

Instruction Material

Simulating quantum many-body dynamics on a current digital quantum computer

Day 2

Practical Training
Condensed Matter Theory
Technical University Munich
Physics Department

Responsible: Prof. Dr. Michael Knap

Dates (Day 1/Day 2):
November 30/ December 01, 2023

1 Summary

In today's part of the training, we apply the concepts introduced yesterday to a relevant many-body system using the Qiskit library. The goal of this session is to study the phenomenon of Dynamical Quantum Phase Transitions (DQPTs) in a transverse field Ising model. Your task will be to convert the closed system quantum dynamics into a corresponding quantum circuit and extract relevant observables such as the magnetization, the Loschmidt echo, and the entanglement dynamics from it. Along the way, we put an emphasis on the required measurement effort and the comparison with the exact solutions.

After the practical training day, please prepare a report in which you answer the questions posed throughout the instructions below, including a (brief) introduction to the topic. You can provide important plots in the main body of your report and attach the associated code in appropriately labeled appendices.

2 Prerequisites

1. Some minimal knowledge about quantum computation will be helpful. If you haven't learned any quantum computation before, don't worry. A comprehensive reference will be the first chapter of *Quantum Computation and Quantum Information* by Nielsen and Chuang.
2. Before we start coding in Qiskit, we will give an introduction and some time for you to install Qiskit.
3. For the coding exercises, we advise you to use interactive Python notebooks. You can for example install your setup via Anaconda, Miniconda or create a Google account to work online with Google Colab.
4. The practical training consists of Day 1 (basics) and Day 2 (application), you are expected to hand in a written report for **both** Day 1 and Day 2, respectively. You can also choose to only participate on Day 1.
5. Please read through the following introduction on dynamical quantum phase transitions (section 3) and the transverse field Ising model (section 4) **ahead** of the practical session. You can follow the instructions even without answering the questions directly.
6. During the exercises, we will either **simulate** the circuits to get full access to the wavefunctions or determine quantities by **measuring/ sampling** circuits, which mimics the use of a real quantum computer. Pay attention to the highlighted keywords.

3 Dynamical Quantum Phase Transitions

In today's example, we investigate the phenomenon of 'dynamical quantum phase transitions' (DQPTs). We provide a short introduction to the most important concepts based on the review of Ref [1]. DQPTs extend the notion of phase transitions to the realm of non-equilibrium physics. Let us recall that for the more conventional equilibrium phase transitions, the central object is the partition function

$$Z = \text{Tr } e^{-\beta \hat{H}(\alpha)}, \quad (3.1)$$

for an inverse temperature $\beta = 1/T$ and a Hamiltonian $\hat{H}(\alpha)$ that depends on a set of parameters α (e.g. the strength of an external magnetic field). The partition function Z provides an implicit definition of a free energy density $f(\beta, \alpha)$ via

$$Z = e^{-\beta N f(\beta, \alpha)}, \quad (3.2)$$

which depends on both β and the collection of parameters α . N denotes the size of the system. Equilibrium phase transitions then occur at points where the free energy density $f(\beta, \alpha)$ becomes *non-analytic* as a function of either β or one of the parameters α . The former are temperature-driven phase transitions at some critical temperature T_c . The latter, if occurring at zero temperature, are called quantum phase transitions.

In the context of DQPTs we now instead consider the real-time evolution of a closed quantum many-body system starting from the ground state $|\psi_0\rangle$ of some Hamiltonian \hat{H}_0 . At the time $t = 0$, the Hamiltonian is abruptly changed from \hat{H}_0 to \hat{H} , a protocol which is called a *quantum quench*. Formally, the time evolution is then solved by

$$|\psi_0(t)\rangle = e^{-i\hat{H}t} |\psi_0\rangle. \quad (3.3)$$

A formal similarity to the above partition functions is achieved by computing the return amplitude to the original ground state $|\psi_0\rangle$,

$$\mathcal{G}(t) = \langle \psi_0 | \psi_0(t) \rangle = \langle \psi_0 | e^{-i\hat{H}t} | \psi_0 \rangle, \quad (3.4)$$

which is called the *Loschmidt amplitude*. The associated return probability

$$\mathcal{L}(t) = |\mathcal{G}(t)|^2 = |\langle \psi_0 | \psi_0(t) \rangle|^2 \quad (3.5)$$

