix, where the main-diagonal blocks are one matrix \( B(w_1) \) and one numerical value \(-1\). Then, \( \{n_x, n_y\} = \{2, 2\} \) and \( \sigma_x, \sigma_y \) are given by

\[
\sigma_x = \begin{bmatrix} \Lambda & 0 \\ 0 & -1 \end{bmatrix}, \quad \sigma_y(w) = \begin{bmatrix} B(w_1) & 0 \\ 0 & -1 \end{bmatrix}. \tag{19}
\]

When \( d = 4 \) is assigned to local observables in \( \mathcal{H}_{222} \), \( \sigma_x \) is a diagonal matrix with diagonal entries \( 1 \) and \(-2\), \( \sigma_y \) is a block diagonal matrix with main-diagonal blocks being two \( 2 \times 2 \) matrices \( B(w_1) \) and \( B(w_2) \). In this case, \( \{n_x, n_y\} = \{2, 2\} \) and \( \sigma_x, \sigma_y \) are

| \( n \) | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|
| \( \text{LTI}_{n-\text{NS}} \) lower bound | \(-\frac{1}{2}\) | \(-\frac{1}{4}\) | \(-\frac{1}{4}\) | \(-\frac{1}{4}\) | \(-\frac{1}{4}\) | \(-\frac{1}{4}\) | \(-\frac{1}{4}\) |

---

**Table 1.** Exact solutions of \( \text{LTI}_{n-\text{NS}} \) approximations of the lower bound of (15) as a function of \( n \).

---

**Table 2.** Ground states and parameters of \( \mathcal{H}_{222} \) with \( d \)-dimensional local observables achieving the classical bound \(-2\).
of the forms

\[
\sigma_x = \begin{bmatrix}
\Lambda & 0 \\
0 & \Lambda
\end{bmatrix}, \quad \sigma_y(w_1, w_2) = \begin{bmatrix}
B(w_1) & 0 \\
0 & B(w_2)
\end{bmatrix}. \tag{20}
\]

When \(d = 5\) is assigned to local observables in \(\mathcal{H}_{222}\), \(\sigma_x\) is a diagonal matrix with diagonal entries two \(-1\) and three \(1\), \(\sigma_y\) is a block diagonal matrix, where the main-diagonal blocks are two \(2 \times 2\) matrices \(B(w_1)\) and \(B(w_2)\) and one numerical number one. Then, \([n_x, n_y] = [2, 2]\) and \(\sigma_x, \sigma_y\) are given by

\[
\sigma_x = \begin{bmatrix}
\Lambda & 0 \\
0 & \Lambda
\end{bmatrix}, \quad \sigma_y(w_1, w_2) = \begin{bmatrix}
B(w_1) & 0 \\
0 & B(w_2)
\end{bmatrix}. \tag{21}
\]

When \(d = 6\) is assigned to local observables in \(\mathcal{H}_{222}\), \(\sigma_x\) is a diagonal matrix, where three \(-1\) and three \(1\) are alternately arranged in the diagonal, \(\sigma_y\) is a block diagonal matrix with main-diagonal blocks being three \(2 \times 2\) matrices \(B(w_1), B(w_2)\) and \(B(w_3)\). Then, \([n_x, n_y] = [3, 3]\) and \(\sigma_x, \sigma_y\) have the forms

\[
\sigma_x = \begin{bmatrix}
\Lambda & 0 & 0 \\
0 & \Lambda & 0 \\
0 & 0 & \Lambda
\end{bmatrix}, \quad \sigma_y(w_1, w_2, w_3) = \begin{bmatrix}
B(w_1) & 0 & 0 \\
0 & B(w_2) & 0 \\
0 & 0 & B(w_3)
\end{bmatrix}. \tag{22}
\]

### Contextuality in 322-type Hamiltonians

The TI-LHV polytope for the 322-type Hamiltonians has been characterized in ref.\(^2\); it has 32,372 facets which can be sorted into 2102 equivalence classes. The general form of the 322-type Hamiltonian is given by

\[
\mathcal{H}_{322} = \sum_{i,j} J_{ij} \sigma_x^i \sigma_x^j + J_{xx}^y \sigma_x^i \sigma_x^j + \sum_{i,j} J_{ij}^y \sigma_y^i \sigma_y^j + \sum_{i,j} J_{ij}^x \sigma_y^i \sigma_y^j + \sum_{i,j} J_{ij}^x \sigma_x^i \sigma_x^j + \sum_{i,j} J_{ij}^y \sigma_x^i \sigma_x^j + \sum_{i,j} J_{ij}^y \sigma_y^i \sigma_y^j
\]

where \(\{ J_{ij}, J_{xx}^y, J_{xx}^x, J_{xx}^y, J_{xx}^x, J_{xx}^y, J_{xx}^x, J_{xx}^y \}\) are the couplings given by the facets inequalities and \(\sigma_x, \sigma_y\) are local observables.

