Machine Learning Detection of Bell Nonlocality in Quantum Many-Body Systems

Dong-Ling Deng*

Center for Quantum Information, IIIS, Tsinghua University, Beijing 100084, China
and Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA

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Machine learning, the core of artificial intelligence and big data science, is one of today's most rapidly growing interdisciplinary fields. Recently, machine learning tools and techniques have been adopted to tackle intricate quantum many-body problems. In this Letter, we introduce machine learning techniques to the detection of quantum nonlocality in many-body systems, with a focus on the restricted-Boltzmann-machine (RBM) architecture. Using reinforcement learning, we demonstrate that RBM is capable of finding the maximum quantum violations of multipartite Bell inequalities with given measurement settings. Our results build a novel bridge between computer-science-based machine learning and quantum many-body nonlocality, which will benefit future studies in both areas.

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Nonlocality is one of the most fascinating and enigmatic features of quantum mechanics that denies any local realistic description of our world [1–3]. It represents the most profound departure of quantum from classical physics and has been experimentally confirmed in a number of systems through violations of Bell inequalities [4–19]. Any quantum state that manifests nonlocality is necessarily entangled, but the opposite is *not* true—there exist quantum states that are entangled but at the same time admit a local-hidden-variable description (thus they do not violate any Bell inequality and cannot show nonlocality properties) [20–22]. In this sense, nonlocality is a stronger property of quantum states and detection of nonlocality is a sufficient condition to demonstrate entanglement. Apart from this fundamental difference, in practical applications nonlocality (rather than entanglement) has been shown to be an indispensable resource for various device-independent quantum technologies, such as secure key distribution [23–25] or certifiable random number generators [26–30]. Thus, characterizing and detecting nonlocality is one of the central problems in both quantum information theory and experiment. Here, we introduce machine learning, a branch of computer science [31–33], to the detection of quantum nonlocality (see Fig. 1 for a pictorial illustration).

For quantum many-body systems, whereas entanglement has been extensively studied [34], nonlocality remains rarely explored. Mathematically, it has been proved that the complete characterization of classical correlations for a generic many-body system is a non-deterministic polynomial (NP)-hard problem [35]. Nevertheless, an incomplete list of multipartite Bell inequalities with high-order correlators has indeed been discovered for a long time [3]. More recently, Bell inequalities with only two-body correlators were constructed [36–40] and multipartite nonlocality has been demonstrated experimentally in a Bose-Einstein condensate by violating one of them [41]. This sparks a new wave of interest in the study of nonlocality in many-body systems.

A particular question of both theoretical and experimental relevance is that for a given multipartite Bell inequality,

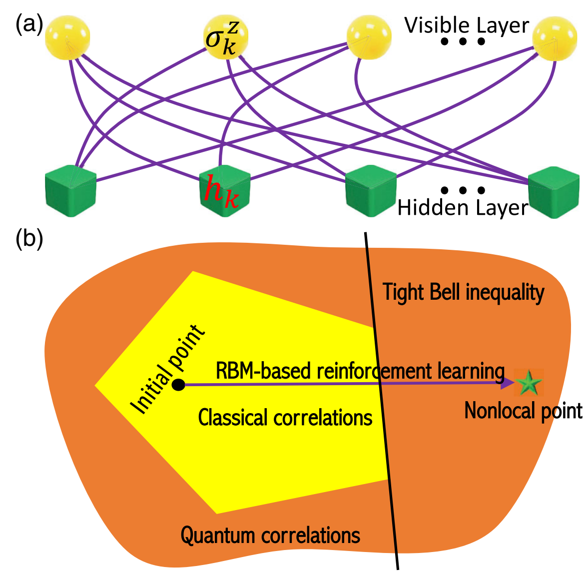

FIG. 1. (a) A sketch of the restricted-Boltzmann-machine (RBM) representation of quantum many-body states. (b) A pictorial illustration of the essential idea of machine learning detection of Bell nonlocality in quantum many-body systems. The set of all classical correlations forms a high-dimensional polytope (yellow region), which is a subset of the quantum-correlation set that consists of all possible correlations allowed by quantum mechanics. The black line represents a tight Bell inequality (facet of the polytope).

