

Synergistic Motifs in Gaussian Systems

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(Received 15 September 2025; accepted 26 February 2026; published 25 March 2026)

High-order interdependencies are central features of complex systems, yet a mechanistic explanation for their emergence remains elusive. Currently, it is unknown under what conditions high-order interdependencies, quantified by the information-theoretic construct of synergy, arise in systems governed by pairwise interactions. We solve this problem by providing precise sufficient and necessary conditions for when synergy prevails over low-order interdependencies in the weak interaction regime; namely, we prove that antibalanced (highly frustrated) correlational structures in Gaussian systems are sufficient for synergy dominance and that antibalanced interaction motifs in Ornstein-Uhlenbeck processes are necessary for synergy dominance. We validate the applicability of these analytical insights beyond the weak interaction regime, as well as in Ising, oscillatory, and empirical networks from multiple domains. Our results demonstrate that pairwise interactions can give rise to synergistic information in the absence of explicit high-order mechanisms, and highlight structural balance theory as an instrumental conceptual framework to study high-order interdependencies.

DOI: [10.1103/179y-qp6j](https://doi.org/10.1103/179y-qp6j)

Introduction—Complex systems are characterized by collective behaviors that cannot be reduced to their components' individual properties. The investigation of the mechanisms that can give rise to these behaviors is at the heart of complexity science [1–3], a central problem across domains of physics [4–6], and a fundamental question in neuroscience [7], genetics [8], ecology [9], and evolutionary biology [10,11].

Recent work has increasingly focused on the intuitive relationship between high-order mechanisms (i.e., beyond pairwise interaction terms in the system's generative process, such as a Hamiltonian) and collective behaviors (i.e., beyond pairwise statistical dependencies in the system's resulting activity) [3–5,12]. Advances in information theory—formalizing high-order interdependencies through the notion of synergy [13,14]—have enabled the systematic study of the interplay between mechanisms and high-order behaviors [15,16]. Surprisingly, while high-order interdependencies are enhanced by high-order mechanisms [15,16], they can also arise purely from low-order mechanisms [17,18]. This puzzle motivates the central question

we address here: Under what precise minimal conditions can low-order mechanisms produce synergistic behaviors?

Early studies in two restricted settings provide some insights. For Ising models of size $N = 3$, frustrated pairwise spin couplings lead to a negative interaction information [17], now understood to be indicative of synergistic interdependencies [13]. In Gaussian systems of size $N = 3$, systems are synergistic if two variables both correlate with a third but are anti- or uncorrelated with each other [18–20]. However, a formal proof linking correlation and anticorrelation patterns to synergy dominance is missing, and whether this intuition translates to larger systems remains unknown.

To address these open problems, we combine two tools: structural balance theory (SBT) and the O-information (Ω). SBT [21] provides a graph-theoretic framework [22,23] to study patterns of signed pairwise relationships across domains [24–33]. In spin glass theory, balanced graphs minimize spins' frustration, while antibalanced graphs maximize it [34–38]. The O-information is a high-order extension of the mutual information [15] whose sign captures the relative strength of synergistic (high-order) vs redundant (low-order) interdependencies in a system [39]. Importantly, it is analytically tractable and readily computable, thus serving as the ideal aggregate measure of high-order interdependencies in large multivariate systems [40–44].

In this Letter, we provide precise conditions under which synergistic interdependencies arise from pairwise mechanisms. For static Gaussian systems, we derive a condition in

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terms of signed patterns in the correlation matrix and prove that, in any dimension, antibalanced structures ensure synergy dominance. Extending this to dynamical systems, we prove that antibalanced interaction motifs in Ornstein-Uhlenbeck processes are necessary for synergy dominance. Finally, we demonstrate the relevance of our results across domains of physics by numerically showing that antibalanced motifs are predictors of synergy dominance in systems taken from statistical mechanics and electrochemical oscillators, as well as in medical, financial, physiological, and epidemiological empirical datasets.

Notation and preliminaries—Let G be a signed graph with adjacency matrix $W \in \mathbb{R}^{N \times N}$, $W_{ii} = 0$. Harary's structure theorem [45] states that a graph G is balanced (antibalanced) if it can be partitioned into two nonoverlapping sets of vertices such that edges between vertices in the same set are positive (negative) and edges between nodes in distinct sets are negative (positive). Let $\mathbf{w}^k$ be the set of all closed walks w of length k in G , and for $w = (i_1, i_2, \dots, i_k, i_1) \in \mathbf{w}^k$ define the weight of a walk as $\sigma(w) = \prod_{i=1}^k W_{w_i, w_{i+1}}$. This theorem implies that if G is antibalanced, then every closed walk of length k satisfies $\text{sign}[\sigma(w)] = (-1)^k$.

