

Lower bounds on entanglement entropy without twin copy

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We discuss the possibility of estimating experimentally the von Neumann entanglement entropy S_A^{vN} of a symmetric bipartite quantum system AB by using the basic measurement counts (bitstrings) for a single copy of a prepared state. Using exact diagonalization and analog simulations performed with the publicly available QuEra facilities for chains and ladders of Rydberg atoms, we calculate the Shannon entropy S_{AB}^X associated with the bitstrings of adiabatically prepared ground states and the reduced entropies S_A^X and S_B^X obtained from the marginal probabilities in A and B . We then calculate the classical mutual information $I_{AB}^X = S_A^X + S_B^X - S_{AB}^X$, which is a lower bound on S_A^{vN} . We show that for a broad range of lattice spacing and detuning, I_{AB}^X is typically 20% below S_A^{vN} in regions where S_A^{vN} is large and a less close bound in regions where S_A^{vN} is low. We argue that this use of the easily available bitstrings provides a robust and efficient way to explore empirically the phase diagram of qubit-based quantum simulators and identify critical regions.

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Introduction. Entanglement entropy is a crucial theoretical concept in quantum physics with applications for many-body physics [1–4], gauge theory [5–8], high-energy collisions [9–11], nuclear physics [12,13], and studies of conformal field theory [14–17]. It provides important information regarding quantum phases transitions. However, the experimental measurement of entanglement entropy is notoriously difficult due to its nonlocal nature. This led to the idea of coupling several copies of the original system [18]. A standard proposal is to measure the second order Rényi entropy S_2 by performing a swap operation between twin copies of a system [19]. Cold atom experimentalists [20,21] were able to prepare and interfere twin copies of a state in small optical lattices to measure S_2 . If practically feasible for larger systems, this would allow the experimental measurement of the central charge which is an important characterization of conformal systems [14–16,22].

Preparing and interfering twin copies of a quantum system are not easy experimental tasks. On the other hand, a generic qubit-based quantum computing device provides counts for bitstrings often given as python dictionaries. For instance, for 1000 shots with a two-qubit universal quantum computer, one gets counts for the four possible states in the form $\{ '01': 269, '00': 251, '10': 247, '11': 233 \}$. As another example, for a ten Rydberg atom analog simulator where g and r represent, for each atom, the ground and Rydberg states, respectively, the counts are given as $\{ 'gggrgrgrgr': 8, 'rgrgrggrgr': 160, \dots \}$. By dividing these counts by the total number of shots, we can estimate the probabilities $p_{\{n\}}$ for the bitstring states $|\{n\}\rangle$. We can

then introduce an AB bipartition and calculate the marginal probabilities in A or B . For instance in the ten atom example, we can estimate the probability to observe $grgrgr$ on the right side of a chain irrespectively of the observations made in B . This reduction process is reminiscent of the tracing over a subsystem used to calculate the von Neumann quantum entanglement S_A^{vN} which is equal to S_B^{vN} for a pure state.

In this Letter, we discuss the applications of concepts introduced by Shannon [23] in the context of the transmission and interpretation of classical bits, to the bitstring measurements of bipartite quantum systems. Using the Shannon entropy associated with these bitstrings and reduced versions obtained from the marginal probabilities, it is easy to calculate the classical mutual information I_{AB}^X , which is a lower bound on S_A^{vN} [24,25]. We show that for a broad range of tunable parameters, I_{AB}^X is typically 20% below S_A^{vN} in regions where S_A^{vN} is large and a less close bound in regions where S_A^{vN} is low. In other words, I_{AB}^X provides unexpectedly good characterizations of the variations of S_A^{vN} and allows an efficient exploration of phase diagrams. The bitstrings are available on many analog and universal quantum computing platforms. In the following, we focus on configurable arrays of Rydberg atoms. We used exact diagonalization and conducted analog simulations using the QuEra device Aquila [26] which is publicly available and can be operated with limited resources.

The presentation is organized as follows. We introduce the bitstring Shannon entropy and mutual information for a bipartite quantum system and then perform calculations for a chain of ten Rydberg atoms with a fixed detuning to Rabi frequency ratio Δ/Ω and a variable lattice spacing. We then extend the numerical calculations for a broad range of Δ/Ω and more general situations.

