Detecting Classical Phase Transitions with Renyi Mutual Information

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By developing a method to represent the Renyi entropies via a replica-trick on classical statistical mechanical systems, we introduce a procedure to calculate the Renyi Mutual Information (RMI) in any Monte Carlo simulation. Through simulations on several classical models, we demonstrate that the RMI can detect finite-temperature critical points, and even identify their universality class, without knowledge of an order parameter or other thermodynamic estimators. Remarkably, in addition to critical points mediated by symmetry breaking, the RMI is able to detect topological vortex-unbinding transitions, as we explicitly demonstrate on simulations of the XY model.

Introduction – The universality and importance of the concept of information is exploited widely in mathematics and the physical sciences. Information sets the fundamental limits in communication (or uncertainty), regardless of system, technology, or physical material. Shannon was the first to quantify information using the concept of entropy – a quantity that has its roots in thermodynamics [1]. It is therefore not surprising that deep ties exist between the measurement of thermodynamic quantities and concepts associated with information theory.

There is already a rich cross-fertilization between ideas in condensed matter physics and the information sciences. Most recently, information measures have been used to quantify “hidden” correlations in materials – exchanges of information that can occur between two parts of a system that are not manifest in traditional condensed-matter estimators (such as correlation functions) [2]. For example, in spin liquid phases, correlation functions can rapidly decay as a function of spatial separation; however, due to constraints, hidden correlations exist across vast distances of the sample [2]. These can be manifest in entropy quantities measuring the amount of communication between two regions of the sample [2]. These transition offer another testing ground for the use of information quantities in condensed matter systems. Critical points are associated with a diverging correlation length, suggesting the existence of long-range channels for information transfer. However, it is not obvious that measurable quantities associated with this information can be exploited to tell us anything about these phase transitions.

In this paper, we examine the Renyi Mutual Information (RMI), a measure that quantifies the amount of information contained in some region of a statistical mechanical system, about the rest of the system. Numerical measurements of classical mutual information [8, 9] typically calculate the reduced density matrix explicitly, a computationally expensive task, and use that to calculate the von Neumann entropy directly. The RMI on the other hand is easily measured in standard Monte Carlo routines via a replica trick [8, 9], rather than calculation of a reduced density matrix, making it immediately amenable to measurement on a vast number of models of interest to condensed matter, biophysics, and physical chemistry. We show that this RMI can be used in a practical way to identify phase transitions through finite-size scaling analysis on lattices of different sizes, without knowledge of an order parameter or any other thermodynamic quantity. We use the standard two-dimensional Ising model as a test case, demonstrating universality when results are compared to vastly different (even quantum mechanical [10]) models that exhibit the same universality class. Finally, we establish the ability of the RMI to detect the Berezinski-Kosterlitz-Thouless (BKT) transition, without relying on knowledge of any thermodynamic estimator such as the spin stiffness. This suggests the power of the RMI for detecting hidden transitions in a variety of other statistical mechanical models in the future.

Information, entropy, and the replica trick – Given a random variable $X$ one can quantify its associated uncertainty, or equivalently, the amount of information one is missing by not knowing the state of $X$. There are various ways that this information can be embodied, for example in the generalized Renyi entropies [11],

$$S_\alpha(X) = \frac{1}{1-\alpha} \ln \left( \sum_{i \in X} p_i^\alpha \right),$$  \hspace{1cm} (1)

where $p_i$ is the probability of outcome $X = i$. Taking the limit $\alpha \to 1$, one recovers Shannon’s familiar entropy, $S_1 = -\sum_i p_i \ln(p_i)$, which can be related to the thermodynamic entropy of a statistical mechanical system $S = \ln \Omega$, where $\Omega$ is the number of microstates, assuming all occur with equal probability. This relationship is often exploited in the study of real physical systems through microscopic statistical mechanical models.

In such systems, one may also ask how much knowledge of a subsystem (call it $A$) is possible, assuming complete knowledge of another subsystem $B$. Correlation functions are a common example that incompletely quantify...
This knowledge. In this paper, let us instead define a spatial subregion \( A \) as the complement of \( B \), so that \( A \cup B \) is the complete system; we could say that \( p_{i A} \) is the probability of state \( i_A \) occurring in region \( A \). The state \( i_A \) can be any classical (or even quantum) state: we will restrict our focus mainly to classical spin systems.

