Detection of quantum criticality in spin-1 chain through multipartite non-locality

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We find non-localities, violation of local realism, in the many-body ground states of spin-1 XXZ chain with on-site anisotropy. In order to identify the non-localities in higher spin systems, we exploit the generalized version of multipartite Bell-type inequalities which characterize symmetric entangled states under the most general settings via combination of high-order correlations. For a given set of unbiased measurements, we obtain a sharp violation of the multipartite Bell-type inequality at the vicinity of the quantum criticality, a type of the first-order, in the regime of large exchanges and strong on-site anisotropies. It signifies that impossibility of local realistic picture is manifested when a system is subjected to quantum phase transition between weekly entangled states via GHZ-like state. Our results provide the first extendible picture on the relationship between the impossibility of local realistic model and many-body quantum phases in higher-spin system as the observable identifies measurable quantities to detect the non-locality on a particular many-body quantum state.

Introduction. — A set of quantum correlations in composite quantum system can be used to demonstrate non-locality when it exceeds the bound imposed by local hidden-variable model \[ \text{[1, 2]} \]. The non-locality shows a counter-intuitive feature of quantum state that has no counterpart in any classical system. Since the first experimental confirmation of the property \[ \text{[3]} \], the validity of the test has been investigated rigorously by the extremely high-precision measurements that close significant possible loopholes \[ \text{[4–6]} \]. As its practical applications, it has been shown that the existence of non-locality is a crucial resource for device-independent (DI) quantum information processing such as protocols of DI quantum key distribution \[ \text{[7, 8]} \] and DI randomness certification \[ \text{[9]} \].

Recently the research on quantum non-locality has been extended to many-body systems \[ \text{[10, 11]} \] similarly to the studies on many-body entanglement a decades ago \[ \text{[12–13]} \]. Although the role of non-locality in many-body systems has not been well established yet, it becomes clearer that the property reveals the important quantum nature of many-body system as Bell-type correlation is closely related to many-body quantum phases. Multipartite Bell-type inequality that involves only one- and two-body correlations with the permutation symmetry is derived a couple of years ago \[ \text{[10]} \] and experimental demonstration of the permutationally invariant non-localities is carried out in a Bose-Einstein condensate \[ \text{[11]} \]. It is also quite recent that violation of a similar Bell-type inequality is observed in the vicinity of the Ising quantum criticality of spin-1/2 systems \[ \text{[13]} \].

In addition, extended version of Bell-type inequalities, including Mermin-type multipartite ones \[ \text{[15]} \], has been tested in many spin systems, such as Ising model and spin-1/2 XXZ model \[ \text{[16, 18]} \]. Since a large number of measurements on all parties can be considered, it is a demanding task to consider the full structure of multipartite Bell correlation for a large number of particles. As its compact form, the ground-state energy is employed as an alternative approach to signal non-locality in numerous many-body systems \[ \text{[19]} \]. Similarly, the ground state of the Ising model with infinite-range interactions in the external field is demonstrated to be non-local at finite temperature \[ \text{[20]} \]. These results were limited in many-body two-level systems only and the behavior was observed by first-order correlations only.

Multipartite Bell-type correlations in the local composite \( d \)-dimensional systems have hardly been studied in many-body systems so far. It is because the approach requires generalization of Bell-type inequalities in higher spin systems whose construction is beyond of exponential complexity, \( d^{2N} \) (\( N \)-party \( d \)-dimensional systems). From the reason, there were only limited number of works done in the direction till now. Here, we exploit a generalized Bell-type correlation which was recently derived under the generic Bell scenario \[ \text{[21]} \] and investigate multipartite non-locality in the spin-1 XXZ chain with the on-site anisotropy \[ \text{[22, 24]} \].

As a result, firstly, we present a Bell-type inequality of the generic \( N \)-parties scenario with two different choices of \( d \)-outcome measurements at each party. In the construction, the optimized local measurements and the symmetry of the spin-1 Hamiltonian are considered to simplify the correlation provided. We then apply it to the ground state of the spin-1 chain and show that multipartite non-locality can be found at the vicinity of the critical points as it signifies the phase transition.

