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Communicating through a sea of frustration: zero-temperature triangular Ising antiferromagnet on a cylinder

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"Communication" through the frustrated ground state of a classical triangular Ising antiferromagnet wrapped on a cylinder is studied via reformulation as imaginary time evolution of a system of fermions on a ring, detailing a breakdown of the ordinary Perron-Frobenius scenario for disordered one-dimensional systems. For instance, constraint of the configuration at one cylinder end allows infinite-range, albeit partial, control of the state. Mutual information between end configurations under open boundary conditions, which measures strength of the correlations, has an asymptotic decay with a complex dependence on cylinder circumference and spin (anti)periodicity. In some cases, the decay is not even exponential in length, but inverse square.

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Introduction. *Frustration* [1] is the presence of interactions that are incompatible in the sense that they cannot simultaneously be brought to lowest energy configurations ("satisfied"). The phenomenon was first recognized in water ice [2, 3] and subsequently in spin systems [4–9], but recent years have witnessed the discovery of many new examples of frustration across an extremely diverse range of physical systems including artificial spin ice [10–12], colloidal assemblies [13, 14], Coulomb liquids [15], lattice gases [16], ferroelectrics [17], coupled lasers [18], and self-assembled lattices of microscopic chemical reactors [19]. The triangular Ising antiferromagnet (TIAFM, see Fig. 1) has a special status as possibly *the* archetype of frustration. In the TIAFM, every elementary triangle must contain at least one unsatisfied bond, hence it is in a disordered state with extensive entropy even at zero temperature. The infinite planar TIAFM is not quite as disordered as it superficially appears, however: zero temperature is a critical point, insofar as the spin correlation length is infinite [20, 21]. At the same time, it is well-known that ordering is suppressed by reducing dimensionality. These observations, plus the rapid recent increase in the number of physical systems that exhibit frustration and have good control of boundary conditions, motivates a study of a zero-temperature TIAFM wrapped on a long cylinder to answer the question: does the state of the cylindrical system resemble an ordinary thermally disordered state where the influence of one end on the other decays exponentially fast with cylinder length, or does hidden structure allow communication through this sea of disorder?

This Rapid Communication is devoted to a detailed negative answer to that question. Reducing the dimension of the zero-temperature TIAFM by one via wrapping onto a cylinder actually *accentuates* the order, insofar as communicating end-to-end through the disordered state is concerned. We can exert an infinite-range influence by constraining the configuration at one end. And, under unconstrained boundary conditions the average information carried about the configuration at one end by that at the other (the mutual information) displays unexpected

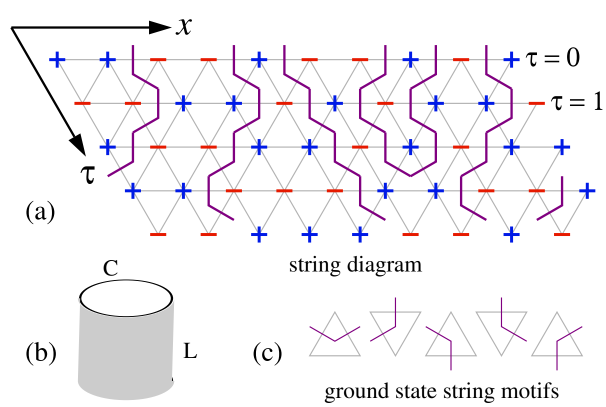

FIG. 1. (a) When each bond belongs to a unique down-pointing triangle (▽), a ground microstate has exactly one unsatisfied bond in each ▽, but may have three in a △. Relative to the ground reference microstate, all spins up/down on even/odd rows, any microstate is represented up to global spin flip by the boundaries (purple "strings" here) between regions matching the reference microstate and its global spin flip. Strings cannot terminate inside the system. (b) Cylindrical geometry. (c) Motifs allowed in string representations of ground microstates. The left-most motif corresponds to pair annihilation when strings are interpreted as particle worldlines.

