

Quantifying Complexity in Quantum Phase Transitions via Mutual Information Complex Networks

David L. Vargas and Lincoln D. Carr

Department of Physics, Colorado School of Mines, Golden, CO 80401, USA

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We quantify the emergent complexity of quantum states near quantum critical points on regular 1D lattices, via complex network measures based on quantum mutual information as the adjacency matrix, in direct analogy to quantifying the complexity of EEG/fMRI measurements of the brain. Using matrix-product-state methods, we show that network density, clustering, disparity, and Pearson's correlation obtain the critical point for both quantum Ising and Bose-Hubbard models to a high degree of accuracy in finite-size scaling for three classes of quantum phase transitions, Z_2 , mean field superfluid/Mott insulator, and a BKT crossover.

Classical statistical physics has developed a powerful set of tools for analyzing complex systems, chief among them complex networks, in which connectivity and topology predominate over other system features [1]. Complex networks model systems as diverse as the brain and the internet; however, up till now they have been obtained in quantum systems by explicitly enforcing complex network structure in their quantum connections [2–7], e.g. entanglement percolation *on* a complex network [4]. In contrast, complexity measures on the brain observe emergent complexity arising *out of*, e.g., a regular array of EEG electrodes placed on the scalp, via an adjacency matrix formed from the classical mutual information calculated between them [8]. We apply the quantum generalization of this measure, an adjacency matrix of the quantum mutual information calculated on quantum states [9], to well known quantum many-body models on regular 1D lattices, and uncover emergent quantum complexity which clearly identifies quantum critical points [10, 11]. Quantum mutual information bounds two-point correlations from above [12], measurable in a precise and tunable fashion in e.g. atom interferometry in 1D Bose gases [13], among many other quantum simulator architectures. Using matrix-product-state computational methods [14, 15], we demonstrate rapid finite size-scaling for both transverse Ising and Bose-Hubbard models, including Z_2 , mean field, and BKT quantum phase transitions.

As we move toward more and more complex quantum systems in materials design and quantum simulators, involving a hierarchy of scales, diverse interacting components, and a structured environment, we expect to observe long-lived dynamical features, fat-tailed distributions, and other key identifiers of complexity [16–18]. Such systems include quantum simulator technologies based on ultracold atoms and molecules [19], trapped ions [20], and Rydberg gases [21], as well as superconducting Josephson-junction based nanoelectromechanical systems in which different quantum subsystems form compound quantum machines with both electrical and mechanical components [22]. A key area in which we

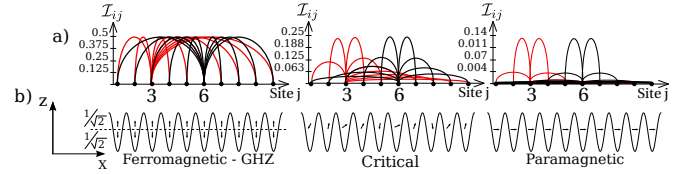


FIG. 1: *Sketch of mutual information complex network.* A chain of L quantum bits (qubits) in a sinusoidal potential, for the transverse Ising model, the “fruit-fly” of quantum many body physics. (a) Links originating from site 3 (red, I_{3j}) and site 6 (black, I_{6j}) for the mutual information complex network I_{ij} , corresponding to phases and critical point in (b). In this weighted complex network, the height of the links in our sketch denotes their relative strength; note descending vertical axes from left to right. The entire complex network is far too dense to depict, so we show just two representative sites. (b) Sketch of ferromagnetic phase (left), critical point (center), and paramagnetic phase (right). The sinusoidal potential corresponds to an optical lattice for ultracold atoms or molecules. In the ferromagnetic case, the dashed line indicates a superposition between the Z_2 symmetric states all spin-up and all spin-down.

have taken a first step beyond phase diagrams and ground state properties is non-equilibrium quantum dynamics, where critical exponents and renormalization group theory are only weakly applicable at best, e.g. in the Kibble-Zurek mechanism, and are hard to find any use for at all in far-from-equilibrium regimes. However, at the most basic level we can first ask, are quantum systems inherently complex? Must we impose complexity on quantum systems to obtain it [2–7], or is there a regime in which complexity naturally emerges, even in ground states of regular lattice models? In this Letter we show that emergent complexity can be well quantified in the simplest of 1D lattice quantum simulator models in terms of complexity measures around critical points in direct analogy to similar measurements on the brain; moreover we establish a much-needed new set of tools for quantifying the complexity of far-from-equilibrium quantum dynamics.