More in details, the strong non-locality is observed in the region of large exchanges and the strong on-site anisotropies along the line of linear proportionality. The violation sectorizes the regions of two different phases, the large-D phase and the Neel-order, as the asymptotic behaviour of the ground state approaches to the gen-

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eralized GHZ-like state. The observation provides the first concrete quantification of criticality appeared at the large-D phase as it exposes the pattern for the violation of local realism in the region of sudden changes of many-body phase. It is also quite interesting to identify the proportionality for the contribution of the first- and the second-order correlations for the maximal violation and it directly indicates the types of measurable physical quantities that is verifiable through the corresponding experimental test.

Generalized Bell correlation for multipartite system.
— Let us consider a generic Bell scenario with \( N \) parties who share a many-particle state performing local measurements on each particle. Each party exploits the \( k \) possible choices of measurements that yield \( d \) different outcomes. Scenario for the generalized Bell-type inequality is suggested under a general symmetric condition \( [21] \). Set of Bell-type correlation appeared in this inequality takes into account two symmetries for the equal distribution of measurements and the site permutation.

For simplicity, we adopt the case of two different measurements for each party only. Generalized Bell correlation for the scenario \((N,d)\) is given by the expectation value of the Bell operator \( \mathcal{B} = \langle \psi | \mathcal{B} | \psi \rangle \) and the Bell operator reads

\[
\mathcal{B} = \sum_{n=0}^{d-1} \left[ f_n \bigotimes_{l=1}^{N} \left( \hat{A}_l^{\alpha_n} + \omega^{\alpha_n} \hat{B}_l^{\alpha_n} \right) \right] + \text{h.c.}, \quad (1)
\]

where \( \omega = \exp(2\pi i/d) \) and \( \text{h.c.} \) denotes the hermitian conjugate. The constant \( c_l \) for a party \( l \) takes value either +1 or −1 and the value −1 of \( c_l \) on an operator implies its conjugate transpose, i.e. \( \hat{O}^{-1} = \hat{O}^\dagger \). The weight \( f_n \), a complex number for an integer \( n \), determines the type of a Bell inequality as it modifies the corresponding probability spectrum. In the \((2,d)\)-class systems, for instance, the weight \( f_n = \frac{n}{2^{d-1}} \sec\left(\frac{\pi n}{d}\right) \) yields the CGLMP Bell correlation together with \( c_1 = c_2 = 1 \) \( [23] \). Furthermore, the \((N,2)\)-class Bell correlation \( \mathcal{B} \) recovers the Mermin-type one when \( f = 1/2 \) and \( c_1 = 1 \) for all \( l \) \( [15] \).

The operators \( \hat{A}_l \) and \( \hat{B}_l \) in Eq. \((1)\) indicate the two different measurement operators for the \( l \)-th party. On the local Hilbert space of dimension \( d \), the quantum measurement in the Fourier spectral eigenbasis whose expectation is obtained from the combination of the probabilities and it can be described as

\[
\hat{A}_l(m_l) = \sum_{\alpha_l=0}^{d-1} \omega^{\alpha_l} |\alpha_l(m_l)\rangle \langle \alpha_l(m_l)| \quad (2)
\]

where \( \omega^n \) is the \( d \)-th roots of unity for distinguishing measurement outcomes \( \alpha_l \in \{0, \ldots, d-1\} \) and \( \{|\alpha_l(m_l)\rangle \rangle_{\hat{A}_l}\} \) denotes a complete set of the orthonormal basis for a local measurement \( m_l \). The choice of measurement for each party \( l \) is denoted by \( m_l \in \{0, 1\} \), and thereby \( \hat{A}_l(m_l = 0) \) and \( \hat{A}_l(m_l = 1) \) correspond to \( \hat{A}_l \) and \( \hat{B}_l \) in Eq. \((1)\) in our notation, respectively.