how to obtain its maximal quantum violation? To tackle this problem, one has to face at least two challenges. First of all, the Hilbert space of a quantum many-body system grows exponentially with the system size and a complete description of its state requires an exponential amount of information in general, rendering the computation of the quantum expectation value corresponding to the inequality a formidably demanding task. Second, the measurement settings for each party involved in a Bell experiment is arbitrary in principle, making the problem even more complicated. In fact, it has been shown that the computation of the maximum violation of a multipartite Bell inequality is an NP problem [42]. In this Letter, we will not attempt to solve this problem completely, which is implausible due to the NP complexity. Instead, we study a simplified scenario where the given multipartite Bell inequality only involves a polynomial number of correlators and the measurement settings for each party are restricted (due to experimental requirements, for instance) and preassigned. Based on Ref. [43], we show that machine learning may provide an unprecedented perspective for solving this simplified, but still sufficiently intricate, quantum many-body problem. Within physics, applications of machine-learning techniques have recently been invoked in various contexts [43–81], such as black hole detection [59], gravitational lenses [60] and wave analysis [61,62], material design [63], glassy dynamics [64], Monte Carlo simulation [65,66], topological codes [82], quantum machine learning [75], and topological phases and phase transitions [45–54], etc. Here, we focus on one of the simplest stochastic neural networks for unsupervised learning—the restricted Boltzmann machine (RBM) [83–85] as an example. We demonstrate, through four concrete examples, that RBM-based reinforcement learning is capable of finding the maximum quantum violations of multipartite Bell inequalities with given measurement settings. Our method works for generic Bell inequalities that involve a polynomial number (in system size) of correlators, independent of dimensionality, the order of the correlators, or whether the correlators are short range or not. Our results showcase the exceptional power of machine learning in the detection of quantum nonlocality for many-body systems and, thus would provide a valuable guide for both theory and experiment.

To begin with, we consider a quantum system with N spin-$\frac{1}{2}$ particles (qubits) $\Xi = (\sigma_1, \sigma_2, \ldots, \sigma_N)$ and use a RBM to describe its many-body wave function [43]:

$$\Phi_M(\Xi, \Omega) = \sum_{\{h_k\}} e^{\sum_k a_k \sigma_k^z + \sum_{k'} b_{k'} h_{k'} + \sum_{kk'} W_{k'k} h_{k'} \sigma_k^z}, \quad (1)$$

where $\Omega \equiv (a, b, W)$ are internal parameters that fully specify the RBM neural network and $\{h_k\} = \{-1, 1\}^M$ denotes the possible hidden neuron configurations. It is worthwhile to clarify that the RBM state defined above is a variational state, with $\Phi_M(\Xi, \Omega)$ specifying the complex coefficient for each component. The actual quantum state should be understood as $|\Psi(\Omega)\rangle \equiv \sum_\Xi \Phi_M(\Xi, \Omega)|\Xi\rangle$ (up to an irrelevant normalization constant). Any quantum state can be approximated to arbitrary accuracy by the above RBM representation, as long as the number of hidden neurons is large enough [86–88].

We consider a standard Bell experiment in which N parties each can freely choose to perform one of K possible measurements $\mathcal{M}_k^{(i)}$ ($i = 1, \ldots, N$ and $k = 0, \ldots, K-1$) with binary outcomes ± 1. We describe the observed correlations by using a collection of correlators $\langle \mathcal{M}_{k_1}^{(i_1)} \cdots \mathcal{M}_{k_\alpha}^{(i_\alpha)} \rangle$. Classical correlations form a high-dimensional (exponential in N) polytope $\mathbb{P}$. Each facet of $\mathbb{P}$ corresponds to a tight Bell inequality and correlations that fall outside of $\mathbb{P}$ will violate a Bell inequality and thus manifest nonlocality. We write the Bell inequalities in a generic form: $\mathcal{I} \geq \mathcal{B}^{(c)}$, where $\mathcal{I}$ is a function of correlators and $\mathcal{B}^{(c)}$ is the classical bound. Within this framework, our general recipe for machine learning detection of nonlocality through violation of a given Bell inequality is as follows: we begin with a random RBM state, whose observed correlations may or may not fall inside $\mathbb{P}$, but typically do not violate the given inequality; we then use a reinforcement learning scheme [43] to iteratively optimize the internal parameters, such that the minimal expectation value of $\mathcal{I}$ within quantum mechanics will be achieved. If the minimal value is smaller than $\mathcal{B}^{(c)}$, the Bell inequality is maximally violated with a given measurement setting and nonlocality is detected. Alternatively, one can think about the problem in another way: for a fixed measurement setting, the corresponding Bell operator reduces to an effective Hamiltonian and finding out the maximal violation is then reduced to finding out the ground state energy, which can be done with RBM-based reinforcement learning. A pictorial illustration of the classical polytope, a tight Bell inequality, and the essential idea of machine learning Bell nonlocality is shown in Fig. 1(b).

