Information Flow in First-Order Potts Model Phase Transition

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Phase transitions abound in nature and society, and, from species extinction to stock market collapse, their prediction is of widespread importance. In earlier work we showed that Global Transfer Entropy, a general measure of information flow, was found to peak away from the transition on the disordered side for the Ising model, a canonical second-order transition [1]. Here we show that (a) global transfer entropy also peaks on the disordered side of the transition of finite first-order transitions, i.e., those which have finite latent heat and no correlation length divergence, such as ecology dynamics on coral reefs [2], and (b) analysis of information flow across state boundaries unifies both transition orders. We obtain the first information-theoretic result for the high-order Potts model and the first demonstration of early warning of a first-order transition. The unexpected earlier finding that global transfer entropy peaks on the disordered side of a transition is also found for finite first-order systems, albeit not in the thermodynamic limit. By noting that the interface length of clusters in each phase is the dominant region of information flow, we unify the information theoretic behaviour of first and second-order transitions.

Numerous mechanisms for predicting phase transitions exist, applied for example, from core science and engineering through biology, ecology, medicine and finance [3]: increased variance and critical slowing down [3]; flickering [4]; and a peak in the global transfer entropy [1, 5] (Eqn. 1). Two important models of equilibrium transitions stand out: the Ising model [6], a binary spin system on a square lattice, where each point on the lattice has a binary spin; and the Potts model, which generalises Ising to spins with an arbitrary number of states, q, and reduces to the Ising model for q = 2.

Transfer entropy, T, measures (Eqn. 2, Eqn. 4, suppl. material) information flow from one stochastic process, Y, to another, X—in this case the states of two neighbouring spins over time. Global transfer entropy, G, measures the average information flow of the entire system to individual spin sites:

\[ G = \frac{1}{N} \sum_i T_{s_i \rightarrow s_i} \]  

We note however, that all information—no matter its origin in the lattice—must flow to s_i via its neighbours or its own past, and thus consider only the immediate neighbourhood of each site (including s_i) rather than s in Eqn. 1 [1]. As with T, G ≥ 0 with G = 0 iff each site s_i, conditioned on its past, is independent of its neighbours.

In the Ising model [6], mutual information peaks at the transition between ordered and disordered phases [7, 8]. The pairwise transfer entropy [9] (Eqn. 4, suppl. material), a measure of information flow between spins also peaks at the transition (suppl. material, but the global transfer entropy (Eqn. 1), measuring information flow from all spins to any given spin, peaks on the disordered side [1] regardless of lattice size.

The q-state Potts model [10] exhibits increasingly first-order phase transitions for q > 4 [11]. At q = 5 the transition is weakly first-order, implying a long correlation length and low latent heat. As q increases the correlation length decreases and the latent heat increases. We show that as the system becomes more strongly first-order (i.e., q > 7) the behaviour of G diverges from the second-order behaviour: in the thermodynamic limit, G becomes discontinuous at the transition temperature, T_c, peaking at T_c^+. We go on to provide a unifying framework for both transitions, based on the phase interface.

The standard Potts model comprises a lattice of spins with periodic boundary conditions and size N = L x L, where the system state is s = s_1, ..., s_N, with s_i ∈ {1, ..., q}. The interaction energy between two neighbouring sites is E_{ij} = -J δ(s_i, s_j) giving the Hamiltonian \[ H = -J \sum_{i,j} \delta(s_i, s_j) \], where interaction strength J = 1, δ(x, y) is the Kronecker delta function which is one if x = y and zero otherwise, and (i, j) are all interacting pairs of sites in the system, in this case nearest cardinal neighbours. Local site energy, E_i, is defined similarly, fixing site i and summing over its four neighbours.

Overall alignment of the lattice is measured by its magnetisation, M = (q<s_m> - 1)/(q - 1) [12], where s_m is the mode state and \[ <s_m> = \sum_s s/s_m/N \] is the proportion of the dominant state over all sites, ranging from q^{-1} to 1, giving magnetisation in the range [0, 1]. M serves as the order parameter with order-disorder transition occurring
at temperature [13]

\[ T_c = \left[ \log(1 + \sqrt{q}) \right]^{-1}, \]  

(2)

where the (thermodynamic) system is disordered (\( M = 0 \)) at temperatures above \( T_c \) and non-zero below \( T_c \). The behaviour at \( T_c \) defines the transition order, where \( q \leq 4 \) has continuous \( M \) (and discontinuous \( dM/dT \)) giving a second-order phase transition.