Quantum phase transitions are often characterized by quantum averages over physical observables such as two-

point correlators. For example, the transverse Ising model (TIM) consists of a chain of qubits with nearest neighbor z - z coupling J and a transverse randomizing field g . For large g the spins tend to be transverse and therefore random in z (meaning an average z -spin measurement of zero), while for small g the spins prefer to align or anti-align, depending on the sign of J . The quantum phase transition between large g (paramagnetic) and small g (ferro/anti-ferromagnetic) at the critical point $g_c = 1$ is evidenced by a change in the long range behavior of the two-point correlator $g_{ij}^{(2)} = \langle \hat{\sigma}_i^z \hat{\sigma}_j^z \rangle - \langle \hat{\sigma}_i^z \rangle \langle \hat{\sigma}_j^z \rangle$, where i, j are sites on a lattice and $\hat{\sigma}^z$ are measurements of spin in the z -direction; alternate measures include the von Neumann entropy and concurrence [23]. The mutual information \mathcal{I}_{ij} is bounded from below by $g_{ij}^{(2)}$, and indeed by any possible two-point correlator in the model [12]. In general for quantum simulator technologies we obtain Hamiltonians for which we do not know *a priori* what the right correlator is or indeed if there is a quantum phase transition at all. Thus mutual information provides a much more general tool to identify such quantum phase transitions than any particular physical correlator.

To establish the usefulness of mutual information complex networks, we consider both the TIM and the Bose-Hubbard model (BHM). The BHM balances particle tunneling J against on-site particle interaction U , with the filling factor controlled by the chemical potential μ ; thus it has a richer phase diagram than the TIM, and exhibits both mean field transitions from Mott insulators to a superfluid phase as well as Berzinskii-Kosterlitz-Thouless (BKT) crossovers at commensurate filling. We emphasize that both these models are studied heavily in quantum simulators experimentally and theoretically [19, 20, 24–26].

Quantum Many-body Hamiltonians and Mutual Information – The 1D transverse Ising model (TIM) takes the form

$$\hat{H}_I = -J \sum_{i=1}^{L-1} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - Jg \sum_{i=1}^L \hat{\sigma}_i^x, \quad (1)$$

where $[\hat{\sigma}_j^\alpha, \hat{\sigma}_k^\beta] = 2i\delta_{jk}\epsilon_{\alpha\beta\gamma}\hat{\sigma}_k^\gamma$. The 1D Bose-Hubbard model (BHM) takes the form

$$\hat{H}_B = -J \sum_{i=1}^{L-1} (\hat{b}_i^\dagger \hat{b}_{i+1} + \hat{b}_i \hat{b}_{i+1}^\dagger) + \frac{1}{2}U \sum_{i=1}^L \hat{n}_i(\hat{n}_i - \hat{1}) - \mu \sum_{i=1}^L \hat{n}_i, \quad (2)$$

where $[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij}$ are bosonic annihilation and creation operators and $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$. Both the TIM and BHM are standard workhorses of quantum many-body lattice physics [11]. The quantum mutual information $\mathcal{I}_{ij} \equiv \frac{1}{2}(S_i + S_j - S_{ij})$ is constructed from the one and two point von Neumann entropies $S_i = -\text{Tr}(\hat{\rho}_i \log_d \hat{\rho}_i)$,

$S_{ij} = -\text{Tr}(\hat{\rho}_{ij} \log_d \hat{\rho}_{ij})$, with reduced density operators defined in terms of the partial trace as $\hat{\rho}_i = \text{Tr}_{k \neq i} \hat{\rho}$ and $\hat{\rho}_{ij} = \text{Tr}_{k \neq i, j} \hat{\rho}$. We take $d = 2$ for the TIM (qubits) and $d = n_{\text{max}} + 1$ for the BHM, since particles can pile up on site in the latter, with n_{max} a truncation parameter converged in our numerical method.