Bipartite setup, bitstring mutual information, and quantum bounds. In the following we focus on the vacuum density matrix $\rho_{AB} = |vac.\rangle \langle vac.|$ of a bipartite AB quantum system. We define the reduced density matrix $\rho_A = \text{Tr}_B \rho_{AB}$ and the

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von Neumann entanglement entropy

$$S_A^{vN} \equiv -\text{Tr}(\rho_A \ln(\rho_A)), \quad (1)$$

which is independent of the bases used in A and B . We now express ρ_{AB} in the computational basis which has a bipartite factorization $|\{n\}_{AB}\rangle = |\{n\}_A\rangle |\{n\}_B\rangle$. In this basis, the diagonal elements are the probabilities for the bitstrings. The Shannon entropy for the experimental probabilities is defined as

$$S_{AB}^X \equiv -\sum_{\{n\}} p_{\{n\}} \ln(p_{\{n\}}). \quad (2)$$

The superscript X is short for eXperimental as opposed to quantum von Neuman (or Rényi).

Similarly, we can consider the diagonal part of ρ_A . Since the partial tracing over B is a diagonal operation, the reduced diagonal elements

$$p_{\{n\}_A} = \sum_{\{n\}_B} p_{\{n\}_A \{n\}_B}. \quad (3)$$

are the marginal probabilities introduced in the 18th century and we define the reduced experimental entropy

$$S_A^X \equiv -\sum_{\{n\}_A} p_{\{n\}_A} \ln(p_{\{n\}_A}). \quad (4)$$

This quantity is basis dependent and its relation to the basis independent S_A^{vN} can in general be expressed as an upper bound using convexity arguments [25,27]:

$$S_A^{vN} \leq S_A^X. \quad (5)$$

The process can be repeated for ρ_B leading to S_B^X . In general, $S_B^X \neq S_A^X$ as it can be easily seen by taking A and B with very different sizes. This is contrast to the quantum symmetry $S_B^{vN} = S_A^{vN}$ for a pure state.

Shannon [23] introduced a manifestly $A - B$ symmetric, non-negative, quantity usually called the mutual information I_{AB} which is a measure of the information shared by A and B . In our bitstring context, it reads

$$I_{AB}^X = S_A^X + S_B^X - S_{AB}^X. \quad (6)$$

It is clear that in the limit where $p_{\{n\}} = p_{\{n\}_A} p_{\{n\}_B}$, the measurements in A and B are completely unrelated and $I_{AB}^X = 0$. At the quantum level, if the pure state is a product of two states in A and B , then $S_B^{vN} = S_A^{vN} = 0$. This suggests that there could exist a relation between I_{AB}^X and S_A^{vN} . We first empirically observed that I_{AB}^X was keeping track of S_A^{vN} from below and it was pointed out to us [28] that a general inequality can be obtained from the Holevo bound discussed in [24,25]:

$$I_{AB}^X \leq S_A^{vN} = S_B^{vN}. \quad (7)$$

In summary, we have provided upper and lower bounds on the von Neumann entanglement that can be easily obtained from bitstring data. The main question addressed hereafter is to decide if some of these bounds can be tight enough to provide reliable information about quantum entanglement.

In the rest of this Letter, we assume that A and B have the same size and can be interchanged by a reflection symmetry. This implies that $S_A^X = S_B^X$ and $I_{AB}^X = 2S_A^X - S_{AB}^X$. Applications

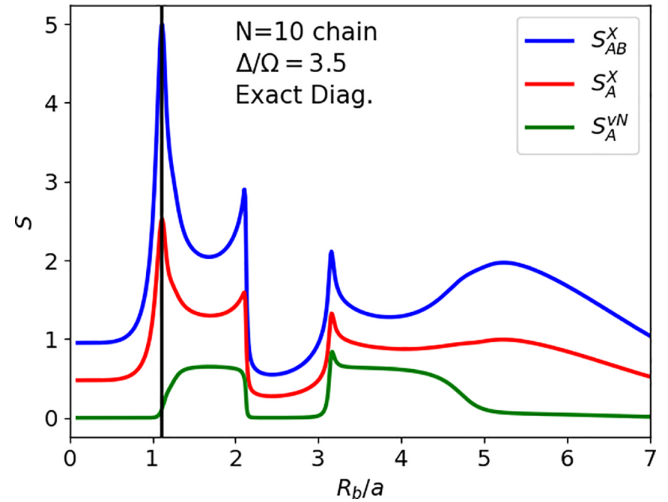


FIG. 1. Entropies for a chain of ten atoms with $\Delta/\Omega = 3.5$ as a function of R_b/a_x : S_{AB}^X , $S_A^X = S_B^X$, $I_{AB}^X = 2S_A^X - S_{AB}^X$, and S_A^{vN} ; the vertical line is at $R_b/a_x = 1.11$.

in asymmetric cases work well and are discussed elsewhere [29,30].