Unlike the Ising model, direct simulation of the Potts models for high \( q \) is not straightforward, since the first-order transition shows a void region of energy space around the phase transition. For temperatures close to the critical temperature, the energy distribution \( P(E) \) is bimodal (See suppl. material, Fig. 1), such that single spin update schemes, such as Glauber dynamics, are very unlikely to enter this region, and thus fully explore the energy space. On the other hand, cluster update schemes such as Swendsen-Wang dynamics [14] flip large groups of spins in each update-step. This can lead to an energy change in the configuration large enough to cross the energy void.

Thus we estimate \( G \) using \( 10^5 \) and \( 10^6 \) Swendsen-Wang cluster updates to approach equilibrium followed by \( 10^5 \) Glauber sweep steps comprising \( N \) spin-flip attempts per sweep. We also estimate \( G \) with a second regime using the density of states, \( d(E) \), calculated with the Wang-Landau algorithm [15]. \( P(E) \) may then be calculated from

\[ P(E) = d(E) \exp(-E/[k_b T]), \]  

(3)

where \( E \) is the lattice energy. Since \( G \) depends upon two consecutive updates it also depends on the temperature, which determines the update statistics. \( G \) may now be determined from its value as a function of \( \Gamma(E,T) \) [16]:

\[ G(T) = \frac{\sum_E \Gamma(E,T)P'(E)}{\sum_E P'(E)}, \]  

(4)

where \( \Gamma \) is \( G \) measured at temperature, \( T \), and energy, \( E \), and \( P'(E) \) is the distribution of energies, and has been rescaled for visualisation and computational reasons [17].

Therefore we in fact need to determine \( \Gamma(E,T) \) for varying \( T \), rather than \( \Gamma(E) \). Additionally, as \( P(E) \to 0 \) for many values, \( \Gamma(E,T) \) can be measured more simply by culling energy values where \( P(E) \) is sufficiently low—that is, reaching every \( E \) is unnecessary and thus \( \Gamma(E,T) \) can be calculated via Glauber dynamics rather than Wang-Landau updating.

In the Swendsen-Wang and Glauber regime, which we denote \( G^{(s)} \), we collate statistics—the site, its neighbours and its future—for each site of the lattice after each Glauber sweep. We collate ensemble statistics for \( \Gamma(E,T) \) in a similar fashion, for varying \( T \) and using lattice energy \( E \) prior to the Glauber sweep. We note however that the choice of \( N \) spin-flip attempts for a Glauber sweep is to reduce intersample correlations compared to individual spin-flips and that each flip happens in serial rather than in parallel. While this is fine in \( G^{(s)} \), as Glauber dynamics maintain detailed balance, for \( \Gamma(E,T) \) we collate statistics according to their specific \( E \) value while also noting that \( G \) is a temporal quantity. Thus each spin-flip attempt during a sweep will have its own \( a priori \) and \( a posteriori \) states as well as its own energy value, \( E' \), which may not necessarily equal \( E \) and therefore statistics should ideally be collated into \( \Gamma(E',T) \) rather than \( \Gamma(E,T) \). Thus to explore the effect of sweep size, we employ two timescales for the density of states approach: the typical \( N \) spin-flip sweep \( (G^{(s)}) \) and the minimum, single spin-flip \( (G^{(f)}) \).

\( G \) is estimated via plug-in discrete entropy histogram-based estimators from a single realisation with settling time of \( 10^5 \) or \( 10^6 \) Swendsen-Wang update-steps, followed by a measurement sequence of \( 10^5 \) time steps (using Glauber dynamics). Standard error is calculated by repeating the experiment 10 times. We optimise simulation by modifying initialisation dependent on \( T \). Realisations are initialised to the disordered regime (i.e., each site is set, independently and uniformly, to a random state). Experiments involving the density of states approaches are constructed likewise, minus the superfluous (in this regime only) settling time. Setting time is unnecessary in this regime since we calculate \( G \) directly via Eqn. 4, where the distribution of energies is calculated beforehand and thus any \( G \) measured is useful, not just those at equilibrium.

