Characterizing correlations with full counting statistics: Classical Ising and quantum XY spin chains

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Characterizing correlations with full counting statistics: classical Ising and quantum XY spin chains

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We propose to describe correlations in classical and quantum systems in terms of full counting statistics of a suitably chosen discrete observable. The method is illustrated with two exactly solvable examples: the classical one-dimensional Ising model and the quantum spin-1/2 XY chain. For the one-dimensional Ising model, our method results in a phase diagram with two phases distinguishable by the long-distance behavior of the Jordan–Wigner strings. For the anisotropic spin-1/2 XY chain in a transverse magnetic field, we compute the full counting statistics of the magnetization and use it to classify quantum phases of the chain. The method, in this case, reproduces the previously known phase diagram. We also discuss the relation between our approach and the Lee–Yang theory of zeros of the partition function.

I. INTRODUCTION

Thermodynamic phases are traditionally described by correlations of local observables. In the simplest case of phase transitions associated with symmetry breaking, phases are distinguished by the expectation value of a local order parameter. In more subtle situations (e.g., Kosterlitz–Thouless phase transition), it is the decay of correlations at large distances that distinguishes between the phases. In recent years, it was realized that other, more sophisticated characteristics of correlations may be useful: e.g., the notion of "topological order" (involving nonlocal order parameters) or entanglement entropy (in the case of quantum systems).

In the present work, we consider yet another *non-local* characteristics of correlations based on the full-counting-statistics (FCS) approach [1] (a related problem of order-parameter statistics was studied in Ref. 2). It was pointed out recently (in the context of temporal correlations) that analytical properties of the *extensive part* of FCS may be used to distinguish between different thermodynamic phases [3]. Related phase-transition effects in FCS were also discussed in various contexts in Refs. 4–7. Here we apply the idea of Ref. [3] to spatial correlations and illustrate it with two examples: the classical Ising and the quantum XY spin chains (see also Ref. 8 for an example of one-dimensional free fermions, which do not exhibit any phase transition).

II. FCS CHARACTERIZATION OF THERMODYNAMIC PHASES

In our approach, a thermodynamic phase is characterized by the singularities of the extensive part of a suitably defined FCS generating function $\chi_0(\lambda)$. This construction is applicable to any infinite system (either classical or quantum, not necessarily one-dimensional) which is periodic in space and possesses an extensive observable taking *quantized discrete values* (e.g., the number of particles or the projection of total spin on a given axis). Consider a large subsystem Σ containing N unit cells of the infinite system. Let Q be our discrete observable restricted to this subsystem and normalized to take integer values. Then one can construct the FCS generating function for the observable Q,

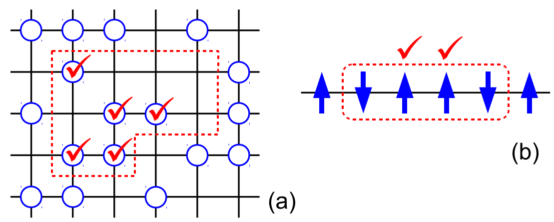

FIG. 1. Two examples of FCS in statistical or quantum systems. In both examples, the subsystem Σ is encircled by a dashed line. **(a)** Particles on a lattice, Q is the number of particles (in the configuration shown, $Q = 5$). **(b)** Spin-1/2 chain, Q is the number of up spins (in the configuration shown, $Q = 2$).

$$\chi_\Sigma(\lambda) = \langle e^{i\lambda Q} \rangle = \sum_m P_m e^{i\lambda m}\,, \tag{1}$$

where the sum is taken over all integer numbers m and P_m is the probability for the observable Q to take the value m. The generating function $\chi_\Sigma(\lambda)$ has the form of a partition function [3] and therefore must depend exponentially on the size of the system Σ [9]:

$$\chi_\Sigma(\lambda) \propto \chi_0(\lambda)^N\,. \tag{2}$$

Here $\chi_0(\lambda)$ plays the role of the *extensive part* of $\chi_\Sigma(\lambda)$. It is periodic in λ (with period 2π), but does not have to be smooth, and it is the singularities of $\chi_0(\lambda)$ at real values of λ that we propose to use as a characteristics of the thermodynamic phase [3].