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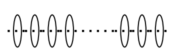
sensitivity to the cylinder circumference — whether it is a multiple of 3 — as well as to whether spin periodicity or antiperiodicity is imposed around the circumference. These features, of the zero-temperature cylindrical TIAFM, which seem bizarre when the system is viewed in its native guise of a spin system, will be addressed here using a simple, exact, mapping to a basic model of solid-state physics, namely fermions hopping on a ring, which will render them transparent. It remains to be seen to what degree results of the sort discussed here carry over to frustrated systems other than cylindrical TIAFM, but one general lesson is that frustration-induced disorder might not effectively screen boundary conditions.

In a little more detail, the cylindrical TIAFM systems we study are formed by identifying the left and right edges of a planar system such as shown in Fig. 1(a). A zero temperature state of the system is equally weighted on all the lowest energy microstates (spin configurations), or some subset picked out by boundary conditions. We consider only boundary conditions, such as specification of all the spins at one end, that actually do this rather than forcing a higher energy.

We intend to view the cylindrical TIAFM as a one-dimensional statistical mechanical lattice model:



The lattice sites of this chain are occupied not by simple spins, but by entire rings of spins. The elementary degrees of freedom of the model are configurations on entire rings, and each such interacts with its nearest neighbors.

Now, before delving into a detailed investigation of the ways the zero-temperature cylindrical TIAFM deviates from normality, it helps to know what "normal" is. For the generic one-dimensional model, we refer to the degrees of freedom residing at the lattice sites as *finite-state units* (FSUs). For instance, an FSU for an ordinary Ising chain is just a single spin, and for the cylindrical TIAFM, a rings of spins (more accurately, the set of configurations of that ring). The statistical mechanics of a chain of FSUs with nearest-neighbor interactions is conveniently treated by means of a transfer matrix [22–24], entries of which are indexed by values of neighboring FSUs. In the normal situation, a sufficiently large power of the transfer matrix has all entries nonzero. This does not preclude the possibility that certain local configurations are forbidden. That is a relevant consideration here since at zero temperature, there are constraints on the elementary triangles of the TIAFM. Now, in this normal situation, the Perron-Frobenius theorem [25, 26] asserts that the transfer matrix eigenvalue λ_0 of largest modulus is positive and nondegenerate. Consequences of this Perron-Frobenius scenario, as we might call it, include (i) a unique macrostate ("phase") in the infinite-length limit, and (ii) correlation functions of the form $\langle f(X_s)g(X_{s+\tau})\rangle - \langle f(X_s)\rangle\langle g(X_{s+\tau})\rangle$, between FSUs separated by τ axial lattice spacings are asymptotically of order $|\lambda_1/\lambda_0|^\tau$, where $|\lambda_1|$ is the second-largest transfer matrix eigenvalue modulus. That behavior of correlation functions holds whether the system is infinite or finite. In particular, the FSUs in question could be at the ends of the system.

Ordinary correlation functions are an awkward tool for probing correlations between the FSUs (rings) of the cylindrical TIAFM. Much more convenient is *mutual information* [27–30], a tool which is finding increasing use in classical statistical mechanics [31–33] and quantum information theory [34]. The mutual information $I(X\!:\!Y)$ between discrete random variables X and Y may be defined as

$$I(X\!:\!Y) = H(Y) - H(Y|X), \tag{1}$$

where $H(Y)$ is the (unconditional) entropy of Y, and $H(Y|X) = -\sum_x P_X(x)\sum_y P_{Y|X}(y|x)\ln P_{Y|X}(y|x)$ is the conditional entropy of Y given X. Thus, $I(X:Y)$ measures the average reduction in uncertainty about Y resulting from learning the value of X. In the Perron-Frobenius scenario, mutual information between FSUs decays asymptotically as $I(X_0 : X_\tau) \sim |\lambda_1/\lambda_0|^{2\tau}$. The difference from ordinary correlation functions is that the decay rate is doubled.