Local realistic bound. — If correlation is allowed by the local hidden variable model, it is possible to establish a Bell-type inequality \( \mathcal{B} \leq \beta_{LR} \) that has a real valued upper bound, \( \beta_{LR} \), often called the classical bound \( [2] \). Through Fourier analysis, it is possible to show that the Bell-type correlation \( \mathcal{B} \) is described as a convex sum of the joint probabilities of relevant measurement outcomes \( [26] \). If the set of probabilities is represented in a vector space, then the local realistic bound \( \beta_{LR} \) can be obtained from the convex properties of probability and from the Farkas’ lemma \( [24] \). Since we are dealing with spin-1 systems, it is enough to consider the local realistic bound of \((N,3)\)-class of Eq. \((1)\), which can be driven as

\[
\beta_{LR} = \max_{\{\alpha_l\}} \left[ 2 \sum_{\{m_l\}} |f_1| \cos \Theta_1 + |f_2| \cos \Theta_2 \right], \quad (3)
\]

where \( \Theta_n = \theta_n + \frac{x_n}{\sqrt{2}} c \cdot \alpha_1 + \frac{x_n}{\sqrt{2}} c \cdot \beta_1 \) and \( f_n = |f_n|e^{i\theta_n} \) and \( 1 \leq l \leq N \) \( [21] \). \( \vec{\alpha}_l = (\alpha_1(m_1), \ldots, \alpha_N(m_N)) \) indicates the outcome configuration for a measurement choice \( m_l \), and \( \vec{c} = (c_1, \ldots, c_N) \) with \( c_l \in \{1, -1\} \). In order to compute the local realistic bound, we are generally confronted with the strategy of optimized term counting for all the deterministic vectors \( \vec{\alpha} \), i.e., all possible outcomes with respect to the possible choices of measurements. Due to the large number of independent parameters, it is notable that the optimization procedure in Eq. \((3)\) falls into the complexity class of \( O(d^{kn}) \). Below, we evaluate the bound numerically. Detailed numerical methods are addressed in \( [27] \).

Maximal test. — As the extension of Pauli spin measurements for spin-1/2 systems, there are \( d^2 - 1 \) measurement bases for the systems in \( d \)-dimensional Hilbert space. The number brings about the computational complexity for the system in the high dimensional Hilbert space. To construct a compact form of correlation, we make a particular choice of measurements using the incompatible bases that are for the maximal tests of the system. The bases is constructed from the Fourier transformation of bases as

\[
|\alpha_l(m_l)\rangle \rangle_{\hat{A}_l} = \frac{1}{\sqrt{d}} \sum_{\beta = 0}^{d-1} \omega^{\beta (\alpha_l + m_l/2 - v_l)} |\beta\rangle_l, \quad (4)
\]

where \( \{|\beta\rangle_l\} \) is the computational basis \( [28] \). Two measurements for each party can be simultaneously shifted by the local phase \( \omega^m \) as for the local choice of measurements and the relative phase between two different measurements remains \( \omega^{1/2} \) due to the even distribution of two measurements. For the spin-1/2 case \((d = 2)\), measurements \( \hat{A}_l(0) \) and \( \hat{A}_l(1) \) for \( v_l = 0 \) are reduced to the Pauli operators \( \hat{\sigma}^x \) and \( \hat{\sigma}^y \), respectively. The measurement choices have been used for generalized Bell-type
Bell-type non-localities. The formal description fixing to the local realistic bound $B$.

### Spin-1 XXZ chain

We consider the spin-1 XXZ chain order to investigate multipartite nonlocality for high-dimensional systems, we consider the spin-1 XXZ chain, means small $N$. We illustrate the procedure for the standard numerical treatment in [27].