The six dimensions (a site, its four neighbours and its future) of \( q \) elements in each dimension necessitate infeasibly many data points to accurately calculate \( \Gamma(E,T) \). But since transition probability of a spin-flip depends only upon the number of spins matching the initial and final spins, rather than the spatial configuration of the neighbouring states, it is possible to substitute the neighbour dimensions with the current site energy \( E_s[18] \). This regime was validated by applying it to \( G^{(f)} \), giving \( G^{(s)} \) (shown in the supplementary materials).

Both timescales exhibit a peak in \( G \) on the disordered side of the transition (Fig. 1), with per-sweep versus per-flip statistics differing by a roughly constant factor: the statistics collated for \( G^{(s)} \) can be considered equivalent to those collated for \( G^{(f)} \) with a small amount of random noise added (i.e., those statistics collated for \( \Gamma(E,T) \) with an initial energy of \( E' \neq E \), as mentioned above), thus reducing the information flow and therefore \( G^{(s)} \approx cG^{(f)} \), with \( 0 < c < 1 \). \( G^{(f)}, G^{(s)} \), exhibit a strong shift in \( G \) peak as \( q \) and lattice size increase, rapidly approaching the critical temperature. Thus for the first-order transition maximum \( G \) occurs at the critical temperature in the thermodynamic limit. Note the system displays strong finite size effects. \( L=128 \) gets very close to
the transition line (computational limitations precluded further increases in \( L \)). The same behaviour is visible in the top tryptich of Fig. 1 using Swendsen-Wang updates to achieve approximate equilibrium.

Conversely, for finite systems, \( \mathbf{G} \) peaks distinctly on the disordered side of \( T_c \) (and the “effective” transition temperature \( T_c(L) \) Fig. 1 [19]), thus demonstrating an early warning of an impending first-order transition when approaching from the disordered side, similar to that previously demonstrated for Ising model systems [1].

Finally, we look at a physical understanding of the behaviour of \( \mathbf{G} \). Intuitively, information flows when neighbour states differ, hence zero information flow in ground states. This behaviour necessarily extends to clusters of states, implying information flow occurs on the boundaries, or interfaces, between clusters (See Fig. 2). It seems reasonable then to assume that information flow scales with number of interfaces. However, such a maximum coincides with the zero-energy fully-disordered regime, where quite clearly \( \mathbf{G} = 0 \). This assumption neglects the temporal nature of \( \mathbf{G} \), which is disrupted at high temperature.

The average interface length is defined as:

\[
\langle I \rangle = \frac{\sum_{x}^{N_I} I_{(x,l)}}{N_I},
\]

where \( N_I \) interface lengths are found by performing a “turn-right walk” procedure, similar to Saberi [20], on every unmarked edge between adjoining lattice sites of differing states. Edges are marked in association with an adjoining site (such that each edge is ultimately marked zero or twice). This prevents a cluster from counting its perimeter (of length \( N_i \)) \( N_i \) separate times, but accounts for interface boundaries between clusters of two or more differing states. This also addresses clusters with two or more disjoint interfaces, i.e., a 2D doughnut.

\( I(T) \) is calculated from \( I(E) \) and Eqn. 4 (where \( I(E) \) replaces \( \Gamma(E,T) \)) with the weighted Wang-Landau update scheme [15]. Each \( E \) value sampled at minimum 5000 times, up to a maximum of 10000 samples.

Remember that \( \mathbf{G} \) is a measure of a site’s dependence on neighbouring sites, conditioned on its own past. At high temperature, spin-flips are essentially random, choosing new states with little influence from neighbours. As temperature decreases, neighbour influence increases, leading to clusters of similar sites. We can thus approximate average influence by probability of cluster size, \( p(c) \). This influence is the manifestation of information flow in the system, but only on cluster boundaries (since information flow is conditioned on its own past), leading to:

\[
\mathbf{G} \propto \sum_{c} p(c)L_c,
\]

where \( L_c \) is the boundary length of cluster of size \( c \). Note however that when clusters get sufficiently large—i.e., on the order of system size \( L \)—they no longer have an outer perimeter and are instead defined by the holes created by other clusters (Fig. 2, bottom). Thus for this dominant cluster to increase in size, the internal holes must shrink and its boundary length \( L_c \) actually falls. As temperature decreases, influence increases, but the available sites to transfer influence decreases, hence total information flow \( \mathbf{G} \) falls.