Note that the definition above is quite general and applies to a vast number of statistical and quantum problems (in many situations, one even has a choice between

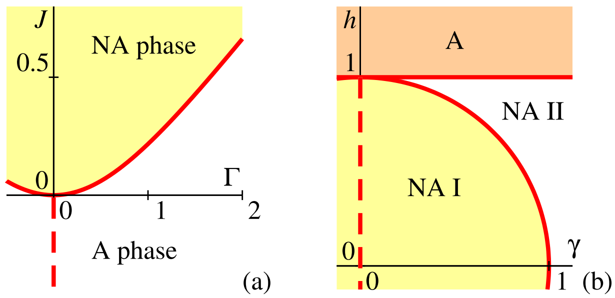

FIG. 2. **(a)** The counting phase diagram of the classical Ising chain. The shaded upper region is the "nonanalytic" (NA) phase, and the lower region is the "analytic" (A) phase [14]. The phase diagram is symmetric with respect to the change of sign of Γ. **(b)** The counting phase diagram of the spin-1/2 XY chain at zero temperature. The three phases are: Nonanalytic I, Nonanalytic II, and Analytic. On the dashed line $\gamma = 0$, $|h| < 1$, the dependence of FCS on γ is nonanalytic. The phase diagram is symmetric with respect to the (independent) changes of sign of γ and h.

different possible observables Q). In Fig. 1, we show two such examples: particles on a lattice (with Q being the number of particles) and a spin-1/2 chain (with Q being the number of up spins).

Our FCS construction is related to other characteristics of correlations. The analytic continuation $\lambda \to i\infty$ produces the "emptiness formation probability" (EFP) [10, 11]. On the other hand, in quantum systems of noninteracting fermions, FCS is known to be related to the entanglement [12].

Singularities in $\chi_0(\lambda)$ is a subtle characteristics of FCS. In Ref. 3 we argued that they are related to pre-exponential factors in staggered cumulants of the observable Q (if the singularity occurs at $\lambda = \pi$). In one-dimensional systems, we can interpret $\ln \chi_0(\lambda)$ as the inverse correlation length of the Jordan–Wigner string $\exp(i\lambda Q)$ (such correlation functions were also discussed in the context of integrable systems [10]). In some situations, Jordan–Wigner strings may be related to physical quantities which are directly observable, e.g., spin correlations in the example of the XY chain below.

We propose to classify thermodynamic phases by the number and type of singularities of $\chi_0(\lambda)$ at real values of λ. Thus obtained *counting phases* do not have to exactly reproduce the conventional phase diagram. Below, we illustrate this proposal with two examples.

III. ONE-DIMENSIONAL ISING MODEL

Our classification results in a nontrivial phase diagram for the one-dimensional Ising model. We consider the classical Ising chain in an external field described by the Hamiltonian

$$H = J \sum_j \sigma_j \sigma_{j+1} + \Gamma \sum_j \sigma_j \, , \tag{3}$$

where the Ising spins σ_j take values ± 1 and the statistical weights of spin configurations are given by $\exp(-H)$ (the temperature is incorporated in the parameters J and Γ). This model is equivalent to the "weather model" considered in Ref. 3, and one finds two different counting phases: "analytic" (A) and "nonanalytic" (NA). In the NA phase, $\chi_0(\lambda)$ has a singularity at $\lambda = \pi$. The phase diagram is shown in Fig. 2a, in coordinates Γ and J [13, 14]. The phase-transition line is given by

$$\cosh \Gamma = e^{2J} \, . \tag{4}$$

This counting phase transition has a simple physical interpretation. If one considers the Jordan–Wigner string

$$V_\pi(j) = \prod_{k=j_0}^{j} \sigma_k \tag{5}$$

(with respect to some reference site j_0), then the counting phase transition corresponds to a nonanalyticity of the correlation length of the exponentially decaying correlation function $\langle V_\pi(0) V_\pi(j) \rangle$, as a function of the parameters J and Γ. In the A phase, the correlation function $\langle V_\pi(0) V_\pi(j) \rangle$ exhibits a pure exponential (at $\Gamma < 0$) or a staggered-exponential (at $\Gamma > 0$) decay as a function of j, while in the NA phase there are additional *incommensurate oscillations* in j. Note that this counting phase transition is not a thermodynamic phase transition in the usual sense: in fact, thermodynamic phase transitions are not possible in statistical one-dimensional systems with local interactions. The thermodynamic partition function of the Ising model does not have a singularity at the counting phase transition, but non-local Jordan-Wigner-type correlations (5) do. This example illustrates a clear distinction between counting and conventional thermodynamic phase transitions.

Finally, we remark that the counting phase diagram of the one-dimensional Ising model found in this Section can also be understood in terms of the Lee–Yang theory of zeros of the partition function. Details of this connection are presented in Section V below.