**Multiparticle nonlocality at the quantum criticality.**— We analyze multipartite nonlocality through the violation of $(N, 3)$-class Bell-type inequalities $\mathcal{B} \leq \beta_{LR}$ for the ground state of the one-dimensional spin-1 chain in Eq. (5). If we take into account the symmetries that leave the hamiltonian invariant, the Bell-type correlation of the ground states in Eq.(1) can be rewritten in a simpler form. The hamiltonian of the spin-1 XXZ chain with on-site anisotropy $J_z$ and the onsite anisotropy $D$, the ground state $\psi_{gs}$ can be transformed into diverse phases one of which is the Haldane phase renowned for the symmetry-protected topological order [22–24]. In this investigation, we focus on the region of non-negative parameters where we found the violation of the generalized Bell-type inequality. When $J_z \geq 0$ and $D \geq 0$, the spin-1 chain in Eq. (5) possesses three different phases and they are the Haldane, the anti-ferromagnetic (AFM), and the large-D phases for the different values of $J_z$ and $D$. The ground state of the system is possible to be obtained by the exact diagonalization as well as using the density-matrix renormalization group (DMRG) method for a small scale chain, means small $N$. We illustrate the procedure for the standard numerical treatment in [27].

**Spin-1 XXZ chain with the on-site anisotropy.**— In order to investigate multipartite nonlocality for high-dimensional systems, we consider the spin-1 XXZ chain model with the on-site anisotropy. The well-studied model has been known that it has many non-trivial phases in it. We in particular has interests on the quantum feature of the system that has various non-trivial phases and whether such phases can be quantifiable through Bell-type non-localities. The formal description of the model is

$$\hat{H} = \sum_{l=1}^{N} \hat{S}_l^a \hat{S}_{l+1}^a + \hat{S}_l^z \hat{S}_{l+1}^z + J_z \hat{S}_l^z \hat{S}_{l+1}^z + D \sum_{l=1}^{N} (\hat{S}_l^z)^2 \tag{5}$$

where $\hat{S}_l^a$ with $a \in \{x, y, z\}$ denotes the spin-1 operator for $l$-th site and $\hat{S}_{N+1}^a \equiv \hat{S}_1^a$ for the periodic boundary conditions.

The Hamiltonian of the spin-1 XXZ chain with on-site anisotropy in Eq.(5) is invariant under the spin rotation along the $z$ axis. It means that the Hamiltonian $\hat{H}$ commutes with the total magnetization $\hat{M}^z = \sum_l \hat{S}_l^z$. Then, the ground state is a simultaneous eigenstate of $\hat{M}^z$ with corresponding eigenvalue $M^z = 0$ that is regarded as an indication of $Z_2$ symmetry. The feature brings about the nonzero value of the $N$-body correlation $\langle \hat{S}_{l=1}^{N+1} \hat{S}_l^{a_{mn}} \rangle$ with the constraint $\sum_{l=1}^{N} \hat{S}_l^z = 0$ only for even $N$, due to the conservation of total parity, which is obvious in the context of the spin-1 basis [30]. In order to satisfy the constraint of symmetry, we specify the constant $c_l$ to take the value 1 for odd $l$ and $-1$ for even $l$.

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**Table I**

| $N$ | $f_{\text{max}}$ | $b$ in $\langle \psi_{\text{max}} | B | \psi_{\text{max}} \rangle / \beta_{LR}$ |
|-----|-----------------|----------------------------------------------------------------------------------|
| 4   | 1.039           | 0.5798                                                                           |
| 6   | 0.7423          | 0.5599                                                                           |
| 8   | 0.5502          | 0.5457                                                                           |
| 10  | 0.4114          | 0.5348                                                                           |

In the $J_z$-$D$ plane (a) the ratio of Bell correlation to the local realistic bound $\mathcal{B} / \beta_{LR}$ maximized over $\hat{f}$ with fixing $\theta_1 = \theta_2 = \pi/2$ and $\theta_2 = \pi$ ($N = 8$). Inset of (a): $\tilde{f}_{\text{max}}$, and (b) the entanglement entropy $S(\hat{\rho}_{N/2})$. The violation of a Bell inequality $\mathcal{B} \geq \beta_{LR}$ arises (the purple). For large positive $J_z$ and $D$, the region in which the ground states lead to the violation of a Bell inequality coincides with the peak of the entanglement entropy.
l. Moreover, it can be found that any ground state with real coefficients satisfies \( \langle \hat{J}_1^n \hat{J}_{-2}^n \cdots \rangle = \langle \hat{J}_{-1}^n \hat{J}_2^n \cdots \rangle \). In accordance with the characteristics, the Bell correlation with a given set of optimal measurements can take a simplified form as