is usually referred to as the *Loschmidt echo*. In analogy to the above equilibrium partition functions, the Loschmidt amplitude takes on a particular dependence on system size N (for large values N), such that we can write

$$\mathcal{G}(t) = e^{-N g(t)}, \quad (3.6)$$

with an associated (complex) rate function $g(t)$. Similarly, the Loschmidt echo is written as

$$\mathcal{L} = e^{-N \lambda(t)}. \quad (3.7)$$

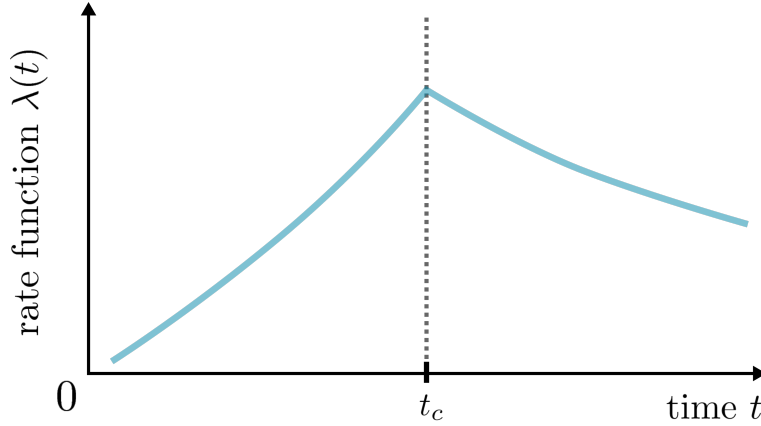


Figure 1: Dynamical Phase Transition. (Figure 1 from Ref. [1]) At critical times t_c , the Loschmidt rate $\lambda(t)$ experiences non-analytic kinks.

We will refer to the rate function $\lambda(t)$, which can alternatively be defined as $\lambda(t) = -\lim_{N \rightarrow \infty} \frac{1}{N} \log \mathcal{L}(t)$ in the thermodynamic limit, as the *Loschmidt rate*.

Exercise 1: Show that $\lambda(t)$ and $g(t)$ are related via $\lambda(t) = 2 \operatorname{Re}[g(t)]$. The exponential dependence of $\mathcal{G}(t)$ and $\mathcal{L}(t)$ on system size N in Eq. (3.6) and Eq. (3.7) is only in general valid if the quench changes the energy density, i.e. inserts an extensive amount of energy into the system. Can you come up with an intuitive reason for this (no calculations necessary)?

Equipped with these definitions, we can now identify DQPTs as points where the rates $\lambda(t)$, $g(t)$ become non-analytic as a function of time. DQPTs occur at *critical times* t_c where the rate $\lambda(t_c)$ typically shows a kink-like behavior in the thermodynamic limit, see Fig. 1 for a sketch.

Technical Note: The analogy between partition functions and the Loschmidt amplitude can be made more concrete by interpreting

$$\mathcal{G}(z) = \langle \psi_0 | e^{-i\hat{H}z} | \psi_0 \rangle, \quad z \in \mathbb{C}, \quad (3.8)$$

as a so-called ‘boundary partition function’ for a general complex parameter z . Non-analyticities of the associated rate function $g(z)$ are then associated with the zeros of $\mathcal{G}(z)$ in the complex plane (called Fisher zeros). A DQPT occurs whenever such Fisher zeros intersect the real axis, see Ref. [1] for more information.

As a final definition for this section, we note that one can generalize the Loschmidt echo $\mathcal{L}(t)$ for situations where the initial Hamiltonian \hat{H}_0 has more than one ground state, i.e. in the presence of spontaneous symmetry breaking: If $|\psi_i\rangle$ with $i =$

$0, \dots, N_{gs} - 1$ labels all the N_{gs} states in the ground state manifold of \hat{H}_0 , the Loschmidt echo becomes

$$\mathcal{L}(t) = \sum_{i=0}^{N_{gs}-1} |\langle \psi_i | \psi_0(t) \rangle|^2, \quad (3.9)$$

and can be interpreted as the return probability to the ground state manifold of \hat{H}_0 . In addition to the usual Loschmidt rate $\lambda(t) = -\lim_{N \rightarrow \infty} \frac{1}{N} \log \mathcal{L}(t)$, we can then also define the individual rates $\lambda_i(t)$ via

$$|\langle \psi_i | \psi_0(t) \rangle|^2 = e^{-N\lambda_i(t)}. \quad (3.10)$$

Exercise 2: Based on the above definitions, show that in the thermodynamic limit $N \rightarrow \infty$, the Loschmidt rate $\lambda(t)$ reduces to the minimum function applied to the set of individual rates $\lambda_i(t)$, i.e. $\lambda(t) = \min_i [\lambda_i(t)]$.