One may also choose another measurement setting and run the same process to obtain the maximal violation for this setting. In order to obtain the maximal violation of the Bell inequality for all measurement settings, one can just scan all possible settings and do the same process repeatedly. An alternative and more efficient way is to regard all the parameters that specify the measurements as variational parameters as well (on an equal footing as the RBM parameters Ω) and optimize them together with the RBM parameters. But this is more technically involved. Here, we will only focus on the former case with preassigned measurements for simplicity and leave the later approach for future studies.

To show more precisely how this protocol works, we give four concrete examples. The first two concern Bell inequalities with short-range two-body correlators in one and two dimensions, respectively. We compare our RBM results with that from exact diagonalization (ED) for small N and density-matrix renormalization group (DMRG) [89–91] for larger N

for the 1D case, and find that they agree excellently. This validates the effectiveness of our RBM approach. The third and fourth examples are about Bell inequalities with either all-to-all but two-body or multipartite correlators. The last three examples are beyond the capacity of the traditional DMRG or ED methods for large system sizes and show a striking advantage of RBMs in detecting many-body nonlocality.

Short-range two-body correlators.—Let us first consider a 1D system with N (an even integer) qubits. A Bell inequality involving only two-body correlators with nearest-neighbor couplings has recently been obtained [38]:

$$\mathcal{I}_1 = \sum_{k=0}^{N/2-1} (1+\delta)\mathcal{I}_{\text{even}}^{(k)} + (1-\delta)\mathcal{I}_{\text{odd}}^{(k)} \geq \mathcal{B}_1^{(c)}, \quad (2)$$

where $\mathcal{I}_{\text{even}}^{(k)} = \sum_{a=0}^{4}\sum_{b=0}^{3}\Lambda_{a,b}(\Delta)\langle\mathcal{M}_a^{(2k)}\mathcal{M}_b^{(2k+1)}\rangle$ and $\mathcal{I}_{\text{odd}}^{(k)} = \mathcal{I}_{\text{even}}^{(k)}(2k \to 2k+1)$ with $\Lambda(\Delta)$ a four-by-three matrix [92]; $\mathcal{B}_1^{(c)}$ is the classical bound depending on the real parameters δ and Δ [93]. By choosing the measurement settings properly [94], the corresponding Bell operator reduces to a XXZ-type Hamiltonian: $H = \sum_{k=0}^{N-1} g_k(\delta)[\hat{\sigma}_k^x\hat{\sigma}_{k+1}^x + \hat{\sigma}_k^y\hat{\sigma}_{k+1}^y + \Delta\hat{\sigma}_k^z\hat{\sigma}_{k+1}^z]$, where $g_k(\delta) = 4[1+(-1)^k\delta]/\sqrt{3}$, and $\hat{\sigma}^x$, $\hat{\sigma}^y$, and $\hat{\sigma}^z$ are the usual Pauli matrices. For this particular setting, the maximal quantum violation of inequality (2) corresponds to the ground state energy of H and can be calculated using DMRG [38]. Here, we use the RBM-based reinforcement learning method to obtain the same violation.

Our results are plotted in Fig. 2. In Fig. 2(a), we compare our results with that from ED for $N = 20$. As shown in this figure, the RBM result matches the ED result very well [95]. We find that the quantum expectation value of $\mathcal{I}_1$, denoted by $\mathcal{Q}_v^{(1)}$, decreases approximately linearly as we increase Δ. There is a critical value $\Delta \approx 2.4$, after which no quantum violation will be observed. In Fig. 2(b), we show the convergence of the RBM learning and compare the obtained results with that of DMRG. We find that the initial random RBM states typically do not violate the Eq. (2), but as the learning process goes on, $\mathcal{Q}_v^{(1)}$ will decrease and begin to violate the inequality after a certain critical iteration number. As the iteration number increases further, $\mathcal{Q}_v^{(1)}$ quickly converges to the DMRG value, validating the effectiveness of the RBM method. Figure 2(c) shows the converged $\mathcal{Q}_v^{(1)}$ as a function of N. We find that $\mathcal{Q}_v^{(1)}$ decreases linearly with increasing N for the chosen parameters $(\delta, \Delta) = (0.9, 2)$. For $\Delta = 2$, the slope for $\mathcal{Q}_v^{(1)}$ is smaller than that of $\mathcal{B}_1^{(c)}$; thus, the larger N is the stronger the quantum violations. For $\Delta = 3$, no violation is observed for all N [95], which is consistent with the results in Ref. [38].