IV. SPIN-1/2 XY CHAIN

We now turn to a quantum example where a nontrivial counting phase diagram may be explicitly constructed: the spin-1/2 XY chain in a transverse magnetic field. The Hamiltonian of the system is [16]

$$\hat{H} = \sum_j \left(\frac{1+\gamma}{2} \, \sigma^x_j \sigma^x_{j+1} + \frac{1-\gamma}{2} \, \sigma^y_j \sigma^y_{j+1} - h \, \sigma^z_j \right) . \tag{6}$$

Without loss of generality, we assume $\gamma \geq 0$ and $h \geq 0$. We are interested in the counting phase diagram with respect to the number of up spins (as the observable Q in our construction) at zero temperature (in the particular case of $\gamma = 1$, the FCS in this system was studied in Ref. 1). By the Jordan–Wigner transformation, this model can be mapped onto a quadratic fermionic system [16, 17], and the generating function $\chi_\Sigma(\lambda)$ for a subchain of N sites can be written as a $N \times N$ Toeplitz determinant. By a simple extension of the derivation in Ref. 11, we find

$$\chi_\Sigma(\lambda) = \det_{1\le j\le k\le N} \int_0^{2\pi} \frac{dq}{2\pi}\, \sigma(q,\lambda) e^{iq(j-k)} \tag{7}$$

with the *symbol* $\sigma(q,\lambda)$ of the Toeplitz determinant given by [cf. Eq. (17) of the first paper of Ref. 11]

$$\sigma(q,\lambda) = \frac{1+e^{i\lambda}}{2} + \left(\frac{1-e^{i\lambda}}{2}\right) \frac{\cos q - h + i\gamma \sin q}{\sqrt{(\cos q - h)^2 + \gamma^2 \sin^2 q}}\,. \tag{8}$$

The exponential asymptotic dependence of such determinants on N is given by the Szegő formula [18]. It immediately produces the result for $\chi_0(\lambda)$:

$$\chi_0(\lambda) = \exp \int_0^{2\pi} \frac{dq}{2\pi}\, \ln \sigma(q,\lambda)\,, \tag{9}$$

provided that $\sigma(q,\lambda)$ has zero winding of the complex phase as q varies from 0 to 2π. In the integral (9), the branch of the logarithm is chosen by the analytic continuation along the real axis of q, and the zero-winding condition implies that $\ln\sigma(2\pi,\lambda) = \ln\sigma(0,\lambda)$ under such an analytic continuation.

For some values of γ, h, and λ, however, the symbol (8) may have winding number one [so that $\ln\sigma(2\pi,\lambda) = \ln\sigma(0,\lambda) + 2\pi i$]. In this case, a modification of the Szegő formula applies [19]:

$$\chi_0(\lambda) = -\exp\left(\int_0^{2\pi} \frac{dq}{2\pi}\, \ln\left[\sigma(q,\lambda)\, e^{-iq}\right] + iq_0\right)\,, \tag{10}$$

where q_0 is the location of the singularity of $\sigma(q,\lambda)$ in the upper half plane of q with the smallest imaginary part.

A tedious, but straightforward application of Eqs. (9) and (10) allows us to calculate explicitly $\chi_0(\lambda)$ at all values of γ and h. As a result, we find three counting phases shown in Fig. 2b: two nonanalytic phases and an analytic one. Note that the same phase diagram appeared previously in the analysis of spin correlations [17] and of EFP [11]. The generating functions $\chi_0(\lambda)$ at typical points in each of the three phases are shown in Fig. 3. Below we summarize some properties of these phases in terms of FCS.

Nonanalytic I phase (NA I): $\gamma^2 + h^2 < 1$. In this phase, we find (assuming $\lambda \in [-\pi,\pi]$, $\gamma \ge 0$, $h \ge 0$) for the absolute value of $\chi_0(\lambda)$:

$$|\chi_0(\lambda)| = \sqrt{\frac{1+\gamma\cos\lambda}{1+\gamma}}\,. \tag{11}$$

Expressions for the phase of $\chi_0(\lambda)$ following from Eqs. (9) and (10) are lengthy for all the three phases, and we do not present them here, except in several particular cases where they can be considerably simplified. In the NA I phase, the only singularity of $\chi_0(\lambda)$ is a phase jump at $\lambda = \pi$:

$$\mathrm{Im}\, \ln \chi_0(\pm\pi) = \pm\left(\pi - \arccos\frac{h}{\sqrt{1-\gamma^2}}\right)\,. \tag{12}$$

In several special cases, $\chi_0(\lambda)$ takes a particularly simple form. At $\gamma = 0$,

$$\chi_0(\lambda) = \exp\left[i\lambda\left(1 - \frac{1}{\pi}\arccos h\right)\right] \tag{13}$$

[in this case, the spin chain is equivalent to free fermions with the density $1 - (1/\pi)\arccos h$].

