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On the singularity structure of the 2D Ising model susceptibility

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Abstract. Some simplifications of the integrals $\chi^{(2n+1)}$, derived by Wu *et al* (1976 *Phys. Rev.* B **13** 316), that contribute to the zero field susceptibility of the 2D square lattice Ising model are reported. In particular, several alternate expressions for the integrands in $\chi^{(2n+1)}$ are determined which greatly facilitate both the generation of high-temperature series and analytical analysis. One can show that as series, $\chi^{(2n+1)} = 2^{2n}(s/2)^{4n(n+1)}(1 + \mathrm{O}(s))$ where s is the high-temperature variable $\sinh(2K)$ with K the conventional normalized inverse temperature. Analysis of the integrals near symmetry points of the integrands shows that $\chi^{(2n+1)}(s)$ is singular on the unit circle at $s_{k\ell} = \exp(\mathrm{i}\theta_{k\ell})$ where $2\cos(\theta_{k\ell}) = \cos(2\pi k/(2n+1)) + \cos(2\pi\ell/(2n+1))$, $-n \leqslant k, \ell \leqslant n$. The singularities, $\theta_{k\ell} = 0$ excepted, are logarithmic branch points of order $\epsilon^{2n(n+1)-1}\ln(\epsilon)$ with $\epsilon = 1 - s/s_{k\ell}$. There is numerical evidence from series that these van Hove points, in addition to the known points at $s = \pm 1$ and $\pm\mathrm{i}$, exhaust the singularities on the unit circle. Barring cancellation from extra (unobserved) singularities one can conclude that $|s| = 1$ is a natural boundary for the susceptibility.

1. Introduction

Although an exact formal expression for the susceptibility of the 2D square lattice Ising model was derived many years ago by Wu *et al* [1], the relative intractability of the integrals appearing there has impeded progress in clarifying the nature of the susceptibility as a function of complex temperature. Detailed information is available at specific points; in particular, Wu *et al* [1] exactly calculated the divergent part of the susceptibility at the ferromagnetic singularity. Aharony and Fisher [2] conjectured that all corrections to the scaling behaviour at this point could be deduced from the nonlinear scaling fields determined entirely by the known free energy and magnetization. This has been verified to quite high order by a high-temperature series analysis by Gartenhaus and McCullough [3]. Amplitudes at the anti-ferromagnetic point have also been determined [4] and series analysis [5] is consistent with the absence of non-analytic corrections to the scaling of the susceptibility just as at the ferromagnetic point. There are also singular points in the complex temperature plane off the real axis; the zero field free energy is singular at $s = v = \pm\mathrm{i}$ where in general

$$s = \sinh(2K) = 2v/(1 - v^2) \qquad v = \tanh(K) \tag{1}$$

with K the conventional Ising model coupling constant $J/k_{\mathrm{B}}T = \beta J$ while v is the more commonly used high-temperature expansion variable for this model†. Not unexpectedly,

† Many of the subsequent formulae are simpler when expressed in terms of s so that I will use it exclusively as the expansion parameter. It is also more 'natural' in that the circle $|s| = 1$ is approximately the locus of zeros of the partition function of a finite system and is the locus of all singularities I find in this paper. A good review with references to earlier work is Fisher [6]. For a discussion of finite system boundary conditions that make the zeros of the partition function fall exactly on $|s| = 1$ see also Brascamp and Kunz [6].

there is evidence [7] that the susceptibility is singular here also; what is of some interest is that conventional scaling relations do not apply†.