Using our umPS-based gradient descent algorithm, a total of 63 Hamiltonians exhibit contextuality. The explicit parameterization of observables \(\sigma_x\) and \(\sigma_y\) is explained at the end of this section. All the contextual Hamiltonians and ground state energy densities are listed in Supplementary Tables 1 and 2, respectively. Among them, we identify some quantum models whose ground state energy density reaches the LTI\(_n\)-NPA\(_1\) lower bounds. For all these contextuality witnesses, we have thus identified translation-invariant quantum models exhibiting the strongest quantum violation. All the matched models are summarized in Table 3. As the reader can appreciate, the first five inequalities seem to require local dimension \(d = 3\) to be saturated; inequality 6, dimension 4; and the last four inequalities, dimension 5.

In Fig. 5, the reader can see the trajectories in parameter space followed by two quantum systems, of dimensions \(d = 3\) and \(d = 4\), undergoing our gradient descent method. This is possible because the number of free continuous parameters in one and another case are 1 and 2.

In Fig. 5a, \(Q_3\) surfaces (blue lines) show that the Hamiltonian exhibits contextuality no matter which values the parameter takes. The trajectory of ground state energy density (black dotted line) in the left subplot decreases along the \(Q_3\) surface to the bottom. Besides, the right enlarged subplot of the trajectory demonstrates that ground state energy density eventually converges to the respective LTI\(_n\)-NPA\(_1\) lower bound. In Fig. 5b, the leftmost subplot shows the trajectory of the ground state energy density on the 3D \(Q_3\) surface, the middle 2D-subplot is the top view of the leftmost one, and the rightmost one only depicts the trajectory of the ground state energy density. Iteratively, our methods guide the initial random ground state energy density converging to the lowest possible one.

We plot the ground state energy density as a function of the parameters defining the local observables for some of the Hamiltonians in Table 3 and Supplementary Table 2 to gauge the robustness of the contextuality violations. The couplings and local observables achieving these values can be found in Supplementary Tables. Five models for \(d = 4\) and another five models for \(d = 5\) are shown in Figs. 6 and 7, respectively. Note that the first two models in Fig. 6a, b and the first four models in Fig. 7a–d exhibit the strongest contextuality.

It can be seen that some Hamiltonians are much more susceptible to small changes in parameters that define the local observables than others. For the Hamiltonians in Figs. 6b, 7b and c, keeping the ground state energy density above the classical bound is unstable, small perturbations in the parameters will make them violate it. In contrast, the remaining Hamiltonians need carefully engineered parameters to violate the classical bound. Especially for the Hamiltonian in Fig. 7e, square-like parameter regions exist in which the corresponding ground state energy density could not violate the classical bound no matter how many times the perturbations are given. These plots help us find suitable Hamiltonians for simulation in trapped-ion or optical lattice systems, where witnessing contextuality (or the strongest contextuality) simply involves cooling the corresponding Hamiltonian to the ground state.

We next describe the parameterization of the 322-type Hamiltonians achieving the minimum quantum values in Table 3. For \(d = 2\) and \(d = 4\), \(\sigma_x, \sigma_y\) have the exact same parameterized forms as the observables in the 222-type Hamiltonians in Eqs. (18) and (20), respectively.

For \(d = 3\) and \(d = 5\), depending on the number of 1’s and \(-1\)’s of each matrix \(\Lambda_n(a=x,y)\) in Eq. (7), two different classes of pairs of local observables \(\sigma_x\) and \(\sigma_y\) are considered. Here, we continue using the notations \(\Lambda\) and \(B(w)\) introduced in Eq. (17).