Let $\mathbf{X} = \{X_1, X_2, \dots, X_N\}$ be a multivariate process of size N and let $\mathbf{X}_{-i} = \mathbf{X} \setminus X_i$ denote the same system with the i th variable removed. The O-information can be written as [42]

$$\Omega(\mathbf{X}) = \sum_{i=1}^N \text{TC}(\mathbf{X}_{-i}) - (N-2)\text{TC}(\mathbf{X}), \quad (1)$$

where the total correlation $\text{TC}(\mathbf{X}) = \sum_j H(X_j) - H(\mathbf{X})$ [46] quantifies the strength of correlations within the system as a whole [15,42]. A negative sign ($\Omega < 0$) indicates that high-order interdependencies dominate (synergy dominance); a positive sign ($\Omega > 0$) instead indicates that low-order interdependencies dominate (redundancy dominance) [15,39,41].

Static Gaussian systems—Information-theoretic quantities can be studied analytically in Gaussian systems, allowing us to derive precise conditions for synergy dominance. In this regime, the O-information can be conveniently written in terms of blocks of the covariance matrix as

$$\Omega(\mathbf{X}) = \frac{N-2}{2} \log[\det(\Sigma)] - \frac{1}{2} \sum_i \log[\det(\Sigma_{-i})], \quad (2)$$

where Σ_{-i} indicates the system's covariance matrix with the i th variable removed (see Supplemental Material [47] for step-by-step derivations). Without loss of generality, in what follows we consider standardized covariances Σ (i.e., unit-variance correlation matrices). To study the signed patterns in Σ using SBT, we represent the correlational structure of Gaussian systems as a complete signed graph G

with adjacency matrix $W = \Sigma - \mathbb{I}$, where $\mathbb{I}$ is the identity matrix. We simplify Eq. (2), following a similar approach as in [54], by expanding the log determinants using the Mercator series

$$\log[\det(\Sigma)] = - \sum_{k=2}^{\infty} \frac{(-1)^k}{k} \text{tr}[W^k]. \quad (3)$$

Importantly, this approximation converges only if the spectral radius of W denoted as $\rho(W)$ is less than 1. As noted in [54], this applies for the case of weakly coupled systems, which are common across the complex systems literature [55–57]. Using the trace identity $\sum_i^N \text{tr}[W_{-i}^k] = (N-k)\text{tr}[W^k]$ for $k = 2, 3$ (see [47]), we can use Eq. (3) to isolate the lowest-order term in Ω :

$$\Omega(\mathbf{X}) = \frac{1}{6} \text{tr}[W^3] + R_4(W), \quad (4)$$

where $R_4(W) \leq \mathcal{O}(\rho(W)^4)$ as $\rho(W) \rightarrow 0$.

This approximation yields an important insight: Since $\text{tr}[W^3] = \sum_{w \in \mathbf{w}^3} \sigma(w)$, whenever $|\frac{1}{6} \text{tr}[W^3]| > |R_4(W)|$ we have that $\mathbf{X}$ is synergy dominated if the triangles (i.e., length-3 walks) are antibalanced. In fact, the lowest-order term in Eq. (4) is, up to normalization and sign, equivalent to the structural balance energy U [35]

$$U = - \frac{1}{\binom{N}{3}} \sum_{\{i,j,k\}} W_{ij} W_{jk} W_{ik}, \quad (5)$$

a measure of balance that is minimized (maximized) if each triangle $\{i, j, k\}$ in the network is balanced (antibalanced). In what follows, we study the higher-order corrections in Eq. (4) and use SBT to provide a stronger condition, proving that systems with antibalanced correlational structures must be synergistic. To do this, we introduce a trace identity valid for any k .

Proposition 1—For $k \in \mathbb{N}$, $k > 0$, we have

$$\sum_i \text{tr}[W_{-i}^k] = N \text{tr}[W^k] - \sum_{w \in \mathbf{w}^k} |w| \sigma(w),$$

where $|w|$ is the number of unique nodes encountered along the closed walk w . See proof in Supplemental Material [47].