Rydberg atoms setup. Recently, optical tweezers have been used to create arrays of Rydberg atoms with adjustable geometries [31–36]. Their Hamiltonian reads

$$H = \frac{\Omega}{2} \sum_i (|g_i\rangle \langle r_i| + |r_i\rangle \langle g_i|) - \Delta \sum_i n_i + \sum_{i<j} V_{ij} n_i n_j, \quad (8)$$

with van der Waals interactions $V_{ij} = \Omega R_b^6 / r_{ij}^6$, for a distance r_{ij} between the atoms labeled as i and j . By definition, $r_{ij} = R_b$, the Rydberg blockade radius, when $V_{ij} = \Omega$ the Rabi frequency. We define the Rydberg occupation $n_i |r_i\rangle = |r_i\rangle$ while $n_i |g_i\rangle = 0$. In the following we use $\Omega = 5\pi$ MHz, which implies $R_b = 8.375 \mu\text{m}$, and a detuning $\Delta = 17.5\pi$ MHz as in [37]. We will consider chains and ladders of atoms with varying lattice spacings. The adiabatic preparation is discussed in *Appendix A: Analog computation methods* and the errors on the bitstring measurements in *Appendix B: Error cancellations*.

Numerical calculations. As a first step to understand the connections among the bitstring entropies and S_A^{vN} , we consider the ground state of a chain of ten Rydberg atoms separated by a varied lattice spacing a_x expressed in units of R_b . A and B are the left and right sides with five atoms each. We used exact diagonalization to calculate S_{AB}^X , S_A^X , I_{AB}^X , and S_A^{vN} for the vacuum. The results are shown in Fig. 1.

We observe that S_{AB}^X has approximately the same shape as S_A^X with a constant of proportionality which is approximately two. In addition, $S_A^{vN} \simeq 1.25(2S_A^X - S_{AB}^X)$. As shown in the SM, the proportionality factor is only approximate, for instance, S_A^{vN} is slightly below (above) this linear combination for smaller (larger) R_b/a_x , respectively. Notice that as R_b/a_x is increased from low values, the onset of S_A^{vN} is marked by a sharp increase S_{AB}^X and S_A^X . However, at the peak of S_{AB}^X and S_A^X , for $R_b/a_x \simeq 1.11$, cancellations occur and S_A^{vN} develops only after S_{AB}^X and S_A^X drop significantly. As expected, $S_A^X \geq S_A^{vN}$ but typically $S_A^X \gg S_A^{vN}$ so this upper bound is not very useful. Other features of Fig. 1 can be understood from

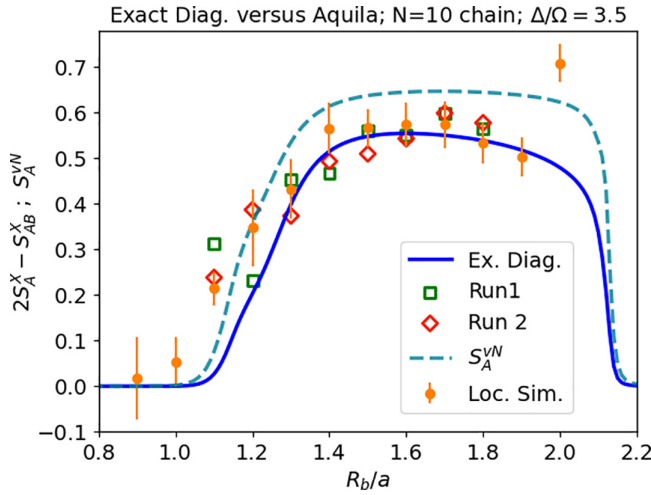


FIG. 2. $2S_A^X - S_{AB}^X$ vs R_b/a_x with three methods: (i) exact diagonalization (continuous curve); (ii) local simulator with no ramping down of Ω at the end (filled circles), the errors bars are calculated using ten independent runs of 1000 shots; (iii) two runs with 1000 shots with Aquila (empty symbols); S_A^{vN} (dashed line) is also given for reference.

elementary considerations that are provided in the Supplemental Material [38]. In summary, we found that whenever S_A^{vN} is not too small, $I_{AB}^X \simeq 0.8 \times S_A^{vN}$ which is 20% below the target value. When S_A^{vN} is small, I_{AB}^X provide a bound that is not so close. Consequently, the mutual information provides a good estimation of the regions of the phase diagram where S_A^{vN} gets large.