All of the results described above would be consistent with a relatively simple functional form for the susceptibility and even possibly a closed form solution. However, Guttmann and Enting [9] following some work by Hansel *et al* [10] have recently argued that the 2D Ising susceptibility should be a function with a natural boundary, distinctly different from the free energy or magnetization which are known in closed form and have singularities only at $s = \pm 1, \pm \mathrm{i}$. They use as evidence the structure of denominators in the generating function for an anisotropic model in which one coupling, say K_y, is held fixed while the other K_x is varied. While suggestive, their argument is ultimately based on series and one does not have the information about high-order terms necessary to make it definitive. In this paper I go much further in that I explicitly find the contribution to an infinite number of singularities to the high-temperature susceptibility χ for the isotropic model on the circle $|s| = 1$. There is no numerical evidence for other singularities that might cancel these and barring this unlikely possibility one can conclude that $|s| = 1$ is a natural boundary‡.

While the emphasis of the paper is on the singularities of χ, these could not have been deduced without also deriving a number of intermediate formulae which represent a formal extension of the work of Wu *et al* [1]. For example, equation (6) below can be used to show that each contributing term $\chi^{(2n+1)}$ is positive definite for real $0 < s < 1$ and this verifies explicitly that the expression in [1] for χ is of the form of a dispersion series§. As another example, equation (7) below shows that the essential part of each integrand in $\chi^{(2n+1)}$ is a 'simple' antisymmetric sum of products. Not only is this suggestive of the fermionic connection [12] but because all remnants of the exponential generator in the formal expressions for $\chi^{(2n+1)}$ in [1] have now disappeared it becomes conceivable that the final answer could be derived by another route. Such an alternative might offer insight that I cannot provide; one might also hope for new derivations simply because those presented here do not qualify as elegant‖.

An important by-product of the intermediate formulae is that it is now much easier to derive high-temperature series for χ and an extension to 84 terms is reported in appendix A. Although possibly counter-intuitive, I believe the characterization of the singularities of χ actually enhances the utility of the series. The point is that the same analysis that shows $|s| = 1$ is very likely a natural boundary also shows that there are no singularities of any practical consequence, i.e. of large amplitude, near the critical point $s = 1$. On the other hand, by knowing the location of the dominant complex singularities of χ, even those very distant, one can perform a better job of estimating the behaviour near the physical critical point. With the new information available it becomes almost certainly worth redoing the Gartenhaus *et al* [3, 5] analyses because, although their results were consistent with the Aharony and Fisher conjectures [2] regarding the nature of corrections to scaling, there was also some hint of effects just beyond what one could convincingly include/exclude.

A summary of the main intermediate results and my conclusions regarding the singularity structure of χ are given in the following section. Section 2 also contains a guide to the more explicit details as given in subsequent sections and the appendices.

† These comments only strictly apply at the singularities $s = \pm\mathrm{i}$ as approached from small s. The same singularities are also present in the magnetization $(1 - s^{-4})^{1/8}$ which is the analytic continuation from the physical ferromagnetic phase $s > 1$. Here the exponent scaling relations do appear to be satisfied (see [7, 8]).

‡ Note that all of the singularities of the generating function coefficients at $v = \tanh(K) = \exp(2\pi\mathrm{i}k/(2n+1))$, $-n \leqslant k \leqslant n$, discussed in [9] lie *outside* the natural boundary circle $|s| = 1$.

§ [11] has emphasized the importance of this information.

‖ A simplification might be achieved just be recasting the formulae in this paper into more conventional form. For example, in equations (4), $x = \mathrm{e}^{-\gamma}$ and $s \cdot y = 1\,\sinh(\gamma)$ where γ is Onsager's variable. A referee has suggested that Onsager's elliptic substitution, as in the proof of equation (5.5) in [13], may also prove fruitful.