We use this identity to eliminate the explicit dependence on W_{-i} in the higher-order terms of Eq. (4), and derive the key theorem for static systems:

Theorem 1—If G is antibalanced, then $\Omega(\mathbf{X}) < 0$.

To prove this, insert Eq. (3) into Eq. (2) and apply Proposition 1 to obtain

$$\Omega(\mathbf{X}) = \sum_{k=3}^{\infty} \left[\frac{(-1)^{k-1}}{2k} \sum_{w \in \mathbf{w}^k} (|w| - 2) \sigma(w) \right]. \quad (6)$$

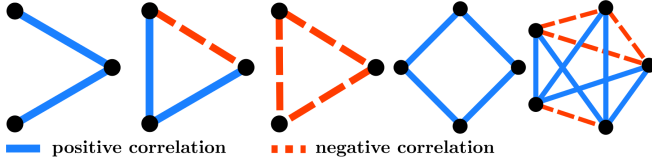


FIG. 1. Examples of synergistic motifs of pairwise correlations that ensure synergy dominance. These structures are either antibalanced or only contain closed walks w of even length with positive weight $\sigma(w)$. Missing edges indicate uncorrelated relationships.

If G is antibalanced, every nonzero closed walk $w \in \mathcal{W}^k$ in G has $(-1)^{k-1}\sigma(w) < 0$, and therefore, $\Omega < 0$.

This result furnishes an exact sufficient condition for synergy dominance and allows us to identify the signed patterns in the correlation matrix (i.e., closed walks w in W) which contribute synergistically. The sign of each summation term in Eq. (6) depends on both the parity of k and the sign of the walk's weight $\sigma(w)$. The synergistic motifs, i.e., the closed walks that contribute negatively in Eq. (6), thus correspond to even-length closed walks with $\sigma(w) > 0$ and odd-length closed walks with $\sigma(w) < 0$ (see examples in Fig. 1).

Notably, while our proof assumes $\rho(W) < 1$, our extensive numerical analyses (see Experimental Validation section and Supplemental Material [47]) have not found any redundancy-dominated antibalanced correlational structures even when $\rho(W) \geq 1$.

Dynamical Gaussian systems—We now ask which patterns of interactions in the coupling matrix of a linear dynamical system can lead to synergistic correlational structures. For example, in diffusive processes with only positive couplings, two variables that both correlate positively with a third tend to be correlated [58]. Synergy-dominated systems instead (Fig. 1) break this, and hence the un- or anticorrelated pair must be negatively coupled. We therefore conjecture that antibalanced interaction motifs are required for dynamical Gaussian processes to be synergy dominated.

Following a similar approach to Ref. [54], we consider Ornstein-Uhlenbeck (OU) processes: $d\mathbf{X}(t) = -\mathbf{X}(t) \cdot (\mathbb{I} - A)dt + d\mathbf{W}(t)$, where $A \in \mathbb{R}^{N \times N}$ is the interaction (or coupling) matrix, and $\mathbf{W}$ is a Wiener process with identity covariance. For symmetric, Schur stable A , the stationary covariance can be written as (see [54,59,60])

$$\tilde{\Sigma} = \frac{1}{2}(\mathbb{I} - A)^{-1}. \quad (7)$$

Then, by normalizing $\tilde{\Sigma}$ we obtain the correlation matrix Σ . With this closed-form expression, we prove our conjecture exactly for $N = 3$ and in the weak interaction regime for arbitrary N . More precisely, we call weak interaction the regime where $\rho(A) \ll 1$ [implying $\rho(W) < 1$], and strong interaction the regime with $0 < \rho(A) < 1$ where the system

is still Schur stable (so information-theoretic quantities are well defined), but correlations are strong and $\rho(W) > 1$ is allowed.

Theorem 2—Let $\mathbf{X}$ be a stable OU process with $A \in \mathbb{R}^{3 \times 3}$. If $\Omega(\mathbf{X}) < 0$, then A is antibalanced.

To derive this, let $a = \Sigma_{12}, b = \Sigma_{13}, c = \Sigma_{23}$. From Eq. (2), the condition $\Omega < 0$ simplifies to $2abc < (ab)^2 + (ac)^2 + (bc)^2 - (abc)^2$. To connect this to the interactions A_{ij} , we use Eq. (7) to write the same condition as $-2xyz > (xy)^2 + (xz)^2 + (yz)^2 - (xyz)^2$, where $x = A_{12}, y = A_{13}, z = A_{23}$ (see Supplemental Material [47]). For Schur-stable A , the rhs is always positive, so this expression is satisfied only if $xyz < 0$. Thus, antibalanced interactions are necessary for synergy dominance when $N = 3$.