Analog simulations. We have repeated parts of the above numerical calculations using the empirical probabilities provided by the Aquila device and the associated Amazon Braket local simulator. As explained in *Appendix A: Analog computation methods*, this imposes size constraints not present in exact diagonalization. Calculations for $1.0 \lesssim R_b/a_x \lesssim 2$ can be performed with the local simulator and, for a slightly shorter range of R_b/a_x , with Aquila. In both cases, we ramped up the vacuum adiabatically starting with all atoms in the atomic ground state, increasing Ω and then Δ , exactly as in [37] and illustrated in *Appendix A: Analog computation methods*. The data is publicly available [39]. The results are shown in Fig. 2 where we see good estimates of $2S_A^X - S_{AB}^X$ with Aquila. The local simulator becomes less accurate when $R_b/a_x \simeq 2$ and the ramping down of Ω at the end involves subtleties discussed in the Supplemental Material [38]. Figure 2 only shows results with no ramping down of Ω at the end for the local simulator.

In *Appendix B: Error cancellations*, we explain that the Aquila values for both S_{AB}^X and $2S_A^X$ are significantly larger than the accurate numerical values, however, these errors appear to cancel in I_{AB}^X . In the Supplemental Material [38], we show that “filtering” the low probabilities tend to increase I_{AB}^X and get it closer to S_A^{vN} . This is discussed in more detail in Ref. [29].

How tight is the lower bound? So far our model calculation shows that the mutual information I_{AB}^X follows rather closely and from below the von Neuman entanglement entropy S_A^{vN} . This is not always the case. An example [40] of state $|\psi\rangle$ with

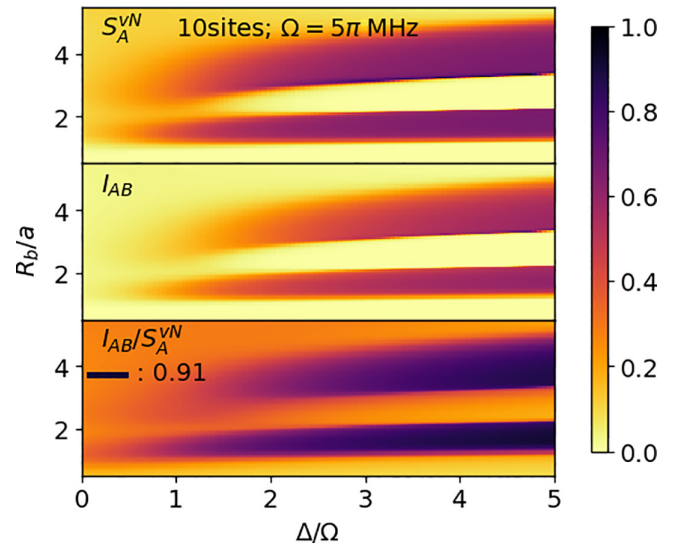


FIG. 3. S_A^{vN} , I_{AB}^X , and I_{AB}^X/S_A^{vN} for a ten site chain.

$I_{AB}^X = 0$ and $S_A^{vN} = \ln 2$ is

$$|\psi\rangle = \frac{1}{2}(|gg\rangle + |gr\rangle + |rg\rangle - |rr\rangle). \quad (9)$$

This state can be obtained by starting with a product state of two $(|g\rangle + |r\rangle)/\sqrt{2}$ and then applying the entangling unitary transformation $\exp(i\pi n_1 n_2)$. All the $p_{\{n\}}$ for both states are 1/4 and the mutual information is zero, but S_A^{vN} changes from zero to $\ln 2$ when the sign of the coefficient of $|rr\rangle$ changes. A discussion of the exactly solvable two qubit case is given in the Supplemental Material [38].

In order to get a better idea about the generic tightness of the bound, we have repeated our numerical calculations over a broad range of values of Δ/Ω . The results are shown in Fig. 3. We see that the shapes of the heatmaps of S_A^{vN} and I_{AB}^X are very similar. The ratio I_{AB}^X/S_A^{vN} reaches a maximal value of 0.91 in regions where S_A^{vN} is large, and small values in regions where S_A^{vN} is close to zero. This confirms our previous observations that I_{AB}^X delimitates reliably the regions of the phase diagram where S_A^{vN} takes its largest values. We have repeated some of the numerical calculations discussed above with two-leg ladders with five rungs and varied the lattice spacings in both directions. We found very similar features that are reported in the Supplemental Material [38].