4 The transverse field Ising model

We now consider a specific example to study DQPTs in the following, the paradigmatic transverse field Ising model (TFI). It is a ubiquitous model in the field of many-body physics and, due to its exact solvability, often used to benchmark numerical methods, including quantum computers.

In one dimension, the TFI consists of a linear chain of N qubits (or spin-1/2 sites) whose time evolution is generated by the following Hamiltonian,

$$\hat{H} = -\frac{1}{2} \sum_{\langle i,j \rangle} Z_i Z_j - \frac{g}{2} \sum_i X_i, \quad (4.1)$$

where $\langle i, j \rangle$ denotes nearest neighbor sites. We set the strength of the ZZ - Ising interaction to unity, but vary the strength g of the transverse field. The computational basis can be chosen as the z -basis in the following.

Before delving into the implementation as a quantum circuit, let us first perform a proper analysis of the model's symmetries and zero temperature (i.e. ground state) phase diagram.

Exercise 3: Show that the parity operator

$$\hat{P} = \prod_i X_i \quad (4.2)$$

commutes with the Hamiltonian, i.e. $[\hat{H}, \hat{P}] = 0$. What is the spectrum of \hat{P} , i.e. its possible eigenvalues? Determine the exact ground states

of \hat{H} in the two limiting cases $g = 0$ and $g \rightarrow \infty$. Notice that for $g = 0$, the symmetry \hat{P} is spontaneously broken, i.e. an infinitesimally small longitudinal field $\pm\epsilon \sum_i Z_i$ induces a finite expectation value of the ground state magnetization $m_z = \frac{1}{N} \sum_i Z_i$. What is the expectation value of m_z in the respective symmetry broken ground states at $g = 0$, and what is $\langle m_z \rangle$ for the ground state at $g \rightarrow \infty$?

From the solution to Exercise 3, we see that the TFI features a symmetry-broken ferromagnetic phase, i.e. $m_z(g) \neq 0$, for $g < g_c$ smaller than some so far unknown critical field strength g_c . As mentioned above, the TFI can be solved exactly and $m_z(g)$ can be computed analytically [2]. However, for our purposes, there is a more direct way to infer the critical field g_c :

Exercise 4: Let us introduce the new Ising variables $\tilde{Z}_n = \prod_{i \leq n} X_i$ and $\tilde{X}_n = Z_n Z_{n+1}$, that can be thought of as living on the bonds of the lattice. Consider an infinite system, i.e. ignoring boundary terms. Show that indeed $\{\tilde{Z}_n, \tilde{X}_n\} = 0$ as required, and express the Hamiltonian in terms of these new variables. Compare the result with the form of the Hamiltonian in terms of the original variables X_i, Z_i . How can you conclude from the resulting self-dual structure that the critical field assumes the value $g_c = 1$? The above transformation is known as the Kramers-Wannier duality transformation.

The previous analysis sets the stage for the investigation of DQPTs in the TFI model. In particular, we now know that for $g < 1$, the ground state manifold contains two degenerate ferromagnetic states $|\psi_0\rangle$ and $|\psi_1\rangle$ which are related by flipping all spins, $|\psi_1\rangle = \hat{P} |\psi_0\rangle$. For $g > 1$ the unique ground state is a paramagnet. Before shifting to numerics, let us answer the following final question:

Exercise 5: We have shown the presence of ferromagnetic order in the ground state for $g < 1$. Does this order survive at finite temperatures? (Hint: How much energy does a domain wall between two ferromagnetic patches cost? Accordingly, how many domain walls as a function of system size do you expect at finite temperatures? Use your result to argue that there can be no long-range ferromagnetic order at finite temperatures.)

5 DQPTs in the TFI using Qiskit

We now turn to the simulation of the time evolution generated by \hat{H} using the methods introduced on Day 1 of the practical. In addition to this manual, your instructors will provide you with a Python notebook containing several pre-defined functions that you may use to perform the following tasks.