For systems of arbitrary dimension, elements in $\tilde{\Sigma}$ are more complex. In the weak interaction regime, Eq. (4) is dominated by the cubic term when A is balanced. Supplemental Material [47] provides the analytical bounds on $R_4(W)$ in the balanced case and numerical tests to identify the range of $\rho(W)$ for which $|\frac{1}{6}\text{tr}[W^3]| > |R_4(W)|$. Under this condition, we prove that antibalanced interaction motifs are necessary for the system to be synergy dominated by studying the sign relationships between A and W .

Theorem 3—Let $\mathbf{X}$ be a stable OU process with $A \in \mathbb{R}^{N \times N}$. In the weak interaction regime, antibalanced interaction motifs in A are necessary for $\Omega(\mathbf{X}) < 0$.

To prove this, we first show in the weak interaction limit that if A is balanced then $\Omega(\mathbf{X}) > 0$. For Schur-stable A , the Neumann series of Eq. (7), after normalization, yields

$$W_{ij} = \frac{1}{2} \frac{\sum_{l=1}^{\infty} (A^l)_{ij}}{\sqrt{d_i d_j}}, \quad i \neq j, \quad d_i = (\tilde{\Sigma})_{ii} > 0. \quad (8)$$

The denominator is positive, so the sign of W_{ij} is the same as that of $\sum_l (A^l)_{ij}$, i.e., the contribution of all length- l interaction walks from i to j . If A is balanced, Harary's structure theorem for balance guarantees that any walk from node i to j satisfies $(A^l)_{ij} > 0$ if i and j are in the same set, and $(A^l)_{ij} < 0$ otherwise. Consequently, $\text{sign}\left(\sum_l (A^l)_{ij}\right) = \text{sign}(A_{ij})$, which implies that W_{ij} and A_{ij} must share the same sign. In the weak interaction regime $|\frac{1}{6}\text{tr}[W^3]| > |R_4(W)|$, such that $\text{sign}[\Omega(\mathbf{X})] = \text{sign}(\text{tr}[W^3])$. Thus, for balanced A we have $\text{sign}[\Omega(\mathbf{X})] = \text{sign}(\text{tr}[A^3]) > 0$, and the stationary dynamics of the resulting OU process is ensured to be redundancy dominated. Consequently, we conclude that antibalanced interaction motifs (e.g., antibalanced triangles of interactions), which leave A not balanced, are necessary for the system to be synergy dominated.

To test our conjecture beyond the weak interaction limit, we performed extensive numerical explorations for systems of size $N \leq 9$ with varied interaction strengths $\rho(A)$ which

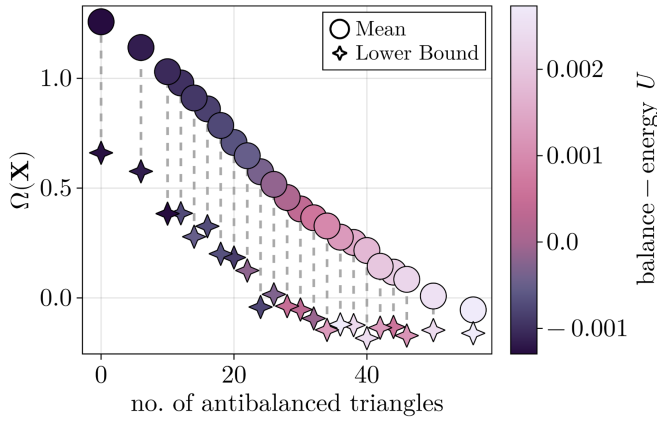


FIG. 2. Antibalanced interaction motifs are necessary for synergy dominance in dynamical Gaussian systems with strong interactions. Mean $\Omega(\mathbf{X})$ as a function of the number of antibalanced triangles in the interaction matrix. Lower bounds indicate the lowest $\Omega(\mathbf{X})$ encountered in our numerical exploration across all configurations with a specific number of antibalanced triangles. Each mean $\Omega(\mathbf{X})$ is colored according to its mean balance-energy value [Eq. (5)]. Lower bounds are colored with the energy value of the configuration that resulted in the lowest recorded $\Omega(\mathbf{X})$, not the highest recorded energy (not shown). Each $A \in \mathbb{R}^{8 \times 8}$ has $\rho(A) \approx 0.88$ (see Supplemental Material [47]).