At $h = 0$,

$$\chi_0(\lambda) = e^{i\lambda/2}\sqrt{\frac{1+\gamma\cos\lambda}{1+\gamma}}\,. \tag{14}$$

At the phase boundary $\gamma^2 + h^2 = 1$,

$$\chi_0(\lambda) = p\, e^{i\lambda} + 1 - p\,, \qquad p = \frac{1}{2}\left(1 + \sqrt{\frac{1-\gamma}{1+\gamma}}\right)\,, \tag{15}$$

which corresponds to independent spins with the probability p of pointing up [17].

Note that Eq. (11) is not even in γ, and therefore $\chi_0(\lambda)$ depends nonanalytically on γ across the line $\gamma = 0$.

Nonanalytic II phase (NA II): $\gamma^2 + h^2 > 1$, $|h| < 1$. In this phase (again assuming $\lambda \in [-\pi,\pi]$, $\gamma \ge 0$, $h \ge 0$), $\chi_0(\lambda)$ has phase jumps at points $\pm\lambda_c$ given by

$$\cos\lambda_c = -\frac{1-z_1^2}{\gamma(1+z_1^2)}\,, \qquad z_1 = \frac{h + \sqrt{\gamma^2 + h^2 - 1}}{1+\gamma}\,. \tag{16}$$

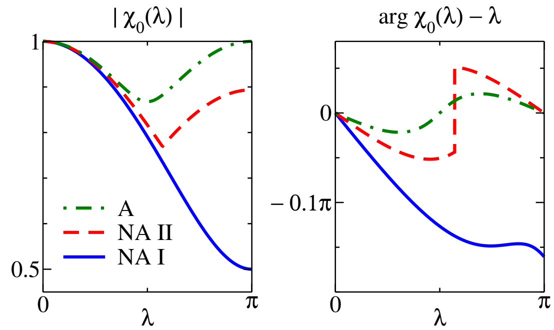

FIG. 3. The absolute value and the phase of the generating function $\chi_0(\lambda)$ at typical points in each of the three counting phases of the XY chain. For better visualization, the linear part λ is subtracted from the phase of $\chi_0(\lambda)$. In each panel, the three curves are (from bottom to top): NA I phase (solid line), $\gamma = 0.6$, $h = 0.7$; NA II phase (dashed line), $\gamma = 0.5$, $h = 0.95$; A phase (dash-dotted line), $\gamma = 0.5$, $h = 1.01$.

For the absolute value of $\chi_0(\lambda)$, we find

$$|\chi_0(\lambda)| = \begin{cases} \sqrt{\frac{1+\gamma\cos\lambda}{1+\gamma}}, & |\lambda| < \lambda_c\,, \\ z_1\sqrt{\frac{1-\gamma\cos\lambda}{1+\gamma}}, & |\lambda| > \lambda_c\,. \end{cases} \tag{17}$$

Once again, we do not present here full expressions for the phase of $\chi_0(\lambda)$. The phase jump at λ_c is given by

$$\operatorname{Im}\ln\frac{\chi_0(\lambda_c+0)}{\chi_0(\lambda_c-0)} = \arccos\frac{h(1+z_1^2)}{2z_1} \tag{18}$$

(this jump tends to zero at the phase boundary). At the boundary with the NA I phase, $\lambda_c \to \pi$, and $\chi_0(\lambda)$ is given by Eq. (15). At the boundary with the Analytic phase $h = 1$, one finds $\lambda_c \to \pi/2$. In the whole NA II phase, $\operatorname{Im}\ln\chi_0(\pm\pi) = \pm\pi$, which implies that $\chi_0(\lambda)$ is smooth at $\lambda = \pi$.

Analytic phase (A): $|h| > 1$. In this phase, $\chi_0(\lambda)$ has no singularities in λ. For its absolute value we find:

$$|\chi_0(\lambda)| = \sqrt{\frac{h+\sqrt{\gamma^2\cos^2\lambda + h^2 - 1}}{h+\sqrt{\gamma^2 + h^2 - 1}}}\,. \tag{19}$$

Throughout this phase, $\operatorname{Im}\ln\chi_0(\pm\pi) = \pm\pi$ (just like in the NA II phase). At $\gamma = 0$, the generating function takes the particularly simple form $\chi_0(\lambda) = i\lambda$ [a completely filled band of free fermions].