5.1 Implementing the time evolution

Given \hat{H} from Eq. (4.1), we want to perform a Trotter decomposition of the unitary operator $U(t) = e^{-i\hat{H}t}$, based on the elementary exponentials $e^{iZ_i Z_j dt/2}$ and $e^{igX_i dt/2}$ that can directly be implemented in Qiskit. To this end, we can rewrite

$$U(t) = e^{-i\hat{H}t} = \left(e^{-i\hat{H} dt} \right)^{t/dt} = \left(e^{\hat{A} + \hat{B}} \right)^{t/dt}, \quad (5.1)$$

with $\hat{A} = idt \frac{g}{2} \sum_i X_i$ and $\hat{B} = idt \frac{1}{2} \sum_{\langle i,j \rangle} Z_i Z_j$.

Exercise 6: Based on the Qiskit's RX -gate and RZZ -gate, define

(a) A function `evolve_basic(circ, g, dt)` that takes the input circuit `circ` and appends a set of operations that evolve the system by a small time step dt based on the first order Trotterization $e^{\hat{A} + \hat{B}} \approx e^{\hat{A}} e^{\hat{B}}$.

(b) A function `evolve_symmetric(circ, g, dt)` that takes the circuit `circ` and appends a set of operations that evolve the system by dt based on the second order Trotterization $e^{\hat{A} + \hat{B}} \approx e^{\hat{A}/2} e^{\hat{B}} e^{\hat{A}/2}$.

In both cases, for the nearest neighbor Ising interaction you can decompose it into two layers of two-qubit gates acting on even and odd bonds, i.e. for even LN :

$$e^{i\delta t/2 \sum_{\langle i,j \rangle} Z_i Z_j} = \prod_{i=0}^{N/2-1} e^{i\delta t/2 Z_{2i} Z_{2i+1}} \prod_{i=0}^{N/2-2} e^{i\delta t/2 Z_{2i+1} Z_{2i+2}}. \quad (5.2)$$

Exercise 7: To benchmark the results from Exercise 6, **simulate** the time evolution and extract the magnetization $m_z(t)$ as a function of time for a system of $N = 10$ qubits at $g = 2$, starting from an initial state $|\psi_0\rangle = |0\dots 0\rangle$ of all spins down. Compare your results to the magnetization obtained through exact diagonalization of the Hamiltonian, which is provided by the pre-defined function

`magn_exact_diagonalization(N, g, t, dt)`

in the Python notebook. How small do you have to choose the time step dt in the circuit to obtain a good approximation to the exact results for a final time of $t = 5$?

5.2 Extracting DQPTs

We now want to evaluate the Loschmidt rate as described at the beginning of this manual. The initial Hamiltonian is chosen as $\hat{H}(g = 0)$, where the two degenerate ferromagnetic ground states are $|\psi_0\rangle = |0\dots 0\rangle$ and $|\psi_1\rangle = |1\dots 1\rangle$.

Exercise 8: Using the same time evolution as above, extract the **simulated** Loschmidt rate by projecting back onto the ground state manifold, see Eq. 3.9. Plot $\lambda(t)$, as well as the individual rates $\lambda_{0/1}(t)$, for

- (a) Different system sizes $N = 6, 8, 10, 12$ and $g = 2$. Can you see DQPTs emerging?
- (b) Different values of g between $0.5 \leq g \leq 1.5$. For which of these values are there DQPTs and for which not?

In the actual quantum device, we do not have access to the simulated wavefunction directly and have to determine observables by repeated measurements.

Exercise 9: Determine both the magnetization and Loschmidt echo again, this time via repeated **measurements**. Plot your results for $N = 10$ and $g = 2$. How much sampling (as a function of system size) is in principle necessary to obtain accurate results?

Exercise 10: Compare the time evolution of the magnetization $m_z(t)$ with the Loschmidt rate $\lambda(t)$ (you may put both quantities into the same plot). Can you see any correspondence between $m_z(t)$ and $\lambda(t)$?