ensure $\rho(W) > 1$. Since the O-information is permutation invariant [15], we explored all nonisomorphic complete signed graphs, each one encoding a unique sign pattern in A . The restriction to complete graphs allowed us to characterize each network of interactions by the number of antibalanced triangles only—balance is fully determined by triangles in this case [34]—and thus compare each graph on equal terms to identify the most synergistic structures. For noncomplete graphs, a similar systematic analysis is not yet obvious due to, for example, degree correlations, which is an interesting direction for future work.

We present our results in Fig. 2 for $N = 8$. For all system sizes studied (see Supplemental Material [47]), we found that the O-information is strongly anticorrelated with the number of antibalanced triangles in A . Importantly, balanced interaction structures (with 0 antibalanced triangles) always result in redundancy-dominated systems, while antibalanced structures [with $\binom{N}{3}$ antibalanced triangles] consistently result in systems with the lowest mean Ω .

Experimental validation—Gaussian systems often serve as an analytically tractable starting point to analyze complex models [18,54]. We now show that the same relationship between antibalanced interactions and synergistic interdependencies extends to two prototypical models of complex systems: the landmark Ising model (see, e.g., [2]) and networks of subcritical Stuart-Landau (SL) oscillators used widely in the modeling of electrochemical and neuronal systems [61]. Additionally, in empirical studies of continuous, high-dimensional data (such as functional magnetic

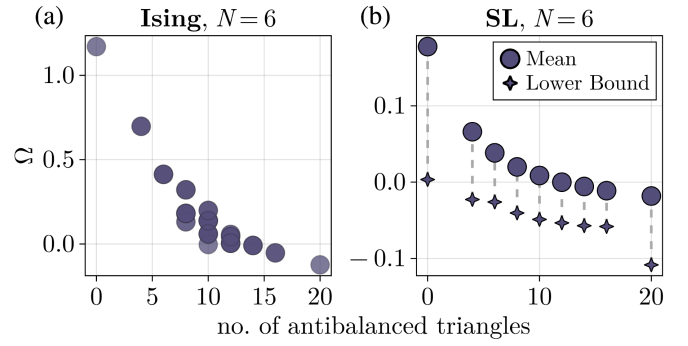


FIG. 3. Antibalanced interaction motifs characterize synergy-dominated complex systems with pairwise coupling. Plots show Ω versus the number of antibalanced triangles in the pairwise coupling matrix. (a) For the Ising model, we compute Ω exactly for each possible coupling configuration ($\beta = 0.25$). Darker markers indicate multiple configurations with identical values of Ω and number of antibalanced triangles (b) For the SL network of oscillators, we report the mean Ω (circle) over 100 initial conditions and the minimum Ω (star) found (lower bound) across configurations with a specific number of antibalanced triangles. See Supplemental Material [47] for implementation details.

resonance imaging (fMRI), biochemical systems, or financial time series), information-theoretic quantities are most commonly estimated using Gaussian (or Gaussian-copula) models [62–65]. Motivated by the widespread use of this approach (see, e.g., [41–44,54,57,66–74]), we demonstrate the practical relevance of our analytical insights [Eq. (4) and Theorem 1] on financial and fMRI brain activity data.

For both the Ising and SL models, we performed a numerical exploration of all possible signed coupling structures, similar to that for the OU process above. For the Ising model, we studied N -spin systems without an external field. For $N < 10$, all the relevant information-theoretic quantities can be calculated exactly. For the SL networks, we numerically solved the system of equations as in [69,75,76] (see also Supplemental Material [47]). Across the board, the coupling structures with the largest number of antibalanced triangles consistently result in those with the lowest O-information, in agreement with our predictions (Fig. 3). Importantly, systems with zero antibalanced triangles consistently showed $\Omega > 0$, confirming our analytical results placing antibalance as a necessary condition for synergy dominance.