Complex Network Measures – We use weighted generalizations of standard measures based on unweighted adjacency matrices [1]; a formal justification for and interpretation of this generalization procedure can be found in [27]. A primitive measure of a node's importance is the sum of the weights connecting it to other nodes in the network, $s_i \equiv \sum_{j=1}^L \mathcal{I}_{ij}$, where, s_i is called the strength of node i . The disparity Y_i of a node i in a network with L nodes is defined as a function over weighted connections to its neighbors,

$$Y_i \equiv \frac{1}{(s_i)^2} \sum_{j=1}^L (\mathcal{I}_{ij})^2 = \frac{\sum_{j=1}^L (\mathcal{I}_{ij})^2}{\left(\sum_{j=1}^L \mathcal{I}_{ij}\right)^2}. \quad (3)$$

Observe that if the mutual information between lattice sites adopts a constant value $\mathcal{I}_{ij} = a$, that $Y_i = a^2(L-1)/a^2(L-1)^2 = 1/(L-1)$, so that if a node has relatively uniform weights across its neighbors the disparity between nodes will be approximately $1/(L-1)$. On the other hand, if a particular \mathcal{I}_{ij} takes on a dominant value b , then $Y_i \approx b^2/b^2 = 1$. The average disparity over all nodes in the network is $Y \equiv \frac{1}{L} \sum_{i=1}^L Y_i$. The clustering coefficient C is 3 times the ratio of triangles (three mutually connected vertices) to connected triples in an unweighted network. In our weighted network,

$$C \equiv \frac{\text{Tr}(\mathcal{I}^3)}{\sum_{j \neq i}^L \sum_{i=1}^L [\mathcal{I}^2]_{ij}}. \quad (4)$$

The density D is the average fraction of the $\binom{L}{2}$ links that are present in the network:

$$D \equiv \frac{1}{L(L-1)} \sum_{i=1}^L s_i. \quad (5)$$

As the number of nodes in an unweighted network is allowed to approach infinity a network is said to be *sparse* if $D \rightarrow 0$, and *dense* if $D > 0$ as the number of nodes in the network L approaches infinity [1]. Finally, a technique for assessing the similarity between two nodes i, j in a network is to compute the Pearson correlation coefficient between them,

$$r_{ij} \equiv \frac{\sum_{k=1}^L (\mathcal{I}_{ik} - \langle \mathcal{I}_i \rangle) (\mathcal{I}_{jk} - \langle \mathcal{I}_j \rangle)}{\sqrt{\sum_{k=1}^L (\mathcal{I}_{ik} - \langle \mathcal{I}_i \rangle)^2} \sqrt{\sum_{k=1}^L (\mathcal{I}_{jk} - \langle \mathcal{I}_j \rangle)^2}}. \quad (6)$$

This is treating link weight as a random variable; the numerator of Eq. (6) is the covariance of the weights of

node i with the weights of node j , while the denominator is the standard deviation in the weights of node i multiplied by the standard deviation in the weights of node j . A Pearson correlation coefficient near zero means the weights of the two nodes are not meaningfully correlated, while larger values mean that the two nodes show a meaningful and linear relationship between their weights. To restrict our study we focus on the Pearson correlation coefficient between the middle two sites of the lattice. These two nodes are spatially close to each other and far from boundaries, making them the most similar nodes in the network whose weights of connection are not strongly modified by boundary conditions; we thus choose $R \equiv r_{\frac{L}{2}, \frac{L}{2}+1}$.