2. Main results

The main results of the paper are summarized here with only a few comments about how these arise. Sketches of the proofs and details of the applications will be left for later sections. I begin with some key formulae from Wu *et al* [1] (hereafter denoted as W with equations from this reference denoted by W $\cdot * \cdot *$) and in particular their reduction of the susceptibility into $2n+1$ particle contributions as (W.7.43)

$$\chi = \beta \sum_{n=0}^{\infty} \chi^{(2n+1)} = \beta \sum_{n=0}^{\infty} \sum_{N=-\infty}^{\infty} \sum_{M=-\infty}^{\infty} \langle \sigma_{00} \sigma_{MN} \rangle^{(2n+1)}. \tag{2}$$

Each $\langle \sigma_{00} \sigma_{MN} \rangle^{(2n+1)}$ is given in W as a $4n+2$ multiple integral (equations W.2.13–2.17) but these can be reduced to $2n$ dimensions by straightforward contour integration methods. Some details about this reduction as well as the derivation of the key formulae (3), (6), (7), (10) below are given in section 3. What appears to be the irreducibly coupled expression for each $\chi^{(2n+1)}$ contribution is

$$\begin{aligned} \chi^{(2n+1)} = (1-s^4)^{1/4} s^{2n} \left(\prod_{m=1}^{2n} \int \frac{\mathrm{d}\phi_m}{2\pi} \right) \left(\prod_{m=1}^{2n+1} y_m \right) \\ \times H^{(2n+1)}\{f_{ij}\} \left(1 + \prod_{m=1}^{2n+1} x_m \right) \Bigg/ \left(1 - \prod_{m=1}^{2n+1} x_m \right) \end{aligned} \tag{3}$$

where the constraint $\sum_{m=1}^{2n+1} \phi_m = 0 \bmod 2\pi$ is understood so that except for the $H^{(2n+1)}$ factor the integrand is completely symmetric in all $2n+1$ variables. The terms in the integrand, valid for small s and elsewhere by analytic continuation, are

$$\begin{aligned} x_m &= s/\{1+s^2 - s\cdot\cos\phi_m + \surd((1+s^2-s\cdot\cos\phi_m)^2 - s^2)\} \\ y_m &= 1/\surd((1+s^2-s\cdot\cos\phi_m)^2 - s^2) \\ f_{ij} &= \tfrac{1}{2}(\sin\phi_i - \sin\phi_j)(1+x_i x_j)/(1-x_i x_j) \end{aligned} \tag{4}$$

while the functions $H\{f_{ij}\}$ can be deduced from the generator equation (W.2.14) and given a graphical interpretation. The first few are

$$\begin{aligned} &H^{(1)} = 1 \qquad H^{(3)} \equiv f_{12} f_{23} - \tfrac{1}{2}(f_{12} f_{21}) \\ &H^{(5)} \equiv f_{12} f_{23} f_{34} f_{45} - \tfrac{1}{2} f_{12} f_{23} (f_{45} f_{54}) - \tfrac{1}{4}(f_{12} f_{23} f_{34} f_{41}) + \tfrac{1}{8}(f_{12} f_{21})(f_{34} f_{43}) \end{aligned} \tag{5}$$

where I use here and throughout the paper $\equiv$ to denote 'is equivalent to, for the purposes of integration in equation (3)'. Because of the symmetric form of the rest of the integrand different labellings of the f_{ij} in (5) are possible. Equation (3) for $\chi^{(1)}$ evaluates directly without integration to $\chi^{(1)} = (1-s^4)^{1/4}/(1-s)^2$ while for $n > 0$ equations (3)–(5) can form the basis for the efficient generation of high temperature series by direct expansion and numerical integration. It was in fact essentially these equations that formed the basis for the series reported at Cargese [14]. However, as shown below, $\chi^{(7)}$ contributes at order s^{48} so that the higher-order terms in the published longer series [3, 15]† need to be corrected by the results below.