For the zero-temperature TIAFM on a cylinder, the Perron-Frobenius scenario breaks down spectacularly. A representation of bond configurations in terms of strings, to be explained shortly (Fig. 1), makes clear the existence of multiple distinct infinite-volume macrostates (pure phases, in a weak sense), labelled by number of satisfied bonds around a circumferential ring. Infinite range communication is possible through this disordered system. The end-to-end mutual information with open boundary conditions does not always decay exponentially in the length. When the circumference C is a multiple of 3, and spin antiperiodicity is imposed around the circumference, the decay is only as the inverse square of the length. In other cases, when the mutual information does decay exponentially, the dependence on circumference is not monotonic, but sensitive to the residue class mod 3 of C (Fig. 3). While not strictly contrary to the Perron-Frobenius scenario, this is highly unexpected behavior.

A unified explanation of these phenomena emerges through a reformulation in terms of non-relativistic fermions hopping on a ring [35–37], a problem amenable to elementary and intuitively appealing techniques widely familiar to physicists. In this picture (see Fig. 1), the circumferential and axial directions on the cylinder correspond to space and imaginary time, respectively; configurational change from one ring to the one immediately below corresponds to evolution through one unit of imaginary time; and satisfied circumferential bonds correspond to the presence of fermions. Although the fermions are noninteracting, neighboring pairs can annihilate. In the limit of infinite length, this *semi-conservation* is effectively promoted to full conservation away from the ends, but the possibility of pair annihilation is crucially important to finite-size effects for systems which are not genuinely infinite. Knowledge of the energies (Fig. 2) and excitation gaps of the fermionic states corresponding to the pure phases elucidates the competition between the pure phases at finite length and explains major features of the decay rate of end-to-end mutual information: sensitivity to the residue class mod three of the circumference, vanishing in some cases, and having the "wrong" dependence on the energy gap.

Fermionic formulation. Two-dimensional Ising models can be reformulated as theories of fermions in one space dimension with imaginary time, by interpreting graphical expansions as depicting worldlines. For ferromagnetic models, these representations originate from high-temperature expansions and feature spontaneous creation and annihilation of fermion pairs [38–41]. For the zero-temperature TIAFM, one needs to proceed in a different way, which leads to semi-conserved particle number; in the thermodynamic limit or with periodic boundary conditions, the slight nonconservation is irrelevant and has therefore usually been implicitly ignored [35–37, 42, 43]. To reach the fermionic formulation, we start from string diagram representations of bond configurations, interpret the strings as fermion worldlines, and deduce a transfer matrix or Hamiltonian in terms of creation and annihilation operators. This fermionic formulation essentially replaces entropy with energy and greatly facilitates calculations.

Only systems which decompose completely into down-pointing triangles ($\bigtriangledown$'s) with no left over bonds, such as that at top of Fig. 1, are considered, because then ground microstates are precisely those with two satisfied bonds in each $\bigtriangledown$. There is no additional restriction related to up-pointing triangles ($\bigtriangleup$'s). Some of them may have *no* satisfied bonds in a ground microstate. Any bond microstate can be represented by a string diagram as in Fig. 1. A bond crossed by a string is satisfied if it is horizontal and unsatisfied if it is diagonal. Notice that the strings separate regions where the considered microstate matches the reference ground microstate with all spins up, down, up, etc. on successive rings, from regions where it matches the spin flip of the reference. That implies that strings cannot end inside the system.