We note that Eqn. 6 is essentially the average interface length as defined in Eqn. 5. There should thus be some relationship between average interface length and net information flow in the lattice.

The intuitive interface model of Eqn. 6, shown in Fig. 3, gives a remarkably good match to the \( \mathbf{G} \) trends, peaking in the disordered regime in all cases, and converging to \( T_c \) only where systems become more strongly first-order (increased \( q \) and increased \( L \) for \( q > 4 \)). In the \( q = 2 \) Ising case, interface peak location remains stable at increasing lattice sizes, as does \( \mathbf{G} \) peak location [1].

Thus the average interface length is a suitable theoretical justification for \( \mathbf{G} \), fitting the behaviour for the first- and second-order transitions into a single unified framework.

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Figure 1. $G$ measured using three methods (top: $G^{(s)}$, bottom: $G^{(f)}, G^{(e)}$), with $q = 5, 7, 10$ (columns) for $L = 32, 64, 128$. $G^{(s)}$ simulated for $10^5$ Swendsen-Wang update-steps, followed by $10^5$ Glauber measurement time-steps. $G^{(f)}, G^{(e)}$ estimated using just $10^5$ Glauber measurement time-steps. Vertical lines indicate $T_c$. Filled symbols indicate “effective” $T_c(L)$, the location where $P(E)$ is precisely bimodal for given $q, L$, corresponding to values found in analytical methods [19]. Error bars calculated from 10 repetitions and are smaller than symbols in some regions. Gap between data included in $G^{(s)}$, with $q \in \{2, 5, 7, 10\}$ for indicated lattice sizes. The behaviour in peak location mimics the behaviour of the $G$ peak in all systems: the first-order cases, $q \in \{5, 7, 10\}$, converge to $T_c$ as the system becomes more strongly first-order (increased $q, L$), while the second-order peak $q = 2$ remains stable above the phase transition. Note the factor of two difference in temperature for $q = 2$ and Ising results is simply due to a slight difference in definition of site energy (i.e., $E_i$), with no further side effects.

Figure 2. Interfaces for $q = 5$ lattice sampled from $T = T_c$ (0.8515) (Top) and $T = 0.5$ (Bottom) where each square is a lattice site. Top: Arrows show the counter-clockwise path interface walker (for large cluster) takes around complex interactions. Labelled clusters, while sharing the same state, are disjoint, and thus have separate interfaces. Average interface length is $(34 + 3\cdot 8 + 3\cdot 6 + 9\cdot 4)/16 = 7$. Bottom: When one cluster dominates, it no longer has an “outer” perimeter. Average interface length is $(6 + 4\cdot 4)/5 = 4.4$.

Figure 3. Average interface length for systems with $q \in \{2, 5, 7, 10\}$ for indicated lattice sizes. The behaviour in peak location mimics the behaviour of the $G$ peak in all systems: the first-order cases, $q \in \{5, 7, 10\}$, converge to $T_c$ as the system becomes more strongly first-order (increased $q, L$), while the second-order peak $q = 2$ remains stable above the phase transition. Note the factor of two difference in temperature for $q = 2$ and Ising results is simply due to a slight difference in definition of site energy (i.e., $E_i$), with no further side effects.

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SUPPLEMENTARY MATERIAL

Glauber Dynamics

The system is updated using Glauber dynamics [1], where site $s_i$ transitions to state $s_k$ with probability

$$P(s_i \rightarrow s_k) = \left[1 + e^{\Delta E_{ki}/(k_B T)}\right]^{-1},$$

where $T$ is the system temperature, Boltzmann’s constant, $k_B$ is taken as one, and $\Delta E_{ki}$ denotes the difference in site (or system) energy should the flip occur—i.e., $\Delta E_{ki} = E_k - E_i$. This transition probability biases spin-flips towards lower energy states—where the ground state occurs at minimum energy when all sites take the same state—while the system temperature inhibits this bias, which disappears as $T \rightarrow \infty$ such that spins flip to random states with probability 0.5. Glauber dynamics satisfy detailed balance [2] and thus yield the thermal equilibrium probabilities at stationarity. However, close to the phase transition, it can take a large number of time steps to reach equilibrium, thus a faster, cluster update, Swendsen-Wang if used. To calculate the information theory quantities a statistics collection series of Glauber updates is carried out.