From Boltzmann, the probability of a state occurring is 
\[
p_{i A, i_B} = e^{-\beta E(i_A, i_B)}/Z,
\]
where \( E(i_A, i_B) \) is the energy associated with states \( i_A \) in region \( A \) and \( i_B \) in region \( B \), and 
\[
Z = \sum_{i_A, i_B} e^{-\beta E(i_A, i_B)}
\]
the partition function. To obtain only the probability of a certain state in \( A \), we can instead sum over all possible states in \( B \), 
\[
p_{i A} = \sum_{i_B} e^{-\beta E(i_A, i_B)}/Z.
\]
The appropriate sums of \( p_{i A, i_B} \) or \( p_{i A} \), raised to the power \( \alpha \), give the Renyi entropies in a straightforward way. In equilibrium statistical mechanical systems, estimators based on sums such as these are commonly calculated using importance sampling techniques, i.e. Markov chain Monte Carlo.

In this paper we mostly restrict our discussion to the second Renyi entropy, which requires sums of the probabilities \( p_{i A, i_B} \) or \( p_{i A} \) squared. For example, to get the entropy of region \( A \) we use, 
\[
p_{i A}^2 = \left( \sum_{i_B} e^{-\beta E(i_A, i_B)} \right) \left( \sum_{i_B} e^{-\beta E(i_A, i_B)} \right)/Z^2,
\]
leading to
\[
S_2(A) = -\ln \left( Z^{-2} \sum_{i_A} \sum_{i_B} e^{-\beta (E(i_A, i_B)+E(i_A, i_B))} \right)
\]
\[
= -\ln(Z[A, 2, T]) + 2\ln(Z[T]),
\]
where we have defined a “replicated” partition function 
\[
Z[A, 2, T][\Omega_0], \text{ which can be sampled via a Monte Carlo simulation procedure described in the next section.}
\]

Note that, while the Renyi entropies tell us about uncertainty in the full system or part of the system, they do not reveal the correlations or information between two regions of a system. For this we introduce the RMI,
\[
I_\alpha(A; B) = S_\alpha(A) + S_\alpha(B) - S_\alpha(A \cup B).
\]
This measure defines in a precise way the information that a full knowledge of \( B \) gives us about \( A \), or vice versa. From \([2]\), the RMI can be related to a difference in free energies. Note, the free energy in a typical condensed-matter system with a \( D-1 \) dimensional boundary generally \([13, 12]\) behaves as 
\[
F = aL^D f(T) + b f_B(T),
\]
where \( f \) and \( f_B \) are the size-independent free energy densities, and \( \ell \propto L^{D-1} \). The thermodynamic behavior of the RMI, which is constructed to cancel contributions arising from the bulk, is determined by this boundary free energy - restricting it to at most “area law” scaling \( I_\alpha \propto \ell \). As we will see next, subleading corrections to this area law make the RMI an extremely useful tool for detecting phase transitions in finite-size systems.

**Thermodynamic behavior** - A key observation that enables the widespread utility of the RMI for integer \( \alpha \geq 2 \) is that, for any physical system, the calculation of \( S_\alpha(A) \) can be accomplished via the replicated system geometry, 
\[
Z[A, \alpha, T] \text{ (Fig. 1).}
\]
For \( S_2(A) \), the form of the Boltzmann factor effectively constrains states in \( A \) to be equal between the two replicas, while states in \( B \) are unconstrained between replicas. This *replica trick* \([12]\) leads to the practical method for measurement of \( S_2 \) in Monte Carlo simulations discussed in the next section. In addition, it facilitates the general understanding of the RMI in the thermodynamic limit, as we now discuss.

We observe that, in addition to the general expectation that the RMI contains an “area law” term, important subleading constant corrections may occur. In the simplest case, where \( \Omega_0 \) symmetry-broken ground states exist at a temperature far below \( T_c \), both \( Z[T] = \Omega_0 \) and 
\[
\Omega_0 = Z[A, 2, T].
\]
Generalizing Eq. (2), the RMI is then,
\[
I_\alpha(A; B) = \frac{1}{1-\alpha} \left( \ln(Z[A, \alpha, T]) + \ln(ZB, B, \alpha, T) \right) - \alpha \ln(Z[T]) + \ln(Z[A \cup B, \alpha, T]) \right) = \ln(\Omega_0),
\]
i.e. some positive constant independent of Renyi index. When \( T > 0 \) and fluctuations are included, this positive constant is added to the area law term discussed above.