The motif occurs in triangles with no satisfied bonds. With strings interpreted as particle worldlines, it represents annihilation of a pair of neighboring particles. One such event is shown in Fig. 1 (a). would also indicate three unsatisfied bonds. But, a down-pointing triangle with three unsatisfied bonds incurs an energy cost, hence this motif does not occur at $T = 0$. In a planar system, particle number $\mathcal{N}$ changes by pair annihilation (decreasing by 2), or by particle entrance or exit at the spatial boundary. On a cylinder, as obtained by identifying left and right edges in Fig. 1 (left), the spatial boundary is eliminated, resulting in a local and global semi-conservation law for particle number. Henceforth, only cylindrical geometries are considered. Generally, we think in terms of classes of systems of differing lengths L, but the same circumference C and with either spin periodicity or spin antiperiodicity around the circumference.

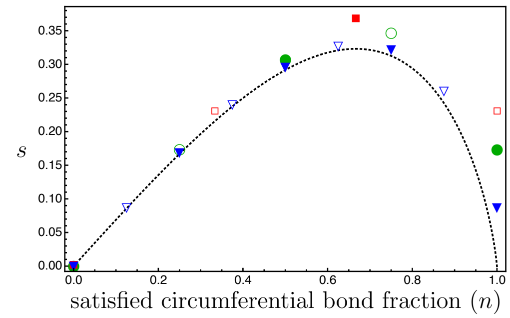


FIG. 2. Entropy density versus fraction of satisfied circumferential bonds (equivalently, the fermion density n) for the zero-temperature TIAFM on a cylinder of circumference C. The solid curve is from Eq. (8). Symbols: exact numerical results, with solid (open) symbols denoting periodic (antiperiodic) boundary conditions, and for circumference C equal to 3 ($\square$), 4 ($\diamondsuit$) and 8 ($\bigtriangledown$). The infinite-C limit is nearly attained already for $C = 8$, except at $n = 1$, for which entropy density is exactly $(\ln 2)/C$.

Spin antiperiodicity can be implemented by means of a seam of ferromagnetic bonds along the cylinder length. This sort of modification, called a gauge transformation by some, preserves the frustration of every individual triangle.

While the string representation provides much qualitative insight, a fermionic representation allows quantitative calculations. A crossing of a horizontal bond by a string is interpreted as presence of a particle, so satisfied circumferential bonds correspond to particles. We take the particles to be fermions so that the prohibition of two occupying the same site is implemented via fermionic statistics rather than an explicit interaction. Now, the possibilities of string movement from time τ to $\tau + 1$ show that the transfer matrix $\mathbb{T}_0$ with the pair annihilation motif held in abeyance satisfies

$$\mathbb{T}_0 c_x^\dagger = (c_{x-1}^\dagger + c_x^\dagger)\mathbb{T}_0, \quad \mathbb{T}_0|\varnothing\rangle = |\varnothing\rangle, \tag{2}$$

where $c_x^\dagger$ creates a fermion at site $x \in \{1, \cdots, C\}$ (mod C), and $|\varnothing\rangle$ is the state with no particles present. In momentum space, one deduces the form

$$\mathbb{T}_0 = e^{-H_0 + iP/2}, \tag{3}$$

where

$$H_0 = \sum_{q\in \mathrm{BZ}} \varepsilon(q) n(q), \qquad P = \sum_{q\in \mathrm{BZ}} q\, n(q), \tag{4}$$

can be considered a Hamiltonian and total momentum operator, respectively, with mode occupation operators $n(k) = c(k)^\dagger c(k)$, effective mode energies

$$\varepsilon(q) = -\ln\left(2\cos\frac{q}{2}\right), \tag{5}$$

and allowed fermion modes depending on the parity of the number of particles $\mathcal{N}$ according to

$$\mathrm{BZ} = \begin{cases} \frac{2\pi}{C}\mathbb{Z} \cap (-\pi, \pi], & \mathcal{N}\,\text{odd} \\ \frac{2\pi}{C}\left(\mathbb{Z}+\frac{1}{2}\right) \cap (-\pi, \pi], & \mathcal{N}\,\text{even}. \end{cases} \tag{6}$$

Since the number of particles is the number of spin reversals around the circumference, even (odd) $\mathcal{N}$ is the same thing as circumferential spin periodicity (antiperiodicity). These being synonymous, we speak henceforth in terms of $\mathcal{N}$ parity rather than circumferential boundary condition, for simplicity.