Transfer Entropy

Transfer entropy measures information flow from one stochastic process, $Y$, to another, $X$—in this case the states of two neighbouring spins over time. It is a non-negative quantity, reaching zero iff process $X$, conditioned on its own past, is independent of the past of $Y$. Positive values indicate a statistical dependency—i.e., a reduction in uncertainty—of $X$ given knowledge of the past of $Y$. Transfer entropy is given by the time-lagged mutual information, conditioned on the past of $X$:

$$T_{Y \rightarrow X} = I(X_t : Y_{t-1} | X_{t-1}) = H(X_t | X_{t-1}) - H(X_t | X_{t-1}, Y_{t-1}),$$

where we use a single-step time-lag and the pairwise transfer entropy is simply the average transfer entropy over all interacting sites:

$$T_{pw} = \frac{1}{N} \sum_{(i,j)} T_{s_i \rightarrow s_j}. \quad (4)$$

Energy Space

First-order transition show a void region of energy space around the phase transition, such that single spin update schemes, such as Glauber dynamics, are very unlikely to enter this region. In fact, for temperatures close to the critical temperature, the energy distribution $P(E)$ is bimodal (See Fig. 1—note a scaling factor is introduced such that peak maximum is one). As $q$ decreases, the peaks shift closer together until they merge into a unimodal peak at $q = 4$ (characteristic of a second-order transition). The valley between peaks is shallower for given lattice size at lower $q$, thus $q = 5$ is considered weakly first-order, while $q = 10$ is strongly first-order. As $L$ increases (with constant $q$) the valley deepens, making simulation for large lattices, particularly at $q = 10$, increasingly difficult.

Neighbourhood Compression

As discussed in the main paper, capturing data for $G$ requires a 6D histogram—one dimension for each neighbour, current spin, and future spin—which requires $q^{12}$ data points for effective estimation (using the heuristic $B = \sqrt{N}$ [3], where $B = q$ is the number of bins in each dimension of the histogram). This volume of data is difficult, yet achievable, for a single histogram (as in $G^{(q)}$), but completely infeasible for $E$ histograms, to calculate $\Gamma(E, t)$ as required in $G^{(s)}$ and $G^{(f)}$. To compress the histogram, we note that the transition probability depends only upon the number of spins matching the initial and final spins, rather than the exact neighbouring states. An intuitive approach replaces the neighbour dimensions with the energy delta term, $\Delta E_{ki}$, as this should encode all transition information. This approach is incorrect however as it incorporates information about the future state directly into the conditioned variables.
in the second term of Eqn. 3—that is, $Y_{i-1}$ incorrectly becomes some function of $X_t$.

Thus we encode just the current site energy, $E_i$, although not without trade-off: removal of neighbour details leads to consistent reduction in total available information (See Fig. 2, top row). This approach was validated with an alternative reduction with consistent results—where the binary function, $\delta(s_i, s_j)$, is used for each neighbour. These approaches give significant reductions in data requirements—$(5q^2)^2$ and $(2^4q^2)^2$ respectively. The former approach was employed as it requires fewer bins, and thus data points, without effect on the result.

### Limiting Behaviour

The limiting behaviour of $G$ can be determined via closer analysis of $\Gamma(E, T)$. Figure 3 shows $G^{(f)}(E, T)$ and $P(E)$ at $q = 10, L = 128$ for selected temperatur-
Figure 2. Figure 1 (main text) repeated with validation from $G^{(e)}$. Note that $G^{(e)}$ tracks $G^{(g)}$ with a constant reduction due to information lost in the compression algorithm.

Figure 3. $G^{(f)}(E,T)$ (top) for selected temperatures at and above $T_c$ with $P(E)$ (middle) for $q=10$, $L=128$ with 10 realisations, half initialised to random ground states and half to disordered states. For temperatures near $T_c$, we observe a valley in $G^{(f)}(E,T)$ as in $P(E)$, where realisations are unable to traverse. As $T$ increases, central energy values are reachable, with lower energy values becoming unreachable—note that $G^{(f)}(E,T)$ drops to zero at $E/N \approx -1.75, -1.3$ for $T = 0.707, 0.710$, respectively. Bottom shows $G^{(f)}(E,T)$ average over $T$ where each $G^{(f)}(E)$ is scaled with respect to frequency over $E$. 