Next, in the intermediate temperature range \( T_c < T < \alpha T_c \), the “unconnected” region \( B \) of the replicated system is above criticality, whereas the “connected” part \( A \) of the simulation is effectively below \( T_c \) due to the constraint on \( A \). If each above-critical degree of freedom in the system can realize \( \sigma \) different states, coarse-graining on the length scale of the correlation length \( \xi \) results in a partition function of 
\[
Z[T] = \sigma^{N/\xi^D}.
\]
The replicated partition function, on the other hand, has a reduction in the number of accessible states since the \( \alpha \) above-critical regions are connected to a below-critical region through the boundary of length \( \ell \), which eliminates \( \mathcal{O}(\ell^D) \) lattice degrees of freedom in each of the unconstrained regions,
giving $Z[A, \alpha, T] = \Omega_0 \sigma^{(\alpha N_\text{tot} - \alpha \xi)} / \xi^D$. Eq. [4] then gives

$$I_\alpha(A;B) = \frac{1}{1 - \alpha} \left( \ln \Omega_0 \sigma^{(\alpha N_\text{tot} - \alpha \xi)} / \xi^D + \ln \Omega_0 \sigma^{(\alpha N_\text{tot} - \alpha \xi)} / \xi^D - \alpha \ln \sigma^N / \xi^D - \ln \Omega_0 \right)$$

$$= \frac{1}{1 - \alpha} \left( \ln \Omega_0 - 2 \alpha \ell / \xi^{D-1} \ln \sigma \right). \quad (5)$$

This gives a constant part of the RMI, $c = - \ln \Omega_0 / (\alpha - 1)$ and a positive area law part $\ell (2 \alpha \ln \sigma / (\alpha - 1) \xi^{D-1})$.

Importantly, we see that the constant part of the RMI changes sign as we pass through $T_c$. It can be seen in our finite-size Monte Carlo data that the presence of this constant $c$ will cause the $I_\alpha/\ell$ curves to “fan out” away from $T_c$ for different $\ell$, while $c = 0$ precisely at $T_c$, producing a striking crossing in the curves.

**Monte Carlo Algorithm** – The form of the replica trick suggests a straightforward way to measure the Renyi entropy using a modified simulation geometry (Fig. 1). The constraint on region $A$ demands that, to be accepted, an update must affect states on the same physical lattice site in all replicas – effectively reducing the temperature of region $A$ by a factor of $\alpha$, as discussed above.

Using this modified simulation we can generate states according to the probability $p^2_\alpha$. In general, generating states from a partition function via Monte Carlo does not allow direct calculation of the partition function (or the free energy) itself in an efficient manner. To overcome this, one approach used previously [12] is to integrate the energy estimator starting from $T \to \infty$, obtaining the Renyi entropy at some finite $T$ from both a replicated simulation and an unreplicated simulation. This necessitates a schedule of simulations over a large range of temperatures to gather enough detailed knowledge of the energy for an accurate integration [17].

**Results on models** – Using conventional Monte Carlo simulations of several models, we demonstrate the use of the second RMI to detect finite-temperature phase transitions. In the following, we use $I_2(A;B)$ where $A$ and $B$ are complementary regions, each defined as an $L \times L/2$ cylinder embedded in the $L \times L$ torus.

The first model we examine is the classical Ising model on a two-dimensional square lattice $H = -J \sum_{\langle i,j \rangle} S_i^z S_j^z$, where $S_i^z = \pm 1/2$. There exists a transition on an ordered phase at a temperature $T_c/J = 2 / \log(1 + \sqrt{2}) \approx 2.269$ [13], which offers us the simplest test for the RMI. Figure 2 illustrates $I_2(A;B)/\ell$ where $\ell$ is the length of the boundary between the regions (in all cases hereafter, $\ell = 2L$). Close inspection indicates approximate crossings of the $I_2(A;B)/\ell$ curves at $T_c$ and $2T_c$. Examining the crossings as we move to larger system sizes we see that they extrapolate towards the transition temperature. Knowing that the correlation length at the Ising transition behaves as $\xi \sim |t|^{-\nu}$ with $t = (T - T_c)/T_c$ and $\nu = 1$, one can derive a finite-size scaling behavior for the crossing temperature $T(L)/T_c \propto 1/L$. This is confirmed by the data in the lower panel of Fig. 2.

Remarkably, this behavior mimics the crossing seen previously in the analogous RMI quantity based on the entanglement entropies in a quantum spin-1/2 XXZ model [12, 16]. That model also realizes a finite-temperature critical point, in the 2D Ising universality class (however at a different $T_c$, which is non-universal). There, it has been argued that the crossings were a manifestation of criticality, with the scaling form [10],

$$I_2(A;B) = [c_1(t) + t \log t] \cdot \ell + c_2(t) + O(1/\ell). \quad (6)$$

It is important to note that $c_1(t)$ can be polynomial in $t$, where the strict “area law” at $t = 0$ is caused entirely by its constant piece crossing zero ($\Omega_0 = 2$ in Eqs. 4 and 5). Divergences in derivatives of $I_2(A;B)$ are caused by the $t \log t$ contribution. This term is known from the $t \log t$ divergence in the boundary free energy as $t \to 0$ for the square lattice Ising model with a field applied to the boundary on an infinite half plane [17, 18]; we can thus use it as a test of universality in this model.