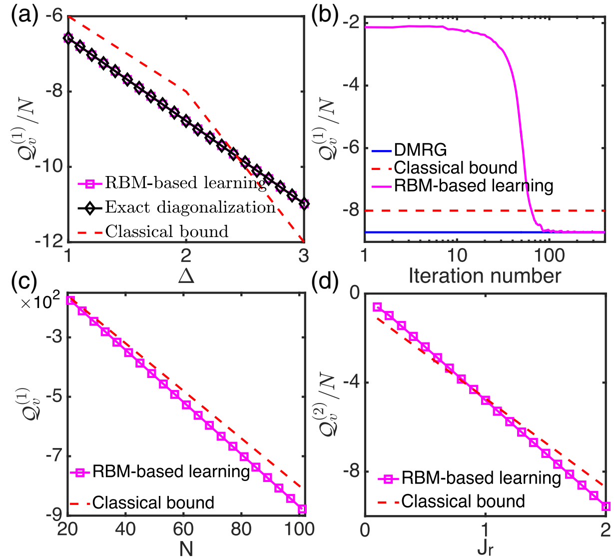

FIG. 2. RBM-based reinforcement learning of many-body Bell nonlocality. The red dashed lines represent the classical bounds, the regions below which show quantum nonlocality. (a), (b), and (c) show the results for the 1D case and we have fixed $\delta = 0.9$ for simplicity. (a) A comparison between results from RBM and exact diagonalization for $N = 20$. (b) The obtained quantum expectation value $\mathcal{Q}_v^{(1)}$ as a function of the iteration number for $N = 100$. For this particular learning process, $\mathcal{Q}_v^{(1)}$ begins to cross the classical bound $\mathcal{B}_1^{(c)}$ after 65 iterations, and all the RBM states thereafter violate Eq. (2) and thus show many-body nonlocality. As the iteration number increases, $\mathcal{Q}_v^{(1)}$ converges quickly to the value computed from DMRG [95]. (c) RBM learned $\mathcal{Q}_v^{(1)}$ as a function of N for $\Delta = 2$. (d) RBM learned $\mathcal{Q}_v^{(2)}$ as a function of J_r for Eq. (3) of the 2D case [95].

Following similar procedures in Ref. [38], the Bell inequality defined in Eq. (2) can be generalized to a 2D honeycomb lattice (see the Supplemental Material [95] for details):

$$\mathcal{I}_2 = \sum_{\tau=\{r,b,g\}} \sum_{\tau-\text{link}} J_\tau \mathcal{I}^{(\tau)} \geq \mathcal{B}_2^{(c)}, \quad (3)$$

where $\mathcal{I}^{(\tau)}$ is defined similar to $\mathcal{I}_{\text{even}}^{(k)}$, J_τ ($\tau = \{r, b, g\}$) is a real parameter characterizing the strength of the τ link of the honeycomb lattice, and $\mathcal{B}_2^{(c)}$ is the corresponding classical bound [95]. We choose similar measurement settings as in the 1D case and calculate the quantum violations of Eq. (3) through RBM-based learning. We plot a partial of our results for a system size as large as $N = 14 \times 12$ in Fig. 2(d) [95]. We find that, for the given parameters, the quantum expectation value $\mathcal{Q}_v^{(2)}$ exhibits roughly a linear decreasing as J_r increases, with a slop smaller than that of the classical bound. When J_r is small, no quantum violation is observed. However, there is a critical value of $J_r \approx 0.9$, after which quantum violations show up and nonlocality is detected. We remark that, unlike in the 1D case, the DMRG method may not be applicable here due to the exponential growing of the bond dimension with $\sim\sqrt{N}$.

All-to-all two-body correlators.—As the third example, we consider the following Bell inequality with *all-to-all* two-body correlators [36]:

$$\mathcal{I}_3 = -2S_0 - S_{01} + \frac{1}{2}(S_{00} + S_{11}) \geq \mathcal{B}_3^{(c)}, \qquad (4)$$