Numerical Techniques – We obtain our data with our widely-used matrix-product-state (MPS) open source code [14], a well-established algorithm [15]. The essence of the approach is data compression of a quantum many-body state onto a classical computer, using singular value decomposition. The key convergence parameter is the bond dimension χ , limiting the growth of spatial entanglement as defined by the truncated Schmidt number of the reduced density matrix [9]; secondary convergence parameters include the local Hilbert space dimension d for the BHM. We use bond dimensions of up to several hundred, which are adequate to establish the usefulness of our complex network measures to pin down quantum critical points, as is our aim (for extremely high accuracy calculations with bond dimensions in the thousands see [28]). Our error estimates are made based on both increased system size L and increased χ . Our largest system sizes are $L = 500$ and $\chi = 2000$. Mesoscopic corrections have been explored for the BHM in detail in our previous work [29].

Emergence of Critical Points – Figure 2 shows a finite-size scaling study of complex network measures on the mutual information calculated with matrix-product-state (MPS) code for these two models, for 1D lattices with $L = 14$ to 500, a range appropriate to experiments. Although we studied twelve measures, we selected the four most relevant for brevity: density of links D , clustering coefficient C , average disparity Y , and Pearson correlation between middle lattice sites, R . All four measures are clearly useful to identify phase transitions in the TIM and highlight different physical aspects. D is high in the TIM ferromagnetic and BHM superfluid phases where the nodes in the lattice are strongly connected, as sketched in Fig. 1(a). However, the quantum phase transition at the critical point is sharp at $L \rightarrow \infty$ for the TIM, where there is a Z_2 transition and $L \simeq 100$ suffices, whereas in the BHM we expect to observe a BKT crossover, which converges only for very large $L \simeq 1000$ [30], and is most apparent in the first and second derivative of D . The TIM paramagnetic and BHM Mott insulating phases are only sparsely connected. C follows a similar behavior except that for both the TIM

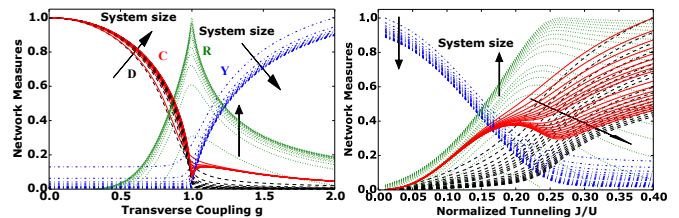


FIG. 2: *Complex network measures on the mutual information.* (a) Transverse quantum Ising model describing quantum spins (qubits). The clustering coefficient C (red) and density D (dashed black) serve as order parameters for the ferromagnetic phase. The average disparity Y (dot-dashed blue) identifies the short range correlations of the paramagnetic ground state. The Pearson correlation coefficient R (dotted green) develops a cusp near the critical point $g_c = 1$, identifying a structured nature to correlations near criticality. (b) Bose Hubbard model describing massive particles for commensurate lattice filling, with BKT crossover occurring in the limit $L \rightarrow \infty$ at a ratio of tunneling J to interaction U of $(J/U)_{\text{BKT}} = 0.305$; for smaller system sizes, the effective critical point [29] can be as small as $(J/U)_{\text{BKT}} \simeq 0.2$. The density and clustering coefficient grow as spatial correlations develop in the superfluid phase. The average disparity is high in the Mott insulator phase where correlations are short-ranged. Critical/crossover behavior is most evident in derivatives of these measures, see Fig. 3 and Table I. Note: all network measures have been self-normalized to unity for display on a single plot.

and BHM it develops a local minimum near the critical point. This reflects the fact that the average number of connected triples is temporarily growing faster the control parameter (g for the TIM, J/U for the BHM) for the average number of triangles. Physically this could be because the length scale of correlations has become as long as one lattice spacing but not two, resulting in a period of rapid increase in mutual information between nearest neighbors relative to second nearest neighbors. In strong contrast to D and C , in the TIM ferromagnetic and BHM superfluid phases Y asymptotically approaches $\frac{1}{L-1}$. In the TIM paramagnetic and BHM Mott insulating phases, where correlations decay exponentially, Y grows as spins become more tightly bound to their nearest neighbor relative to other qubits in the complex network. Finally, R has a completely different behavior, and clearly develops a cusp at the TIM critical point. Qualitatively, R is low in both the ferromagnetic and paramagnetic phases due to the collapse of the data onto single points in the $(\mathcal{I}_{\frac{L}{2},j}, \mathcal{I}_{\frac{L}{2}+1,j})$ plane when $g \ll 1$ and when $g \gtrsim 2$. In contrast, near criticality the weights display an approximately linear relationship. In this way R measures the non-trivial correlation that occurs near criticality.