The transfer matrix (3) is a quantum imaginary-time evolution operator (ignoring P in the exponent, which vanishes for physical states anyway), so this is an example of the ubiquitous [44, 45] correspondence between imaginary-time quantum evolution and classical statistical systems.

Entropy. Imposing periodic boundary conditions end-to-end, but with particle number density fixed at $n = \mathcal{N}/C$, the partition function of a length L cylinder is expressed in terms of entropy density s as

$$e^{CLs} = \mathrm{Tr}_{\mathcal{N}}\mathbb{T}_0^L = \sum_{E\in\,\mathrm{spec}\,H_0} e^{-EL} \sim e^{-E_0(n)L}. \tag{7}$$

The final expression is the $L \to \infty$ asymptote, with $E_0(n)$ the energy of a Fermi sea. For large C and Fermi wavevector $k_F = \pi n$,

$$s = -\frac{E_0}{C} = -\int_0^{k_F} \varepsilon(q)\,\frac{dq}{\pi}. \tag{8}$$

This entropy density is plotted in Fig. 2, along with exact calculations for small circumferences. The limit is reached very quickly with C.

Although it is not particularly difficult to write a complete transfer matrix which formally incorporates pair annihilation, we find it just as effective, and more intuitive, to simply consider pair annihilation as a supplementary process to the number-conserving evolution (3). If boundary conditions are imposed to fix the particle number at the top and bottom ends of a very long cylinder to n_{top} and n_{bot}, with $n_{\mathrm{top}} \geq n_{\mathrm{bot}}$, the particle density n in the bulk will be such as to maximize $s(n)$. For most combinations of circumference C and $\mathcal{N}$ parity, there is a unique n maximizing $s(n)$. The exceptions are the systems with zero modes ($C \in 3\mathbb{Z}$ and odd $\mathcal{N}$). In those cases, the two values of n closest to $2/3$ have equal entropies; the case $C = 3$ can be seen on Fig. 2. Considering the exact (discrete) counterpart of Eq. (8) for entropy, it is clear that this situation is atributable to single-particle modes at exactly zero energy.

In the limit $C \to \infty$, semi-conservation of particle number is effectively promoted to a full conservation law as far as the bulk is concerned. Depending upon what $\mathcal{N}$ one wishes to stabilize, it can be done by controlling the configuration at one end or the other. These different bulk macrostates are in a sense, zero-temperature pure phases. They are, however, delicate insofar as only those maximizing $s(\mathcal{N}/C)$ are accessible if the infinite-length limit precedes the zero-temperature limit. As noted above, there is a unique such $\mathcal{N}$, except in the anomalous cases with zero modes.

Mutual information on infinite cylinders. Turning now to mutual information, we consider first the mutual information between configurations X_0 and X_τ on rings 0 and τ in the bulk of a cylinder in the zero-temperature pure phase labelled by particle number $\mathcal{N}$. Asymptotically in τ, the mutual information is

$$I_{\infty,\mathcal{N}}(X_0 : X_\tau) \sim \left|\frac{\lambda_{\mathcal{N},1}}{\lambda_{\mathcal{N},0}}\right|^{2\tau} = e^{-2\Delta\varepsilon_{\mathcal{N}}\tau}, \tag{9}$$

where $\lambda_{\mathcal{N},0}$ and $\lambda_{\mathcal{N},1}$ are the leading and subleading eigenvalue of $\mathbb{T}_0$ in the $\mathcal{N}$-particle subspace, respectively. $\Delta\varepsilon_{\mathcal{N}}$, the excitation gap in the fermionic $\mathcal{N}$-particle subspace, corresponds to a minimum energy particle-hole excitation. Actually, $\lambda_{\mathcal{N},1}$ is not unique, but its modulus is. Remarkably, the coefficient is exactly one, but with $\mathcal{N}$ fixed, this formula does conform to the Perron-Frobenius scenario. The variation of the decay rate with circumference is smooth and monotonic.