5.3 Tracking the entanglement production

During the time evolution following the quantum quench, the system builds up entanglement. The increase in entanglement is responsible for the limitations on using classically efficient methods (e.g. matrix product states) to simulate the dynamics up to arbitrary times. To quantify the amount of entanglement in the system we consider the half-chain entanglement von Neumann entropy as well as the second Rényi entropy. For this purpose, we first define the reduced density matrix ρ_ℓ of the left half of the system,

$$\rho_\ell = \text{Tr}_r [\rho], \quad (5.3)$$

with ρ the density matrix of the full system. The von Neumann entanglement entropy S is then defined as

$$S = -\text{Tr}[\rho_\ell \log(\rho_\ell)]. \quad (5.4)$$

The second Rényi entropy on the other hand is obtained from ρ_ℓ via

$$S^{(2)} = -\log(\text{Tr}[\rho_\ell^2]). \quad (5.5)$$

Exercise 11: We first extract the entanglement from the **simulated** wave function of the quantum circuit. Do so in the following way:

(a) Define two functions `vN_entropy(rho)` and `renyi2_entropy(rho)` that return S and $S^{(2)}$ from Eqs. (5.4) and (5.5) for a given density matrix ρ , respectively.

(Hint: In order to compute S , express the trace in Eq. (5.4) in the eigenbasis of ρ .)

(b) Use the functions from part (a) to compute and plot both $S(t)$ and $S^{(2)}(t)$ as a function of time for $g = 2$ (again starting from the ferromagnetic initial state $|\psi_0\rangle = |0\dots 0\rangle$). Verify that both $S(t)$ and $S^{(2)}(t)$ grow *linearly* in time.

For the final report, it is sufficient to implement only one of the following two options to measure the entanglement production. Of course, you can also compare both alternatives.

Option I: State Tomography

In order to obtain the reduced density matrix from the measured data, one needs to use state tomography. The principle of state tomography is readily explained (following Ref. [3]): Consider a single qubit (compare also with Day 1 of the practical), whose state is described by a point on (or within for mixed states) the Bloch sphere, i.e. three independent coordinates. Measuring the state of the qubit in the computational z -basis yields the z -component $\langle z \rangle = p_0 - p_1$ on the Bloch sphere. In order to determine the y -component, we simply rotate around the x -axis by $\pi/2$ before measuring, in order to bring the y -axis upright. Analogously, rotation around the y -axis by $-\pi/2$ brings the x -axis upright and allows to determine the x -component.

For a system of N qubits with density matrix ρ , the above Ansatz is straightforwardly generalized: We apply all 3^N possible combinations of rotations of the individual qubits before measuring, denoted by U_j with $j \in \{1, \dots, 3^N\}$. For a given rotation U_j , we then measure the probabilities p_{jk} of all basis states $|k\rangle$, with $k = 1, \dots, 2^N$. This can be expressed as

$$p_{jk} = \langle k | U_j^\dagger \rho U_j | k \rangle. \quad (5.6)$$

Using the measured probabilities p_{jk} as inputs, Eq. (5.6) can straightforwardly be solved for the density matrix ρ by linear inversion. Notice, however, that due to the limited amount of measurements, the resulting ρ is not guaranteed to be physical. Therefore, the ρ extracted from the measurements has to be post-processed in order to find the physical density matrix that provides the best fit to the measured ρ . This is done automatically in Qiskit if you run the default options of `StateTomography`. If you are interested, it is instructive to read through Ref. [4] (accessible at <https://arxiv.org/abs/1106.5458>) to see how the corresponding algorithm works.

Exercise 12: For $N = 10$ and $g = 2$, perform a state tomography experiment with `tomo_rep = 400` repeated **measurements** for each basis

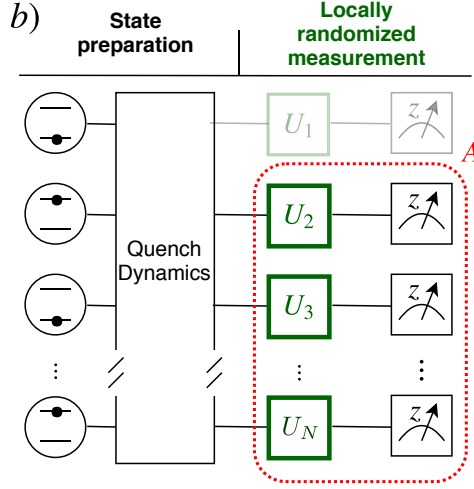


Figure 2: Randomized Measurements (Figure 1b from Ref. [5]) Before measuring the qubits of subsystem A , random unitaries U_i are applied to the individual qubits. Correlations between these randomized measurement outcomes yields the second Rényi entropy according to Eq. (5.8).

rotation. From the results extract the associated density matrix. Compute the corresponding von Neumann and second Rényi entropies as a function of time and compare them to the above exact results. How do your results change if you increase `tomo_rep` to 1000 or 2000?