Finite-size scaling – Figure 2(b) shows the BKT crossover transition for commensurate filling (average one particle per lattice site). However, a mean field phase transition at non-commensurate filling also appears in

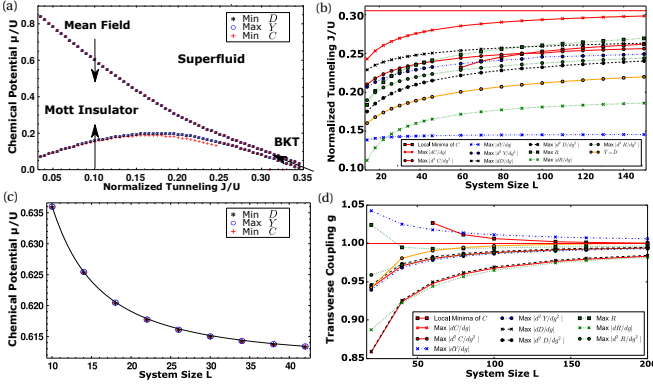


FIG. 3: *Finite-size scaling for the Bose-Hubbard model and transverse Ising model.* (a) BHM quantum phase diagram for fixed $L = 42$ showing superfluid and Mott Insulating phases with mean field phase transition along the Mott lobe and a BKT transition at its tip. (b) BHM BKT transition at unit filling. Scaling in $1/L$ places the critical point at $(J/U)_{\text{BKT}} = 0.316$ (clustering, solid red), 0.284 (average disparity, blue dot-dashed) and 0.281 (density, black dashed), respectively. Compare to the best value to date [28, 31] of 0.305, or the Luttinger liquid prediction of 0.328. (c) Approaching the BHM mean field superfluid/Mott insulator transition for fixed $(J/U) = 0.1$. Maximum disparity (blue circles), minimum clustering (red plus signs), and minimum density (black star) scale towards the commensurate-incommensurate phase boundary and lie closely on top of each other. (d) Scaling of multiple measures and their derivatives for the TIM, see also Table I.

the BHM. As the Mott insulating phase is gapped (meaning the energy to create an excitation, even in the $L \rightarrow \infty$ limit, is non-zero), the usual way to find the boundaries of the Mott lobe (the region encompassing the Mott insulating phase) is to compute the energy required to add a particle or a hole to the insulator: the chemical potentials $\mu_c^p = E^p - E_0$ and $-\mu_c^h = E^h - E_0$, respectively [30]. Then one uses finite-size scaling to extrapolate μ_c^p and μ_c^h in L^{-1} to estimate the phase boundary. Instead of working with chemical potentials, in Fig. 3(a) we use Y to obtain the first Mott lobe with both mean field and BKT crossover, shown here for $L = 42$. Figures 3(b)-(c) show finite size scaling in L towards the BKT crossover and the mean field phase transitions indicated in Fig. 3(a). Minimization of D results in similar estimates to Y . However minimization of C leads to slightly worse estimates as shown in Fig. 3(b). The BKT transition has been estimated by many methods in the past, including from the correlator $\langle \hat{b}_i^\dagger \hat{b}_{i+r} \rangle \sim r^{-K/2}$, taking advantage of the fact that at the critical point $K = 1/2$ [30], predicting $(J/U)_{\text{BKT}} = 0.29 \pm 0.01$; more recent results estimate $(J/U)_{\text{BKT}} = 0.305$ [28, 31]. By fitting curves like those shown in Fig. 3(b)-(c) (BHM) and Fig. 3(d) (TIM), to power laws of the form $(J/U)_c(L) = (J/U)_c + AL^{-1/\nu'}$ (BHM) and $g_c(L) = g_c + AL^{-1/\nu}$ (TIM) we perform