End-to-end mutual information. Mutual information between the ends of a finite cylinder with free boundary conditions has a much richer structure. The relevant spectral gap is that above the minimum energy state ($n \approx 2/3$, see Fig. 2) in the *full* fermionic configuration space. These never correspond to particle-hole excitations, but rather particle-particle (pp) or hole-hole (hh), as tabulated in Table I. Not listed are the anomalous cases of odd $\mathcal{N}$ and $C \in \mathbb{Z}$, which have zero spectral gap.

Putting those cases aside, asymptotically in the length L of the cylinder the end-to-end mutual information behaves as

$$I_L(X_0 : X_L) \sim A(C)\left(\frac{\lambda_1}{\lambda_0}\right)^L = A(C)e^{-\Delta\varepsilon\,L}, \tag{10}$$

where the amplitudes $A(C)$ for small values of C are plotted in Fig. 3. Here, λ_0 and λ_1 are the nondegenerate, real, leading and subleading eigenvalues of $\mathbb{T}$ for the given $\mathcal{N}$ parity and circumference C.

$\mathcal{N}$ parity	even			odd		
C mod 3	0	1	2	0	1	2
excitation type	hh	pp	hh	hh	hh	pp
$\Delta\varepsilon \cdot C/(\pi\sqrt{3})$	1	1/3	1/3	0	2/3	2/3

TABLE I. Linearized fundamental energy gaps $\Delta\varepsilon$ of $\mathbb{T}_0$ and corresponding excitation types. 'hh' and 'pp' indicate excitations involving removal (addition) of two particles. Using a linearization of $\varepsilon(q)$ around $q = q_0 = 2\pi/3$, energies are effectively reported in units of $v(q_0)(\Delta q) = (\sqrt{3}/2)(2\pi/C) = \pi\sqrt{3}/C$. Due to the strict convexity of $\varepsilon(q)$, energies reported for hh (pp) excitations are overestimates (underestimates), though the relative error goes to zero as $C \to \infty$.

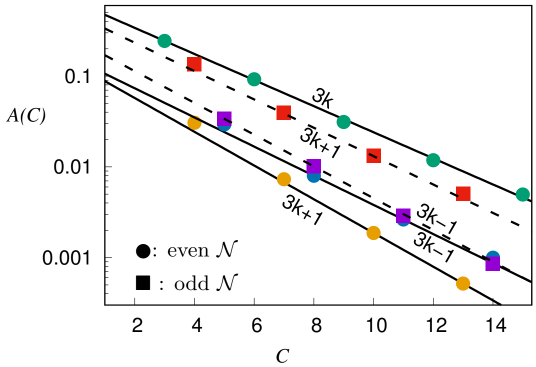


FIG. 3. Amplitudes of the asymptotic decay of end-to-end mutual information break into families labelled by $\mathcal{N}$ parity and mod 3 residue class of C ($3k+m$, $m=0,\pm1$). Within each family, $A(C)$ decays approximately exponentially in C.

The plot of $A(C)$ in Fig. 3 makes evident that there are distinct families labelled by $\mathcal{N}$ parity and the residue class of C mod 3. That is expected. A very nearly exponential dependence on C within each family, however, is unexplained. The ratio of the exact mutual information (from numerical calculations) to the asymptotic formula in plotted in Fig. 4. It appears that the asymptotic formula is good for L at least a few times C.