where the one- and two-body correlators are defined as $S_a = \sum_{k=1}^{N} \langle \mathcal{M}_a^{(k)} \rangle$ and $S_{ab} = \sum_{k\neq l}^{N} \langle \mathcal{M}_a^{(k)} \mathcal{M}_b^{(l)} \rangle$ $(a,\ b = 0,\ 1)$, and the classical bound $\mathcal{B}_3^{(c)} = -2N$. This inequality has been used in a recent experiment to demonstrate many-body nonlocality of about 480 atoms in a Bose-Einstein condensate [41]. For permutationally symmetric measurement settings, its quantum violations were numerically studied in Ref. [36]. Here, we find that, using the RBM approach, one can obtain the same maximal violations readily if one chooses a permutation-invariant neural network. More interestingly, we find that the RBM approach also works for the cases where the permutation symmetry is released. To this end, we consider a scenario where the measurement settings are chosen as $\mathcal{M}_0^{(k)} = \sigma^z$ and $\mathcal{M}_1^{(k)} = \cos\theta_k \sigma^z + \sin\theta_k \sigma^x$, where θ_k are random rotation angles drawn from some uniform distributions [95]. We mention that in a real experiment, the measurement angles will never be exact due to various control imperfections or system noises. For instance, in quantum dot spin-qubit experiments, the precision of single qubit rotations is typically limited due to charge fluctuations [96] and Overhauser noise [97,98]. Thus, our consideration of random measurement settings is of both theoretical and experimental relevance. In Fig. 3(a), we show the quantum expectation value $\mathcal{Q}_v^{(3)}$ corresponding to $\mathcal{I}_3$ as a function of the iteration number for a typical random sample of θ_ks, for a system size as large as $N = 60$, which is inaccessible with ED. It is clear that $\mathcal{Q}_v^{(3)}$ decreases as the learning process continues and becomes smaller than the classical bound at a critical iteration number. For smaller system sizes, we have compared our RBM results with that from ED and find that they agree excellently [95].

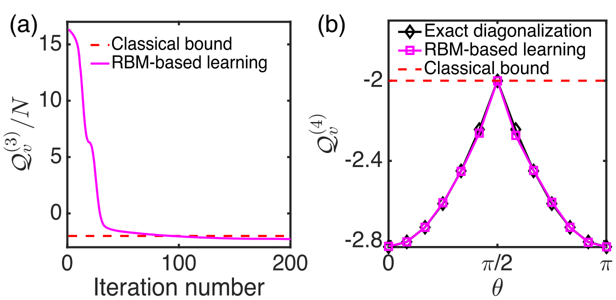

FIG. 3. (a) RBM-learned quantum expectation value $\mathcal{Q}_v^{(3)}$ as a function of the iteration number, for a typical random sample of measurement angles (see Ref. [95]). (b) RBM-learned quantum violations $\mathcal{Q}_v^{(4)}$ of Eq. (5) as a function of measurement angle θ. In (a) and (b), the system sizes are chosen to be $N = 60$ and $N = 20$, respectively.

Multipartite correlators.—To show that our RBM approach also works for Bell inequalities with multipartite correlators, we consider the following Bell inequality [99]:

$$\mathcal{I}_4 = -\langle \mathcal{M}_0^{(1)} \mathcal{M}_0^{(2)} \cdots \mathcal{M}_0^{(N)} \rangle - \langle \mathcal{M}_1^{(1)} \mathcal{M}_0^{(2)} \cdots \mathcal{M}_0^{(N)} \rangle + \frac{1}{N-1} \sum_{k=2}^{N} [\langle \mathcal{M}_0^{(1)} \mathcal{M}_1^{(k)} \rangle - \langle \mathcal{M}_1^{(1)} \mathcal{M}_1^{(k)} \rangle] \geq -2, \qquad (5)$$

with measurements [100]: $\mathcal{M}_0^{(1)} = \hat{\sigma}^z$, $\mathcal{M}_1^{(1)} = \cos\theta \hat{\sigma}^x + \sin\theta \hat{\sigma}^z$, $\mathcal{M}_0^{(k)} = \hat{\sigma}^z$ and $\mathcal{M}_1^{(k)} = \hat{\sigma}^x$ for all $k = 2, \ldots, N$. Using RBM-based reinforcement learning, we have computed the quantum violations of Eq. (5) and part of our results are plotted in Fig. 3(b) [95]. From this figure, we find that Eq. (5) is always violated when $\theta \neq \pi/2$ and the maximal violation is achieved at $\theta = 0$ or π. When $\theta = \pi/2$, $\mathcal{M}_0^{(1)} = \mathcal{M}_1^{(1)} = \hat{\sigma}^z$ and the first party actually has only one measurement; hence, no quantum violation can be obtained. In addition, from our numerical results we also find that the maximal violation of Eq. (5) is always $-2\sqrt{2}$, independent of the system size [95]. This can be understood from the observation that Eq. (5) is in fact reminiscent of the Clauser-Horne-Shimony-Holt inequality [103], whose maximal quantum violation has proved to be bounded by $2\sqrt{2}$ [104].