Other bitstring proxies. In Ref. [37], we found a detailed correspondence between the contour plots in the $(\Delta/\Omega, R_b/a)$ plane of the peak height of the structure factors, which can be reconstructed from the $p_{\{n\}}$ only, and the contour plots of S_A^{vN} which require the knowledge of the vacuum wave function. This motivated the idea of finding proxies of S_A^{vN} that depends on the $p_{\{n\}}$ only. Besides I_{AB}^X , one can also construct a second order Rényi version of the S^X quantities defined above:

$$S_{2AB}^X \equiv -\ln \sum_{\{n\}} p_{\{n\}}^2, \text{ and } S_{2A}^X \equiv -\ln \sum_{\{n\}_A} p_{\{n\}_A}^2. \quad (10)$$

As shown in the Supplemental Material [38], we found numerically that for the ten atom chain,

$$S_{2A}^R \approx 2S_{2A}^X - S_{2AB}^X. \quad (11)$$

with $S_{2A}^R = -\ln(\text{Tr}\rho_A^2)$. Another possibility is the configurational entanglement entropy. The connection between correlations and purity [41] or the reconstruction of quantum states using a restricted Boltzmann machine based on single-basis measurements [42] could help develop a more general understanding of our observations. Ref. [41] introduces another proxy C for S_A^{vN} in the case of the Bose-Hubbard model called the configurational entanglement entropy. Adapting their definition for the case where the particle number is not conserved and where there is no number entropy, and introducing a function of C that reproduces S_A^{vN} for a two-qubit Bell state, we propose to use

$$LC \equiv \ln \left(1 + \sum_{\{n\}} |p_{\{n\}} - p_{\{n\}_A} p_{\{n\}_B}| \right). \quad (12)$$

This quantity provides good estimates of S_A^{vN} but has a more intricate behavior which will be discussed separately.

Applications. Arrays of Rydberg atoms have been proposed for quantum simulation of lattice gauge theories [43–52]. More specifically, ladder arrays have been considered as quantum simulators for scalar electrodynamics [47] and their phase diagram has been studied experimentally [37] and with effective Hamiltonian methods [53]. These results show a very rich phase diagram and the need to study the regions of parameter spaces where the correlation lengths are much larger than the lattice spacing (continuum limits). This has possible relevance for the study of inhomogeneous phases and the Lifshitz regime of lattice quantum chromodynamics [54,55]. Entanglement entropy considerations play an important role in the tentative designs of hybrid algorithms for collider event generators [50].

Generalizations. It is possible to extend our procedure for arbitrary AB partitions where A and B have different sizes. This allows us to study the conjectured lower bound for multipartite entropies which are of great interest in the context of conformal field theory [56–58]. Ongoing calculations show that our proxy provide reasonably tight lower bounds for digitized ϕ^4 models with qudits [30], Ising models in curved space [59], and larger Rydberg arrays than the ones considered here [29].

Conclusions. We have shown that the bitstring mutual information provides robust and reliable estimates for the order of magnitude of the von Neumann entanglement entropy. This works efficiently for a broad range of adjustable parameters available in arrays of Rydberg atoms. The method can be applied to any qubit based universal or analog quantum computing device. This provides a quick way to map the phase diagram and identify regions of interest from the point of view of approaching continuum limits with quantum simulators.

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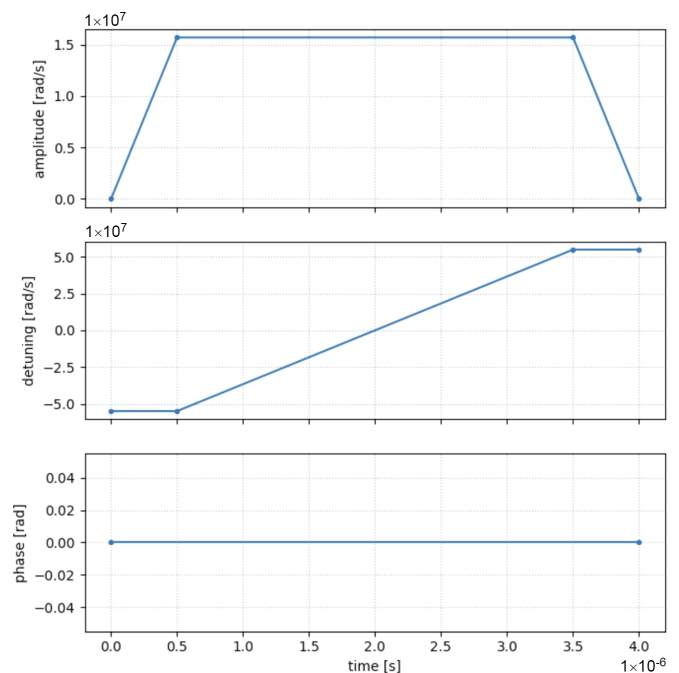