Option II: Randomized Measurements

Above, we extracted the von Neumann and second Rényi entanglement entropies through state tomography. However, for the second Rényi entropy (as well as for even higher Rényi entropies), there is a less costly way to extract $S^{(2)}(t)$ via *randomized measurements*. In this procedure, following Ref. [5], before the qubits are measured, we apply a random unitary operation $U = \prod_i U_i$ (with $i = 1, \dots, N$) to each individual qubit of the chain, see Fig. 2, and use the statistical correlations between such randomized measurements in order to determine $S^{(2)}(t)$.

Let us go through the individual steps of this scheme more specifically:

1. Each U_i is chosen randomly from the so-called *circular unitary ensemble* (CUE). This can be achieved by the following parametrization,

$$U_i(a, b, c) = \begin{pmatrix} e^{ia} \cos(b) & e^{ic} \sin(b) \\ e^{-ic} \sin(b) & e^{-ia} \cos(b) \end{pmatrix}, \quad (5.7)$$

where a and c are uniformly sampled from $[0, 2\pi]$, and $b = \arcsin(k)$ with k uniformly in $[0, 1]$. In Qiskit, you can either realize Eq. (5.7) via a param-

terized circuit with a generic single-qubit rotation `Ugate()` or directly use the built-in function `quantum_info.random_unitary()`.

2. Once a set of U_i has been chosen, we perform repeated measurements with this given instance of random unitaries to extract the probabilities $P_U(s_A)$ of measuring a bitstring s_A of the subsystem A .
3. Finally, we repeat the above procedure many times and compute the probabilities $P_U(s_A)$ for different random operations $U = \prod_i U_i$. The second Rényi entropy of the subsystem A is then obtained from [5]

$$S^{(2)} = -\log \bar{X}, \quad \text{with } X = 2^{L_A} \sum_{s_A, s'_A} (-2)^{-D(s_A, s'_A)} P_U(s_A) P_U(s'_A), \quad (5.8)$$

where the overbar \bar{X} denotes the average over different random unitaries $U = \prod_i U_i$ with the U_i chosen independently from the CUE. $D(s_A, s'_A)$ denotes the *hamming distance* between the two bitstrings s_A and s'_A , which is defined as the number of bits where the two bitstring differ, i.e. $D(s_A, s'_A) = \#\{i : s_A(i) \neq s'_A(i)\}$.

Exercise 13: To implement the above algorithm, go through the following steps.

- (a) Write a function `hamming(s1,s2)` that implements the above hamming distance.
- (b) Choose around 2000 **measurement** repetitions for each instance of the CUE and around 200 different instances of the CUE to compute $S^{(2)}(t)$ for selected time steps between $t = 0$ and $t = 5$, again for $g = 2$ (running the algorithm with these parameters might take a while, so you can experiment with smaller values first). Use the parametrized circuits introduced on the first day of the practical. Plot and compare your result to the exact value of $S^{(2)}(t)$ from the simulated wave function.

References

- [1] M. Heyl, “Dynamical quantum phase transitions: a review,” *Reports on Progress in Physics*, vol. 81, p. 054001, apr 2018.
- [2] P. Pfeuty, “The one-dimensional Ising model with a transverse field,” *Annals of Physics*, vol. 57, no. 1, pp. 79 – 90, 1970.
- [3] M. G. Neeley, *Generation of Three-Qubit Entanglement Using Josephson Phase Qubits*. PhD thesis, 2010.

- [4] J. A. Smolin, J. M. Gambetta, and G. Smith, “Efficient Method for Computing the Maximum-Likelihood Quantum State from Measurements with Additive Gaussian Noise,” *Phys. Rev. Lett.*, vol. 108, p. 070502, Feb 2012.
- [5] A. Elben, B. Vermersch, C. F. Roos, and P. Zoller, “Statistical correlations between locally randomized measurements: A toolbox for probing entanglement in many-body quantum states,” *Phys. Rev. A*, vol. 99, p. 052323, May 2019.