For local dimension \(d = 3\), the first class of pairs of local observables is of the form \([n_x, n_y] = [1, 2]\). More specifically

\[
\sigma_x = \begin{bmatrix}
\Lambda & 0 \\
0 & 1
\end{bmatrix}, \quad \sigma_y(w_1) = \begin{bmatrix}
B(w_1) & 0 \\
0 & -1
\end{bmatrix}. \tag{24}
\]
The general form of this type of Hamiltonian is given by
\[ H_{232} = \sum_{i=1}^{\infty} J_{xx} \sigma_i^x \sigma_i^{x+1} + J_{xx} \sigma_i^y \sigma_i^{y+1} + J_{xx} \sigma_i^z \sigma_i^{z+1} + J_{yy} \sigma_i^x \sigma_i^{x+1} + J_{yy} \sigma_i^y \sigma_i^{y+1} + J_{yy} \sigma_i^z \sigma_i^{z+1} + J_{zz} \sigma_i^x \sigma_i^{x+1} + J_{zz} \sigma_i^y \sigma_i^{y+1} + J_{zz} \sigma_i^z \sigma_i^{z+1}. \]

We consider \( H_{232} \) when \( d = 2, 3, 4 \) and perform the optimizations on one representative facet from each of the 652 classes. For \( d = 3, 4 \), we only consider real parameters. For \( d = 2 \), we allow the most general measurements in quantum theory: complex POVMs.

While this step is straightforward, different combinations of ±1 in \( \Lambda_\sigma \) may lead to different ground state energy density.

Since the number of 1 and -1 on the diagonal of \( \Lambda_\sigma \) in three local observables is not necessarily the same, there is more than one combination of three parameterized local observables. We consider every possible combination of 1 and -1 in \( \Lambda_\sigma \) for each \( a \in \{x, y, z\} \). We only show combinations of parameterized local observables used in Table 4. Here, we denote the 2 × 2 identity matrix by \( I \), and continue using the notation \( \Lambda \) introduced in Eq. (17).

When \( d = 2 \), the classical bound can be achieved via three local observables determined by two parameters, where \[ n_x, n_y, n_z = \{2, 1, 1\} \]. The first local observable \( \sigma_x \) is minus the identity matrix:
\[ \sigma_x = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}. \]

For the second and third local observables \( \sigma_y(a = y, z), \Lambda_\sigma \) has entries one 1 and one -1 on the main diagonal, and \( S_\sigma \) is.

\[ \text{Fig. 5} \quad \text{Trajectories of ground state energy from our algorithm.} \quad \text{Two models from Table 3 are selected. a} \quad \text{Has two subplots, and the right panel gives a more detailed view of the trajectory in the left one when ground state energy density converges to the minimum. b} \quad \text{Gives two different views for the ground state energy surface, while the last panel shows the trajectory in parameter space. a} \quad \text{No. 3 in Table 3,} \quad \mathcal{L} = -3. \quad \text{b} \quad \text{No. 6 in Table 3,} \quad \mathcal{L} = -4. \]
Fig. 6  Ground state energy surfaces for selected Hamiltonians with local dimension 4. $Q_4$ surfaces of five models in Table 3 and Supplementary Table 2, where $w_1, w_2$ both take discrete values on $[-2, 2]$ at the interval 0.1. Three different viewing angles are shown for each model. The leftmost panel is a 3D overview, the middle panel is for better visualizing the internal structure, and the rightmost panel gives the top-down view. a No. 1 in Table 3, $\mathcal{L} = -6$. b No. 5 in Table 3, $\mathcal{L} = -8$. c No. 8 in Supplementary Table 2, $\mathcal{L} = -4$. d No. 19 in Supplementary Table 2, $\mathcal{L} = -11$. e No. 23 in Supplementary Table 2, $\mathcal{L} = -8$. 
Fig. 7 Ground state energy surfaces for selected Hamiltonians with local dimension 5. $Q_5$ surfaces of five models in Table 3 and Supplementary Table 2, where $w_1, w_2$ both take discrete values on $[-2, 2]$ at the interval 0.1. Three different viewing angles are shown for each model. The leftmost panel is a 3D overview, the middle panel is for better visualizing the internal structure, and the rightmost panel gives the top-down view. 