quantitative analysis of critical points in Table I. In particular, examining this data we observe that by measuring the complex network structure present in the quantum mutual information, we can estimate the critical point of the TIM to within 0.01% of its known value; that the Mott-insulator phase boundary can be reliably estimated by extremization of network quantities; and that the BKT transition at the tip of the Mott lobe, famously difficult to pin down without going to extremely large systems with 1000s of sites with high accuracy, can already be estimated to within 3.6% of its accepted value with just 80 sites.

Conclusions – We have shown that quantum complexity already emerges in a clearly quantifiable way in quantum states near quantum phase transitions in regular 1D lattices. In direct analogy to complexity of EEG/fMRI measurements on the brain, our measures are built on taking the quantum mutual information as a weighted adjacency matrix, and reliably estimate quantum critical points for well-known quantum-many body models, in particular the transverse Ising and Bose-Hubbard models. These models include three classes of phase transitions, Z_2 , mean field superfluid/Mott insulator, and a BKT crossover; in each case we obtain rapidly converging accuracy for critical point values, a demonstrable improvement in finite-size scaling over all other known methods including e.g. high order perturbation theory. Our work sets the stage for application of a new set of quantum measures to quantify complexity of quantum systems where traditional correlation measures are at best weakly applicable. In future work we will apply our new methods to far-from-equilibrium dynamics in such systems, for instance, quantum cellular automata [17, 18, 32, 33] and quantum degenerate ultracold molecules with a multiscale hierarchy of internal and external degrees of freedom.

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TABLE I: *Quantitative finite-size scaling analysis of quantum critical points.* Estimates for the critical point g_c and $(J/U)_{\text{BKT}}$ and scaling exponents ν, ν' for the transverse Ising and Bose Hubbard models, respectively, based on three complex network measures on the mutual information. We include in our analysis first and second derivatives (F.D., S.D.) since bare measures are often insufficient, an effect well-known from one-point entanglement measures like von Neumann entropy. We also note two other features: the local minimum in the clustering coefficient C (L.M.), and an intriguing point where normalized average disparity is equal to normalized density ($\tilde{Y} = \tilde{D}$). Entries are left blank where no significant feature appears in the complex network curves. Our complex network measures clearly perform as well or better than standard measures, particularly for the still improving estimates for the BHM BKT point [28].

Fit Parameter	Network Density D		Average Disparity Y		Clustering Coefficient C			Pearson Correlation R			$\tilde{Y} = \tilde{D}$
	F.D.	S.D.	F.D.	S.D.	L.M.	F.D.	S.D.	L.M.	F.D.	S.D.	
g_c	1.001 ± 0.001	1.001 ± 0.001	1.000 ± 0.002	0.999 ± 0.001	0.999 ± 0.001	1.000 ± 0.001	1.001 ± 0.001		1.02 ± 0.001	1.007 ± 0.001	1.002 ± 0.001
ν	1.07 ± 0.01	1.02 ± 0.03	1.2 ± 0.05	1.03 ± 0.02	0.352 ± 0.008	1.09 ± 0.01	1.05 ± 0.02		1.76 ± 0.16	1.82 ± 0.15	0.65 ± 0.01
$(J/U)_{\text{BKT}}$	0.281 ± 0.001	0.282 ± 0.001	0.146 ± 0.001	0.284 ± 0.001	0.275 ± 0.001	0.316 ± 0.001	0.278 ± 0.001	0.291 ± 0.06	0.199 ± 0.001	0.272 ± 0.002	
ν'	2.27 ± 0.06	2.58 ± 0.04	0.933 ± 0.02	2.88 ± 0.17	0.79 ± 0.03	1.69 ± 0.01	2.07 ± 0.07	1.56 ± 0.06	1.25 ± 0.01	2.3 ± 0.1	

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