Since all terms in the integrand in (3) are of order unity the naive expectation is that $\chi^{(2n+1)}$ is of order s^{2n}, a bound already remarked on in W as very poor. Twenty orders were observed to cancel in $\chi^{(5)}$ yet there is nothing in the structure of the integrand as written above to suggest

† The term $90466431959611708308v^{49}$ should replace a misprint in the series on p 9 in [15].

why this might happen. To verify this cancellation one needs alternate representations for the H functions. A very useful reduction for analytical work is

$$H^{(2n+1)} \equiv (G^{(2n+1)})^2/(2n+1)! \equiv \left(\prod_{m=1}^{n} f_{2m-1,2m}\right) G^{(2n+1)}/(2^n n!) \tag{6}$$

where $G^{(2n+1)}$ is the totally anti-symmetric sum of products

$$G^{(2n+1)} = \sum_{\mathrm{p}} \delta_{\mathrm{p}} P\left(\prod_{m=1}^{n} f_{2m-1,2m}\right)/(2^n n!). \tag{7}$$

The permutation operator P is to be understood to generate all possible $(2n+1)!$ terms using $2n+1$ labels. A normalization $2^n n!$ is included in (6) and (7) to correct for the redundancy that arises because the f_{ij} are anti-symmetric and the ordering of the f_{ij} factors does not matter. Thus there are only $(2n+1)!!$ distinct terms in the sum (7) each with weight ± 1 as given by the parity factor δ_{p} depending on whether the permutation is even or odd†. It is this reduction to the anti-symmetric form that suggests why there is so much cancellation in the evaluation of the integrals. The details of the additional analysis to prove the cancellation observed in the high-temperature expansions are given in section 4. Here I only quote the final result for the susceptibility from equation (3) which is

$$\chi^{(2n+1)} = s^{2n}(s/2)^{2n(2n+1)}(1 + \mathrm{O}(s)). \tag{8}$$

Another reduction verified in section 4 that is useful for extended numerical work is

$$H^{(3)} \equiv f_{12}(f_{23} + \tfrac{1}{2} f_{12}) \qquad H^{(5)} \equiv f_{12}(f_{23} f_{14} + \tfrac{1}{2} f_{12} f_{34})(f_{45} + \tfrac{1}{4} f_{34}) \tag{9}$$

and for the general term the product

$$H^{(2n+1)} \equiv f_{12}\left(\prod_{m=1}^{n-1}\left(f_{2m,2m+1} f_{2m-1,2m+2} + \frac{1}{2m} f_{2m-1,2m} f_{2m+1,2m+2}\right)\right) \times \left(f_{2n,2n+1} + \frac{1}{2n} f_{2n-1,2n}\right). \tag{10}$$

Furthermore, as part of the proof of the cancellation leading to equation (8) one finds that the f_{ij} to be used in (10) need not be restricted to the form given in (4). Instead one can use the equivalent

$$f_{ij} \equiv (\sin\phi_i - \sin\phi_j)(x_i x_j/(1 - x_i x_j) - s^2/4) \tag{11}$$

which is $\mathrm{O}(s^3)$. Since $2n$ factors of f_{ij} appear in the integrand for $\chi^{(2n+1)}$ in equation (3), use of the f_{ij} from equation (11) gives as a bound for $\chi^{(2n+1)}$ order s^{8n} and while much better than the naive s^{2n} is still nowhere near the actual result in equation (8) except for $n = 1$. The use of these representations and the further manipulations necessary to derive high-temperature series efficiently are described in appendix A where also series to order s^{84} are given. Longer series for $\chi^{(3)}$ and $\chi^{(5)}$ have been useful in confirming some of the analytical work described here. In connection with this I discuss in appendix B a series analysis method that is particularly well suited to long series.

For a determination of the singularities of $\chi^{(2n+1)}$ I have guessed that at least a subset of them should arise from the symmetry points of the integrand in analogy with the van Hove singularities seen in periodic systems such as typically studied in solid state physics. The most obvious symmetry point is that at which all ϕ_m are equal and equal $\phi^{(k)} = 2\pi k/(2n+1)$

† The fact that the permutation sum in equation (7) is over $2n+1$ labels means that $G^{(2n+1)}$ is a sum of $2n+1$ Pfaffians obtained by cyclically permuting indices starting from $1, 2, \ldots, 2n$ with index $2n+1$ initially missing. A discussion of Pfaffians can be found in [16].