\[
B = 2^{N+1} \sum_{n=1}^{2} |f_n| \cos (\theta_n - n\theta) \left( \bigotimes_{i=1}^{N} \hat{J}_i^{c_n} \right), \tag{6}
\]

where \( \nu_{tot} = \sum_i c_i \nu_i \) is for the total phase shift of any real \( \nu_i \)'s and \( \theta = 2\pi \nu_{tot}/3 \). We only consider spin-1 system of small size chain, \( N = 4, 6, 8, \) and 10, and it is because the \( N \)-body correlations vanish for odd \( N \).

Let us exploit the weighted sum of multi-order Bell-type correlation in Eq.\( (6) \) to detect the multi-partite nonlocality. Since the local realistic bound of Eq.\( (6) \) is determined by the weights \( f_n \), we take the ratio of Bell correlation to local realistic bound \( B/\beta_{LR} \) as a function of \( f \equiv |f_2|/|f_1| \) as well as \( \theta_1, \theta_2, \) and \( \theta_\nu \). We numerically maximize the correlation \( B \) over these variables. For a given ground state \( |\psi_{gs} \rangle \) of Eq.\( (5) \), we find that the angles \( \theta_{1,\text{max}} = (-1)^{N/2} \pi/2, \theta_{2,\text{max}} = \pi, \) and \( \theta_{\nu,\text{max}} = \pi/2 \) result in the maximum value of \( B/\beta_{LR} \) from simple substitution. The sign of \( \theta_{1,\text{max}} \) is flipped by the number of particles due to the negative value of the first-order correlation \( \langle \hat{J}_1 \hat{J}_{-2} \cdots \rangle \) when \( N/2 \) is odd but the alternating sign does not affect to the value of the local realistic bound.

With the substitution of \( \theta_{1,\text{max}}, \theta_{2,\text{max}} \) and \( \theta_{\nu,\text{max}}, \)

Bell-type correlation Eq.\( ( \ref{eq:bell} ) \) normalized by the local realistic bound is maximized over \( f \). The normalized function is plotted, when \( N = 8 \), in the \( J_z-D \) plane on Fig.\( (3) \). The multipartite nonlocality is then revealed where the ground state gives the violation of a Bell inequality \( B/\beta_{LR} \leq 1 \). We find two weights \( f_{\text{max}} \) that give the maximal value of \( B/\beta_{LR} \) in the ground state and one of them, denoted by \( f_{\text{max}}^c \), has to do with the Bell inequality violation depicted in inset of Fig.\( (1) \). For a given weight \( f_{\text{max}} \), we take the ratio of Bell-type correlation Eq.\( ( \ref{eq:bell} ) \) normalized by the local realistic bound is maximized over \( f \) when \( f_{\text{max}} \) is nothing but the generalized GHZ state

\[
|\psi_{\text{max}} \rangle = b|02 \cdots \rangle + \sqrt{1-2b^2}|11 \cdots \rangle + b|20 \cdots \rangle \tag{7}
\]
gives the maximal value of Eq.\( ( \ref{eq:bell} ) \) where a real \( b \) is determined by \( f_{\text{max}} \) in Table\( I \). This state can be achieved by solving the eigenvalue equation of \( B \) with \( f_{\text{max}} \), where the Bell operator is \( B = \sum_{n=1}^{2} (-1)^{N/2} |f_n| \hat{J}_1^n \hat{J}_2^n + h.c. \). With \( |f_1| = 1 \) and \( |f_2| = f_{\text{max}}^c \). Note that for \( f = 1 \) the state \( |\psi_{\text{max}} \rangle \) is nothing but the generalized GHZ state.