We notice a remarkable property of the A phase: throughout this phase, $\chi_0(\pi) = -1$. This means that the correlations of the Jordan–Wigner operators (5) [where σ_k denote now the z components σ_k^z] decay slower than exponentially. This property was described in Ref. 1 as "confinement of dual domain walls", and it can also be understood in the fermionic language. At $|h| > 1$, fermions form a completely filled (or completely empty) band, and the anisotropy terms (involving γ) introduce local Cooper pairs, which, however, change the number of particles by two. Thus the expectation value of the Jordan–Wigner parity string $\langle V_\pi(0)V_\pi(j)\rangle$ is only affected by Cooper pairs intersecting one of the end points of the string (0 or j). But, since pairs are local, the number of such pairs remains finite for long strings, which leads to a saturation of the correlations $\langle V_\pi(0)V_\pi(j)\rangle$ at large j.

The counting phase diagram of the XY chain (Fig. 2b) coincides with that obtained from spin correlations: different phases are distinguished by the transverse long-range order, presence or absence of incommensurate oscillations in spin correlations and by pre-exponential factors in exponentially decaying spin correlations [17]. This coincidence is not surprising, since, by the Jordan–Wigner transformation, transverse spin operators $\sigma_j^\pm$ are represented by the product of the string operator (5) and a fermion operator [16]. As a consequence, transverse spin correlations are given by the Toeplitz determinants which differ from Eqs. (7) and (8) only by a shift of the winding number (and by fixing $\lambda = \pi$) [17].

The phase diagram in Fig. 2b also resembles those based on EFP in Ref. 11 and on entanglement entropy in Ref. 20. Indeed, the EFP is given by the same Toeplitz determinant (7), (8) with $\lambda \to i\infty$ [11], and the entanglement entropy depends on the spectrum of a closely related block Toeplitz matrix [20]. Therefore the phase boundaries which are determined by the geometry of the square-root branching points in Eq. (8) coincide in all the three problems. However the FCS classification contains additional details related to the positions of λ-dependent logarithmic branching points in Eq. (9).

Finally, we remark that, even though the XY spin chain considered in our work maps onto a quadratic fermionic system, it does not obey the theorem on factorization of FCS for noninteracting fermions of Ref. 21: the phase NA II with a singularity at an intermediate value of λ would not be allowed by that theorem. The reason for this discrepancy is that the corresponding fermionic system contains pairing terms [16], and the theorem of Ref. 21 is not, in general, valid for quadratic Hamiltonians with pairing (see also discussion in the supplementary material of the last paper of Ref. 12). Thus the NA II phase presents an example of an *interacting* system with singularitites of $\chi_0(\lambda)$ shifted away from $\lambda = \pi$.

V. RELATION TO LEE–YANG ZEROS

Our theory of counting phase transitions is closely related to the approach of Lee and Yang considering zeros of the partition function in the complex plane of a parameter of the model (fugacity or magnetic field) [15]. Namely, in many (but not all) situations, the counting phase transitions are determined by the locations of zeros of the partition function in the complex fugacity (or magnetic-field) plane.

Consider first the case of a classical system. Then the generating function (1) can be understood as the partition function of the system with the imaginary part $-i\lambda$ added to the chemical potential dual to the observable Q in the subsystem Σ. Thus we study the same analytic continuation of the partition function as Lee–Yang's one, but with a different order of thermodynamic limits. In Lee–Yang theory, the chemical potential acquires a uniform imaginary component in the whole system, and then the system size tends to infinity. In contrast, in our construction, the system size is infinite from the very beginning, it is only the subsystem Σ where the chemical potential has an imaginary part, and the thermodynamic limit is defined by expanding the subsystem Σ within the same infinite system.

We believe that in most situations this difference in the order of the thermodynamic limits is unimportant and the extensive part of the generating function $\chi_0(\lambda)$ simply equals the Lee–Yang partition function per unit cell of the system. In this case, the counting phase diagram and the positions of singularities of $\chi_0(\lambda)$ can be easily read off the locus of the Lee–Yang zeros in the thermodynamic limit. The irrelevance of the order of the thermodynamic limits can be most easily understood in the case of one-dimensional classical systems: there, both $\chi_0(\lambda)$ and the asymptotic behavior of the Lee–Yang partition function in the thermodynamic limit are given by the leading eigenvalue of the corresponding transfer matrix. This connection to Lee–Yang zeros was also discussed in Ref. [22] in the context of "dynamical phase transitions".