In Fig. 2, $\partial I_2/\partial t$ shows the predicted log $t$ singularity, confirming that this critical point lives within the 2D Ising universality class.

We turn now to Monte Carlo simulations of the classical 2D XY model on a square lattice, $H = -J_{XY} \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)$. This is a model with continuous spin variable $0 \leq \theta_i < 2\pi$ that undergoes a BKT transition from a phase with free vortices to one with bound vortex-antivortex pairs. Numerically, the detection of the BKT transition is much more subtle than the Ising phase transition, since it has no local order parameter and standard scaling theory on thermodynamic
estimators (such as the specific heat) does not work. In 2D, this is circumvented by measuring the “spin stiffness” and making use of a special universal jump condition, $T_{\text{BKT}} = \pi \rho_s/2$. – a procedure that has found $T_{\text{BKT}} = 0.89294(8)$ [21]. However, one may wonder if the RMI can detect this phase transition without any need for such specialized measurements.

To address this, we examine the RMI for the classical XY model, shown in Figure 3. One can clearly see the development of crossings in the quantity $I_2/\ell$ near the value of $T_{\text{BKT}}$ and $2T_{\text{BKT}}$ – strong indication that universal scaling is coming into play. To examine this further, in the inset we illustrate the RMI for a completely different model, the quantum XY model

$$H = -t \sum_{(ij)} \left( b_i^\dagger b_j + b_i b_j^\dagger \right),$$

computed using Stochastic Series Expansion QMC where the quantum RMI is generated using a broad histogram approach [14]. In this case, similar crossings appear at the (non-universal) $T_{\text{BKT}} \approx 0.343$, giving strong evidence in support of the universality of our result that the RMI can detect the BKT transition.

However, unlike the relatively “clean” crossing of the 2D Ising critical point, these crossings have a larger finite-size scaling component. Figure 4 contains a detailed finite-size scaling analysis for the XY model. This shows fits to two finite-size scaling forms which are derived by setting the correlation length near the critical temperature, $\xi = e^{-b/\sqrt{3}(1+O(t))}$ [22], equal to the linear system size $L/L_0$ with $t = (T - T_{\text{BKT}})/T_{\text{BKT}}$. Then by relating the temperature $T$ with the finite-size transition temperature $T(L)$, we derive:

$$T_{\text{BKT}}(L) = T_{\text{BKT}}(\infty) \left[ 1 + \frac{b^2}{\log^2(L/L_0)} + \frac{c}{\log^2(L/L_0)} \right].$$

Note, typical finite-size scaling analyses set the coefficient $c$ equal to zero, effectively ignoring subleading $O(t)$ corrections to the correlation length. Using this finite-size scaling form, the data for the crossing of $I_2/\ell$ convincingly approaches $T_{\text{BKT}}$ in the limit of $L \to \infty$.

Discussion – The Renyi Mutual Information (RMI) is a quantity able to detect all correlations in a physical system, even those missed by traditional connected correlation functions. We have introduced a practical method to calculate the RMI using a modification of standard Monte Carlo techniques for classical statistical mechanical systems. We demonstrated that the RMI associated with the second Renyi entropy, $I_2$, is able to identify both conventional critical points, as well as the BKT transition where standard scaling theory breaks down. A straightforward finite-size scaling analysis of $I_2$ is sufficient to identify each phase transition, without knowledge of an order parameter, broken symmetry, or critical theory.

The ease of implementation of the RMI measurement in any standard Monte Carlo routine could stimulate adoption to simulation studies in many fields of the physical sciences and beyond. The RMI will likely find great utility in many classes of classical models, such as generalized XY models with “hidden” transitions [23] or loop [24, 25] and dimer models [26, 27] where universal properties of exotic criticality may be manifested [28]. Also particularly pressing is the question [29] of whether RMI can detect unconventional transitions in disordered or glassy systems [30, 31]. Finally, the ubiquity of the Monte Carlo method in such far-reaching fields as humanities or finance may precipitate the use of RMI in a host of unforeseen applications, such as detecting transitions linked to financial market crashes [34].
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[37] Alternatively, it may be possible to use methods able to directly extract the ratio of partition functions at a given temperature, as done previously for the analogous quantum method 33.