It is notable that the violation of a generalized Bell inequality \( B/\beta_{LR} \) with \( f_{\text{max}}^c \) appears in the vicinity of the criticality only. As \( J_z \) and \( D \) increase almost at the same time, the violation of this Bell inequality occurs more clearly on Fig.\( (1) \). For large positive \( J_z \) and \( D \), the ground state undergoes two different phases, the AFM and large-D phases. Ideally, the ground state is \( |11 \cdots 1 \rangle \) for large-D phase and \( |02 \cdots 02 \rangle + |20 \cdots 20 \rangle \) for the AFM phase. On Fig.\( (2) \) multipartite nonlocality is shown to be located between the large-D and AFM phases and generalized Bell correlation reaches to its maximal value \( \langle B_{\text{max}} \psi_{\text{max}} \rangle \) when \( J_z \) and \( D \) increase along the critical line. This feature guarantees that the ground state is close to GHZ-like state \( |\psi_{\text{max}} \rangle \) Eq.\( (7) \), which can be verified by the fidelity \( F = \langle |\psi_{\text{max}} \rangle | \psi_{\text{gs}} \rangle \) between the ground state \( |\psi_{\text{gs}} \rangle \) and the state \( |\psi_{\text{max}} \rangle \) on Fig.\( (4) \). This criticality is known as the first-order phase transition where the discontinuity of the staggered magnetization in large-scale systems appears.

Interestingly, for large values of \( J_z \) and \( D \), the behavior of the ratio \( B/\beta_{LR} \) corresponds to that of the entanglement entropy \( S(\rho_{1/2}) \), a measure of the bipartite entanglement between two halves of the system, on
The various characteristics of the spin-1 chain, Bell-type correlation can be modified in virtue of this optimal measurement and the symmetry of the Fourier transformed states, which is considered to be optimal -optimal to detect maximally entangled state. By virtue of this optimal measurement and the symmetry of the spin-1 chain, Bell-type correlation can be modified in simple generic form. We maximize the ratio of the Bell correlation to the local realistic bound $B/\beta_{LR}$ over the weight $f_n$.

The violation of this Bell inequality in the Bell scenario $(N, 3)$ is then prominently revealed in the vicinity of the first-order quantum phase transition. This result for multipartite nonlocality is close to the existence of the multipartite entanglement at the same criticality $[31, 33]$. Consequently, we can affirm that Bell correlation Eq. (6) is associated with the quantum criticality. This phenomenon is also seen in a recent work that shows the violation of the Bell inequality measuring by one- and two-body correlations at the Ising quantum criticality $[14]$. It is noted that quantum simulation for spin models has achieved many big advances in a variety of physical systems and platforms $[30]$.

Especially, experimental realization of the spin-1 XXZ chain with on-site anisotropy has been proposed in trapped ions $[37, 38]$ and implemented in ultracold atoms $[39]$. This result has thus a potential to be realized in these experiments beyond the theoretical demonstration.

We would like to thank to L. Amico and K. Bae for their useful comments. The DMRG method was performed by using the Tensor Network Python (TeNPy) library (version 0.7.2) $[40]$. This work was supported by National Research Foundation and Samsung Research Funding & Incubation Center of Samsung Electronics.

Conclusion. — We investigate multi-partite non-locality at the quantum criticality of the spin-1 chain by employing a generalized Bell-type correlation. We apply a set of the specific measurements consisting of the Fourier transformed states, which is considered to be optimal -optimal to detect maximally entangled state. By virtue of this optimal measurement and the symmetry of the spin-1 chain, Bell-type correlation can be modified in simple generic form. We maximize the ratio of the Bell correlation to the local realistic bound $B/\beta_{LR}$ over the weight $f_n$.

The violation of this Bell inequality in the Bell scenario $(N, 3)$ is then prominently revealed in the vicinity of the first-order quantum phase transition. This result for multipartite nonlocality is close to the existence of the multipartite entanglement at the same criticality $[31, 33]$. Consequently, we can affirm that Bell correlation Eq. (6) is associated with the quantum criticality. This phenomenon is also seen in a recent work that shows the violation of the Bell inequality measuring by one- and two-body correlations at the Ising quantum criticality $[14]$. It is noted that quantum simulation for spin models has achieved many big advances in a variety of physical systems and platforms $[30]$.

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