with $-n \leqslant k \leqslant n$. Furthermore, I require a potential divergence in the integrand in equation (3) and an obvious point for this criterion is the vanishing of the denominator factor $1 - \prod_m x_m = 1 - x^{2n+1}$ with all $x_m = x(\phi_m) = x$ equal. This combination $\phi_m = \phi^{(k)}$ and $x = \exp(\mathrm{i}\phi^{(\ell)})$ requires $s = s_{k\ell}$ where from equation (4) for $x_m(s)$ one obtains

$$\begin{aligned} &s_{k\ell} = \exp(\mathrm{i}\theta_{k\ell}) \qquad 2\cos(\theta_{k\ell}) = \cos(\phi^{(k)}) + \cos(\phi^{(\ell)}) \\ &\phi^{(k)} = 2\pi k/(2n+1) \qquad \phi^{(\ell)} = 2\pi\ell/(2n+1) \qquad -n \leqslant k, \ell \leqslant n. \end{aligned} \tag{12}$$

The details of the expansion of the integrand in equation (3) about the symmetry points and the determination of the leading singularity structure of $\chi^{(2n+1)}$ in the neighbourhood of $s_{k\ell}$ are given in section 5. The general result, from equation (42), is that the singular part of $\chi^{(2n+1)}$ is

$$\chi_{k\ell}^{(2n+1)} = \mathrm{O}(\epsilon^{2n(n+1)-1}\ln(\epsilon)) \qquad \epsilon = 1 - s/s_{k\ell} \tag{13}$$

with the ferromagnetic point $k = \ell = 0$ excepted. With all amplitude information included,

$$\begin{aligned} \chi_{k\ell}^{(2n+1)}/(1-s_{k\ell}^4)^{1/4} \simeq{} & (\mathrm{i}/s_{k\ell})\left(\prod_{m=1}^{2n}(m!/2^m)\right)\Bigg/(\pi^n\Gamma(2n(n+1))\sqrt{(2n+1)}) \\ & \times(\epsilon(2n+1)\sin(\theta_{k\ell}))^{2n(n+1)-1}\ln\epsilon \\ & \times[(\sin^2(\phi^{(\ell)})\cos(\phi^{(k)}) + \sin^2(\phi^{(k)})\cos(\phi^{(\ell)}))^{2n(n+1)}]^{-1}. \end{aligned} \tag{14}$$

There is an ambiguity in equations (12)–(14) with regard to the sign of $\theta_{k\ell}$ but this is to be resolved simply by symmetrizing the contributions between $\theta_{k\ell}$ and $-\theta_{k\ell}$. That is, of all the solutions related by the $|k| \leftrightarrow |\ell|$ symmetries, exactly $\frac{1}{2}$ are to be identified with $0 < \theta_{k\ell} < \pi$ and $\frac{1}{2}$ with $-\pi < \theta_{k\ell} < 0$ so that the total $\chi^{(2n+1)}$ is real.

The singularities as given by equations (12)–(14) imply a definite asymptotic contribution to the series expansion of each $\chi^{(2n+1)}/(1-s^4)^{1/4} = \sum K_N^{(2n+1)} s^N$. For the case $n = 1$ these contributions, obtained most simply by expanding $\epsilon^3\ln(\epsilon)$ for each k, ℓ pair, combine to give in the limit $N \to \infty$ the coefficients

$$\Delta K_N^{(3)} = N^{-4}(4/\pi)(8\sin((N+1)2\pi/3) + 5\sqrt{5}\sin((N+1)\arccos(\tfrac{1}{4}))) \tag{15}$$

and while much smaller than the contributions from singularities at $s = \pm 1, \pm \mathrm{i}$, they are easily observed in the series analysis described in appendix B. Some of the corresponding $\Delta K_N^{(5)}$ contributions are also observed. There is no evidence in either series for additional $|s| = 1$ singularities. Thus the infinite number of singularities described in this paper are very unlikely to be cancelled and the conclusion that the circle $|s| = 1$ is a natural boundary for χ becomes very compelling.