FIG. 4. Standard ramping up or down of Ω (top), Δ (middle), and ϕ (bottom) as appearing in the Amazon Braket notebook tutorials.

Holevo bound. We thank the Amazon Web Services and S. Hassinger for facilitating remote access to QuEra through the Amazon Braket while teaching quantum mechanics and our Department of Physics and Astronomy for supporting the cost of the analog simulations presented here.

Data availability. The data that support the findings of this article are openly available [39], embargo periods may apply.

Appendix A: Analog computation methods. Analog calculations with arrays of Rydberg atoms have been performed with Aquila using the Amazon Braket services. We used the Amazon Braket SDK for local simulations. The actual device imposes constraints not present in exact diagonalization. Analog calculations were performed with a single chain model with ten sites, $\Omega = 5\pi$ MHz, which implies $R_b = 8.375 \mu$, and a detuning $\Delta = 17.5\pi$ MHz. The linear size of the system needs to be less than 100μ . This means that we need $R_b/a_x \gtrsim 0.9$. The distance between the atoms needs to be more than 4μ which implies $R_b/a_x \lesssim 2.0$. We used the values $R_b/a_x = 0.9, 1.0, \dots, 2.0$. The ground state needs to be prepared adiabatically and actual measurements with Aquila are performed after turning off Ω . The procedure suggested on the Amazon Braket tutorials lasts 4μ s and involves ramping down Ω during the last 0.5μ s, as illustrated in Fig. 4. This protocol was used for our Aquila calculations. Different rampings down were studied with the local simulator and reported in the Supplemental Material [38]. We used 1000 shots ten times for the local simulator and had two runs with 1000 shots for Aquila. The raw data files are available in [39].

Appendix B: Error cancellations. An important aspect of the results presented in Fig. 2 is that the errors (the difference between the analog estimates and the values calculated accurately with numerical methods) for S_{AB}^X and $2S_A^X$ are significant and actually larger than I_{AB}^X . This is illustrated in

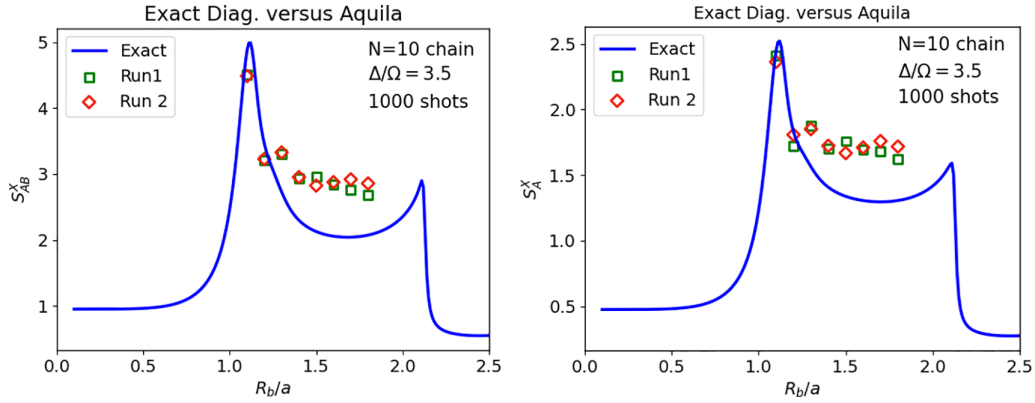


FIG. 5. Top: S_{AB}^X (left), S_A^X (right) vs R_b/a_x with exact diagonalization (continuous curves) and with Aquila with two runs of 1000 shots.

a specific way in Fig. 5. Near $R_b/a = 1.5$, the difference between Aquila and exact diagonalization for both $2S_A^X$ and S_{AB}^X are both positive and close to one while their difference

$I_{AB}^X = 2S_A^X - S_{AB}^X$ is of order 0.5 with an estimated error of order 0.1. More details can be found in the Supplemental Material [38].

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