- (a) No. 7 in Table 3, $\mathcal{L} = -5$.
- (b) No. 8 in Table 3, $\mathcal{L} = -4$.
- (c) No. 9 in Table 3, $\mathcal{L} = -4$.
- (d) No. 10 in Table 3, $\mathcal{L} = -5$.
- (e) No. 11 in Supplementary Table 2, $\mathcal{L} = -3$. 
Table 4. Ground state energy density for five 232-type TI Hamiltonians with different local observable dimensions.

| No. | $\mathcal{L}$ | $Q_2$ | $Q_3$ | $Q_4$ | LTJ$_{\alpha}$–NPA$_1$ |
|-----|---------------|--------|--------|--------|---------------------|
| 1   | 1            | 0      | 1      | 0      | 0.00000             |
| 2   | 1            | 0      | 1      | 0      | 0.00000             |
| 3   | 1            | 0      | 1      | 0      | 0.00000             |
| 4   | 1            | 0      | 1      | 0      | 0.00000             |
| 5   | 1            | 0      | 1      | 0      | 0.00000             |

The first class is of the form $[n_x, n_y, n_z] = [3, 1, 1]$, where $\Lambda_x$ has one 1 and three $-1$ on the main diagonal, and $\Lambda_y$ and $\Lambda_z$ both have three 1 and one $-1$ being main diagonal entries. Then, $\Lambda_x$, $\Lambda_y$, and $\Lambda_z$ are given by

$$\Lambda_x = \begin{bmatrix} \Lambda & 0 \\ 0 & -1 \end{bmatrix}, \quad \Lambda_y = \begin{bmatrix} 1 & 0 \\ 0 & \Lambda \end{bmatrix}, \quad \Lambda_z = \begin{bmatrix} 1 & 0 \\ 0 & \Lambda \end{bmatrix}.$$  

The second class is of the form $[n_x, n_y, n_z] = [3, 2, 3]$, where $\Lambda_x$ and $\Lambda_y$ both have one 1 and three $-1$ on the main diagonal, and $\Lambda_z$ has two 1 and two $-1$ being main diagonal entries. Then, $\Lambda_x$, $\Lambda_y$, and $\Lambda_z$ are given by

$$\Lambda_x = \begin{bmatrix} \Lambda & 0 \\ 0 & -1 \end{bmatrix}, \quad \Lambda_y = \begin{bmatrix} 1 & 0 \\ 0 & \Lambda \end{bmatrix}, \quad \Lambda_z = \begin{bmatrix} 1 & 0 \\ 0 & \Lambda \end{bmatrix}.$$  

The third class is of the form $[n_x, n_y, n_z] = [3, 2, 1]$, where $\Lambda_x$ has one 1 and three $-1$ on the main diagonal, $\Lambda_y$ has two 1 and two $-1$ being main diagonal entries, and $\Lambda_z$ takes three 1 and one $-1$ on the main diagonal. Then, $\Lambda_x$, $\Lambda_y$, and $\Lambda_z$ are given by

$$\Lambda_x = \begin{bmatrix} \Lambda & 0 \\ 0 & -1 \end{bmatrix}, \quad \Lambda_y = \begin{bmatrix} 1 & 0 \\ 0 & \Lambda \end{bmatrix}, \quad \Lambda_z = \begin{bmatrix} 1 & 0 \\ 0 & \Lambda \end{bmatrix}.$$  

The fourth class is of the form $[n_x, n_y, n_z] = [2, 1, 2]$, where $\Lambda_x$ and $\Lambda_y$ have two 1 and two $-1$ on the main diagonal, $\Lambda_z$ has one 1 and one $-1$ being the main diagonal entries. Then, $\Lambda_x$, $\Lambda_y$, and $\Lambda_z$ are given by

$$\Lambda_x = \begin{bmatrix} \Lambda & 0 \\ 0 & \Lambda \end{bmatrix}, \quad \Lambda_y = \begin{bmatrix} 1 & 0 \\ 0 & \Lambda \end{bmatrix}, \quad \Lambda_z = \begin{bmatrix} 1 & 0 \\ 0 & \Lambda \end{bmatrix}.$$  

DISCUSSION

In this paper, we investigate the contextuality of several types of infinite one-dimensional translation-invariant local quantum Hamiltonians. We found that it is very likely that all quantum Hamiltonians with nearest-neighbor-only interactions and two dichotomic observables per site admit local hidden variable models. Violation of contextuality witnesses is only possible when we either increase the interaction distance to include next-nearest neighbor terms or have three dichotomic observables per site. In the former case, we identified several Hamiltonians with the lowest possible ground state energy density in quantum theory. In the latter case, we give strong evidence that contextuality is only present if the dimension of local observables is greater than or equal to 2, which excludes the usual Heisenberg-type models where local observables are Pauli matrices.