In the empirical datasets, where the underlying interaction matrix A was not available, we studied the O-information as a function of the structural balance-energy U of various N -plets (i.e., correlation matrix of subsystems) of size N (Fig. 4). In both datasets, in which the majority of subsystems display $\rho(W) > 1$ (indicative of strong interactions; see Supplemental Material [47]), our results demonstrate a systematic relationship between patterns of pairwise correlations (quantified by U) and high-order interdependencies (quantified by Ω), confirming our analytical insights [Eq. (4) and Theorem 1]

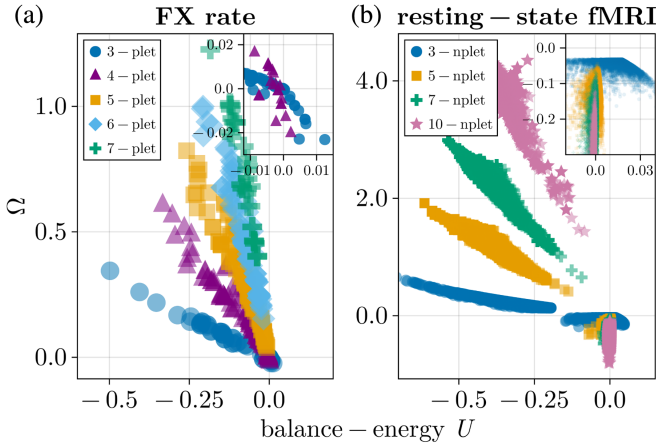


FIG. 4. Structural balance energy predicts synergy: the most synergistic N -plets maximize U and positive U guarantees synergy dominance. (a) N -plets from a multivariate time series of nine foreign-exchange (FX) rate logarithmic returns. (b) N -plets from resting-state fMRI functional-connectivity matrices (229 brain regions).

that predominantly antibalanced subsystems with $U > 0$ are synergy dominated (and conversely, predominantly balanced systems with $U < 0$ are redundancy dominated). Specifically, the results in Fig. 4 show that (i) the most synergistic (redundant) subsystems have the highest (lowest) energy; (ii) if an N -plet has $U > 0$, it is always synergy dominated (Fig. 4 insets). To test the robustness of our conclusions, we additionally report in Supplemental Material [47] a comparison between O-information estimates obtained using Gaussian copula and Kraskov estimators (which capture nonlinear dependencies), as well as further analyses on medical, epidemiological, financial, and physiological datasets.

Conclusion—We have established, for the first time, analytical sufficient and necessary conditions for the emergence of high-order behaviors from low-order mechanisms, providing a theoretical ground to a rapidly growing line of research [3–5,16,68,77–80]. Specifically, we proved that antibalanced correlations are sufficient for synergy dominance in Gaussian systems and that antibalanced interaction motifs are necessary for synergy dominance in OU processes. While our analytical results are derived in the weak interaction regime [except for Theorem 2, which is valid for any $\rho(W)$], numerical simulations and empirical data analyses show that the same qualitative behavior strongly persists beyond the weak interaction regime. Our results are therefore directly applicable whenever multivariate dynamics are modeled as approximately stationary linear processes with Gaussian statistics, which is a widely used approach in information-theoretic analyses of multivariate continuous data in neuroscience and biology. Moreover, our analyses of Ising and SL oscillator networks, together with the comparison between Gaussian and non-linear Kraskov estimators on empirical datasets, indicate

that the same relationship between antibalanced motifs and synergy extends beyond linear Gaussian models. These results provide a novel mechanistic link between low-order mechanisms and high-order interdependencies, establishing SBT as a natural framework for modeling and analyzing synergistic complex systems with pairwise interactions. The expansion of the O-information in terms of signed closed walks has immediate implications for empirical analyses: (i) We expect our motifs analysis to point to faster and more principled algorithms for detecting synergistic subsystems in real datasets whenever the Gaussian approximation is justified [42,43,81]. (ii) The leading, normalized term of the expansion is mathematically identical to the structural balance-energy U , explaining the similarities and uncovering novel connections between two previously disconnected lines of work, namely, information-theoretic [40,41,43] and SBT-based studies [30–33]. We demonstrate this connection explicitly in Supplemental Material [47] by reanalyzing an existing SBT-based study using the O-information instead of U . Finally, our Ising results motivate exploring frustrated quantum magnets, including spin liquids [82,83], using quantum measures of high-order interdependencies [84,85].

Acknowledgments—Network controllability and Connectivity Inference grant from Moogsoft Ltd to L. B.

Data availability—The fMRI correlation matrices data which support the findings of this article are openly available [86,87], as well as the multivariate time series financial data [88] (see also [89]). To construct the non-isomorphic signed graphs used throughout the study, we used the openly available dataset [90]. The code used to collect the data and produce the figures is available at [91].

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