It is worthwhile to clarify that our RBM approach may in principle only converge to some local minima. This is a common issue in machine learning and might be overcome [31]. For the examples shown in this Letter, the RBM approach seems always to find the global minimum (its accuracy can be systematically improved by increasing the number of hidden neurons or iterations in the training process). We stress the difference between DMRG and our RBM approach. Generally speaking, DMRG is limited to short-range 1D problems and is not applicable to Bell inequalities with multipartite correlators (since for this case there is no apparent way to write down a local matrix product operator) [90]. In stark contrast, our RBM approach does not suffer from these limitations, as explicitly demonstrated by the last three examples. In addition, entanglement is not a limiting factor for the efficiency of the RBM representation of quantum many-body states [81]. Thus, we expect that RBM can be used to detect many-body nonlocality for quantum states with massive (e.g., volume-law) entanglement as well. This implies another unparalleled advantage of the RBM approach, when compared with traditional methods, such as DMRG, [105] projected entangled pair states (PEPS), or [106] multiscale entanglement renormalization ansatz (MERA), which are limited to problems with low entanglement. We also note that one may use other types of neural networks (e.g., deep Boltzmann machine [68] or feedforward neural networks [107], etc.) with different learning algorithms to detect many-body nonlocality. A complete study on detecting nonlocality with different neural networks would not only bring new powerful tools for solving complex problems in the quantum information area, but also provide helpful insight in understanding the internal data structures of the networks themselves. We leave this interesting and important topic for future investigation.

Discussion and conclusion.—Finding out experimentally friendly Bell inequalities for a given many-body system is a challenging problem, since in general the complexity of characterizing the set of classical correlations scales exponentially with the system size. In the future, it would also be interesting to study how machine learning can provide valuable ideas in designing optimal Bell inequalities for many-body systems. Particularly, recent experiments in cold atomic [108] and trapped ion [109] systems have realized programmable quantum simulators with more than fifty qubits and observed exotic quantum dynamics and phases transitions. It is highly desirable to find appropriate Bell inequalities that can be used in these experiments to demonstrate many-body nonlocality. We believe that machine learning will provide valuable wisdom in tackling this problem as well.

In summary, we have introduced machine learning to the detection of quantum nonlocality in many-body systems based on Ref. [43]. Our discussion is mainly focused on the RBM architecture, but its generalizations to other artificial neural networks are possible and straightforward. Through four concrete examples, we have demonstrated that RBM-based reinforcement learning shows remarkable power in computing quantum violations of generic multipartite Bell inequalities. Our results not only opened a door for machine learning detection of Bell nonlocality, but also clearly demonstrate the great potential of machine learning techniques in solving other quantum many-body problems that are beyond the scope of DMRG and other traditional methods, which would benefit future studies across quantum information, condensed matter physics, machine learning, and artificial intelligence.

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*dldeng@tsinghua.edu.cn

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[93] The classical bound $\mathcal{B}_1^{(c)}$ is defined as $\mathcal{B}_1^{(c)} = -(4 + 2|\Delta|)N$ for $|\Delta| \leq 2$ and $|\delta| \leq 1$, and $\mathcal{B}_1^{(c)} = -4|\Delta|N$ for $2 \leq |\Delta| \leq 3$ and $|\delta| \leq 1$.

[94] On the even sites, we choose the measurements as $\mathcal{M}_0^{(2k)}=(\hat{\sigma}^x+\hat{\sigma}^y+\hat{\sigma}^z)/3$, $\mathcal{M}_0^{(2k)}=(\hat{\sigma}^x-\hat{\sigma}^y-\hat{\sigma}^z)/3$, $\mathcal{M}_0^{(2k)}=(-\hat{\sigma}^x+\hat{\sigma}^y-\hat{\sigma}^z)/3$, and $\mathcal{M}_0^{(2k)}=(-\hat{\sigma}^x-\hat{\sigma}^y+\hat{\sigma}^z)/3$; whereas on the odd sites, the measurements are $\mathcal{M}_0^{(2k+1)}=\hat{\sigma}^x$, $\mathcal{M}_1^{(2k+1)}=\hat{\sigma}^y$, $\mathcal{M}_2^{(2k+1)}=\hat{\sigma}^z$.

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