In the case of a quantum system, the relation to the locus of Lee–Yang zeros is more complicated. Here one should distinguish two possibilities: either the observable Q (defined for the full system) commutes with the Hamiltonian H or it does not.

In the case of Q commuting with H, the Lee-Yang partition function $Z_{\rm LY}$ may be related to the FCS generating function for the full system in the grand-canonical ensemble, just like in the classical case discussed above:

$$Z_{\rm LY} = \operatorname{tr} e^{-\beta H + i\lambda Q} = \operatorname{tr} e^{-\beta H} e^{i\lambda Q} = \langle e^{i\lambda Q}\rangle \operatorname{tr} e^{-\beta H} \tag{20}$$

(here β is the inverse temperature). Therefore, one may draw the same relation between the locus of Lee–Yang zeros and counting phase transitions as in classical systems, provided the order of the thermodynamic limits is unimportant. The latter is, however, not always the case, at least for systems with sufficiently slowly decaying correlations. An example where the Lee–Yang approach and FCS give different results is one-dimensional fermions at zero temperature (equivalent to the spin-1/2 XY chain considered in Section IV at $\gamma = 0$). There, the FCS approach leads to a well defined generating function $\chi_0(\lambda)$ [8], while the Lee–Yang approach provides neither a good locus of zeros nor a good thermodynamic partition function per unit cell of the lattice. The question about the general conditions under which the two orders of the thermodynamic limit are equivalent, goes beyond the scope of the present paper, and we leave it for future studies.

Finally, in the case of Q not commuting with H (which applies to our example of spin-1/2 XY chain in Section IV at $\gamma \neq 0$), the relation (20) between the Lee–Yang partition function and full counting statistics no longer holds, and we conclude that there is no obvious relation between the two approaches.

VI. CONCLUSION

We have proposed a classification scheme of thermodynamic phases and correlations in general in terms of the analytical properties of the extensive part of FCS for a suitably chosen discrete observable. Using FCS for describing correlations involves nonlocal observables (1) and therefore allows us to capture subtle details of correlations inaccessible with local observables. In this way, *counting phases* may be distinguished: sometimes they coincide with conventional thermodynamic phases, but sometimes one thermodynamic phase may be further subdivided into several counting phases reflecting differences in statistics of fluctuations of a certain discrete variable. The physical meaning of counting phase transitions is often subtle. In some situations it is related to the structure of zeros of the partition function in Lee–Yang theory, and in one-dimensional situations we relate FCS physics to the correlations of nonlocal string observables of Jordan–Wigner type. Deeper physical implications of these counting phase transitions are still to be understood.

In our work, we have illustrated our proposal with two simplest examples: one-dimensional Ising model as a classical example and spin-1/2 XY model as a quantum one. We have chosen those examples, since they allow an analytical calculation of the counting phases and an easy comparison with other available results. Studying counting phases in systems with more complicated interactions is interesting but requires more involved analytical or numerical methods.

In general, the role of interactions in counting phase transitions is not yet fully understood. While it has been shown in Ref. 21 that fermionic systems in the absence of interactions can only exhibit singularities in $\chi_0(\lambda)$ at real negative $e^{i\lambda}$, the absence of interactions is not a necessary condition for this property. Indeed, for the spin-1/2 XY chain at a finite anisotropy γ (see Section IV) both phases with singularities at $\lambda = \pi$ and those with singularities at $\lambda \neq \pi$ are present.

Finally, we remark that here we have only focused on analytic properties of the generating function $\chi_0(\lambda)$ at real values of λ. It may also be instructive to analyze, more generally, the structure of singularities of $\chi_0(\lambda)$ in the complex plane of $e^{i\lambda}$. This would, on one hand, provide a closer connection to the theory of Lee–Yang zeros [15], and on the other hand, relate it to the theory of the emptiness formation probability [10, 11].

VII. ACKNOWLEDGMENTS

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[14] The phase diagram in Fig. 2a shows an additional singular line $\Gamma = 0$, $J < 0$, which was omitted in Ref. 3. This line separates two regions of the same analytic phase (one with exponential and the other with staggered-exponential correlations $\langle V_\pi(0)V_\pi(i)\rangle$). On this line, the function $\chi_0(\lambda)$ is nonanalytic with a singularity at an intermediate value of λ (between 0 and π).
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