Not only does the end-to-end mutual information depend on different spectral gaps than ring-to-ring mutual information in the bulk, but the decay rate is precisely the energy gap, rather than twice it. These features are

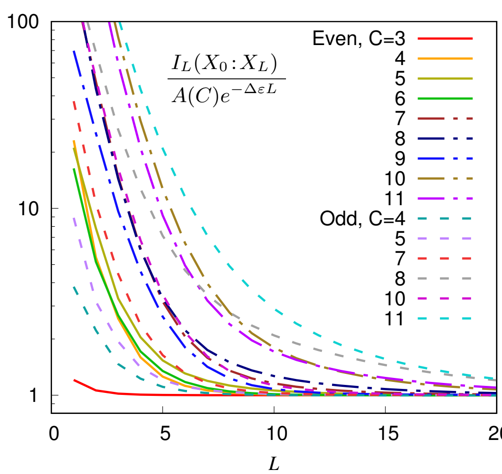


FIG. 4. Ratio of the numerically computed end-to-end mutual information $I_L(X_0:X_L)$ to the leading behavior $A(C)e^{-\Delta\varepsilon L}$ from Eq. (10), for cases without zero-energy modes and $3 \le C \le 11$. The approach is always from above because the leading behavior correctly accounts for information transmission only via the two largest eigenvectors of the transfer matrix. The numerical results are found by directly computing powers of the exact transfer matrix in a fermionic basis.

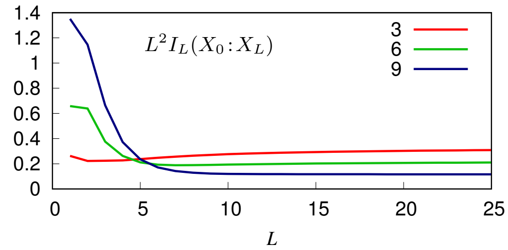


FIG. 5. End-to-end mutual information $I_L(X_0:X_L)$ multiplied by L^2 for the anomalous systems with zero modes (odd $\mathcal{N}$ and $C \in 3\mathbb{N}$).

related. Fluctuations in an infinite cylinder are typical of the zero-temperature phase it is in, and their correlations decay with distance. In contrast, the fluctuations which dominate the end-to-end mutual information are fluctuations of the entire system between phases. As a result, the expansion in powers of the deviations described above is invalid because the relevant deviations are comparable to the unconditioned probabilities.

Now we turn to consideration of the systems with zero-energy fermion modes, those with odd $\mathcal{N}$ and $C \in 3\mathbb{Z}$. Since the energy gap is zero in these cases, subexponential decay of end-to-end mutual information, possibly a power law, is to be expected. Precisely, the dependence is inverse square:

$$I_L(X_0:X_L) \sim a(C)L^{-2}, \tag{11}$$

for some $a(C)$, as demonstrated by the plot of $L^2 I_L(X_0:X_L)$ in Fig. 5 for $C = 3, 6, 9$. *Semi*-conservation of particle number is critical to the explanation of this result. For a cylinder without zero modes, the dominant contribution to the partition function has rings away from the cylinder ends in a Fermi sea with all non-positive energy modes occupied. In the presence of zero modes, the Fermi sea may include or exclude them. Due to particle semi-conservation, there can be only one "domain wall" between the regions including and excluding them. In the statistical mechanical language, it is entropically neutral whether the domain wall occurs in one place, or another, or not at all. The degree of freedom represented by the presence and placement of the domain wall is the only significant freedom in the bulk state, and it alone accounts for the L^{-2} dependence in (11).

Conclusion. Although the zero-temperature TIAFM on a cylinder appears to casual inspection much like an ordinary (e.g., thermally) disordered one-dimensional system, that appearance is deceptive. The system actually embodies a complete breakdown of the Perron-Frobenius scenario, including dependence of the decay rate of end-to-end mutual information on the circumference which is very puzzling in the native formulation as a spin model. A well-known string representation elucidates some of this, and the representation in terms of fermions on a ring evolving in imaginary time matters quantitatively transparent. The pure frustration-induced disorder in this model is significantly different from thermal disorder. Thus, while the TIAFM is an archetype of frustration, it is certainly not entirely representative. Determining which frustrated systems are like the TIAFM in this respect and which are not is an important task.

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