States and measurements which exhibit the strongest violations of Bell inequalities are essential ingredients in device-independent certifications and self-testing. So far the possibility of self-testing...
in quantum many-body systems has not been thoroughly established, due to a lack of tools to certify the strongest violation of Bell inequalities or contextuality witnesses, without having to solve the corresponding quantum model analytically. Our results pave the way for self-testing quantum many-body systems in the thermodynamic limit.

The ground states of our models are computed using uMPS, and they are global approximations of the true ground state of the corresponding quantum models. However, in applications such as quantum simulation, we will only have access to local approximations of the ground state. Moreover, the quality we are interested in, such as the ground state energy density and the expectation values of local observables all depended on the accuracy of the local description. Finding locally accurate approximations of properties of one-dimensional local quantum Hamiltonians has yielded many interesting results. However, most of these results assume the models to have nearest-neighbor interactions. As we can see from our results, the models with next-to-nearest neighbor interactions are surprisingly the most interesting in terms of contextuality.

In two dimensions, very little is known about the contextuality of translation-invariant local Hamiltonians. We know that when the number of inputs and outputs is unrestricted, the set of local hidden variable models becomes non-semi-algebraic and eventually characterized by the set of the is impossible. Properties of 2D classical and quantum models differ so markedly from their 1D counterparts that most intuitions and tools we gained in 1D break down. However, in 2D a powerful mathematical tool, tiling, has been repeatedly employed to solve questions about the computability and complexity of classical and quantum models. The number of tiles in an aperiodic tiling would correspond to the number of states in a local hidden variable model, so it would be interesting to explore the connection between tiling and contextuality.

METHODS
Optimization of 1D TI Hamiltonians with POVMs as local observables

We describe an extension of the algorithm used to minimize the ground state energy density to include the most general quantum measurements: POVMs. The extended algorithm is used to minimize 232-type Hamiltonians when the dimension of local observables is 2. These local observables $\{a_i : C^2 \to C^2, a \in X\}$ are constructed from POVM elements $M_{00}, M_{01}$. In a gradient descent algorithm, at iteration $k$ the current gradient is subtracted from the parameters, which may take the local observables out of the space of POVMs. To correct this issue we project the local observables after the gradient has been subtracted onto the closest POVM found via semidefinite programming:

$$\min ||a_k - a_0||_2$$

s.t. $a_0 = M_{00} - M_{01}$

$$M_{00} + M_{01} = \mathbb{I}$$

$$M_{00} \geq 0, M_{01} \geq 0.$$

Here, $a_k = a_{k-1}(k + 1)$. The parameters $W(k)$ are complex decision variables for the SDP, whose value at each iteration will be given by the solver.

Even though the extended algorithm based on projected gradient descent works in principle, we have encountered a number of numerical issues which require additional tweaks. The main issue affecting convergence is that it takes many iterations to traverse a nearly flat region in the parameter space. It is one of the most common problems affecting the performance of gradient descent algorithms, and it is very common to encounter such regions in our Hamiltonians. We use a well-known remedy, using momentum to speed up the traversal of nearly flat regions. At each iteration $k$, the parameters $W(k)$ defining the local observables $a_i(k) | a \in X$ are updated by

$$V(k + 1) = \eta - V(k) - \gamma(k) \cdot \nabla_W(W(k));$$

$$W(k + 1) = W(k) + V(k + 1),$$

where $V(k)$ is the momentum and $\eta$ is the decay factor.
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ACKNOWLEDGEMENTS
This work is supported by the National Key R&D Program of China (Nos. 2018YFA0306703, 2021YFE0113100). Z.W. is supported by the Sichuan Innovative Research Team Support Fund (No. 2021JDTD0028). G.Y. is supported by the National Natural Science Foundation of China (No. 62172075). We thank Wei He for helping with some of the illustrations.

AUTHOR CONTRIBUTIONS
Z.W. and M.N. conceived the project. K.Y., X.Z. and Y.L. performed the numerical computation. Z.W., G.Y. and L.S. supervised the project. All authors contributed to the development of the manuscript.

COMPETING INTERESTS
The authors declare no competing interests.

ADDITIONAL INFORMATION
Supplementary information The online version contains supplementary material available at https://doi.org/10.1038/s41534-022-00598-0.
Correspondence and requests for materials should be addressed to Zizhu Wang.

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