3. Alternate integrand representations

Any particular term generated by (W.2.14) for $\langle\sigma_{00}\sigma_{MN}\rangle^{(2n+1)}$ is the product of combinatorial factors to be discussed below, a factor $(1-s^4)^{1/4}s^{2n}$, $2n+1$ double phase integrals of the form

$$\int\frac{\mathrm{d}\phi}{2\pi}\int\frac{\mathrm{d}\psi}{2\pi}(1+s^2-s(\cos\phi+\cos\psi))^{-1}\exp(-\mathrm{i}M\phi-\mathrm{i}N\psi) \tag{16}$$

and a further $2n$ integrand factors

$$\tfrac{1}{2}(\sin\phi-\sin\phi')(1+\exp(-\mathrm{i}\psi-\mathrm{i}\psi'))/(1-\exp(-\mathrm{i}\psi-\mathrm{i}\psi')). \tag{17}$$

Here I have used ϕ and ψ in place of the odd and even phases of W. The phases ϕ' and ψ' are integration variables associated with a factor not explicitly shown but which is identical to (16) except for the replacements $\phi \to \phi'$ and $\psi \to \psi'$; conversely there may be other occurrences of $\exp(-\mathrm{i}\phi)$ and $z = \exp(-\mathrm{i}\psi)$ in factors like (17) not explicitly shown. It is to be understood that $N \geqslant 0$ and the phases ψ have an infinitesimal negative imaginary part so that none of the factors (17) are singular and the $N \to \infty$ limit of $\exp(-\mathrm{i}N\psi)$ exists. The integral $\int \mathrm{d}\psi$ can be done by residue calculus with the zero of the denominator in (16) being the only singularity to consider; one gets for small s

$$\int \frac{\mathrm{d}\psi}{2\pi}(1+s^2-s(\cos\phi+\cos\psi))^{-1} = y = 1/\surd((1+s^2-s\cdot\cos\phi)^2-s^2) \tag{18}$$

and elsewhere the replacement

$$z = \exp(-\mathrm{i}\psi) \to x = s/\{1+s^2-s\cdot\cos\phi+\surd((1+s^2-s\cdot\cos\phi)^2-s^2)\}. \tag{19}$$

Similar replacements will be generated after integration over ψ'. The result of these integrations is that the product of integrals (16) becomes

$$\prod\left(\int \frac{\mathrm{d}\phi}{2\pi} y x^N \exp(-\mathrm{i}M\phi)\right) \tag{20}$$

and the dependence of $\langle\sigma_{00}\sigma_{MN}\rangle^{(2n+1)}$ on the lattice site M, N is contained entirely in (20). The lattice sum over the integers M, N can therefore be done on this expression alone; the x^N product in (20) converts to†

$$\left(1+\prod_{m=1}^{2n+1} x_m\right)\Big/\left(1-\prod_{m=1}^{2n+1} x_m\right) \tag{21}$$

in $\chi^{(2n+1)}$ and appears as the last factor in equation (3). The $\exp(-\mathrm{i}M\phi)$ product in (20) is replaced by $2\pi\delta(2\pi k-\Sigma\phi_m)$, $k = 0, \pm 1, \pm 2, \ldots$, and eliminates one of the $2n+1$ remaining ϕ integrations in $\chi^{(2n+1)}$. Finally, the integrand factor (17) reduces to $\frac{1}{2}(\sin\phi-\sin\phi')(1+x\cdot x')/(1-x\cdot x')$ which is one of the $2nf_{ij}$ factors that contribute to the $H\{f\}$ function in (3). Included in the definition of $H\{f\}$ are the combinatorial factors that depend on the specific structure of each f_{ij} product.

An f_{ij} can be viewed as a propagator from site i to j and the products of propagators will form either closed loops of even length or a combination of closed loops and an open line of even length‡. The loops originate in the $F^{(2n)}_{>MN}$ and the line in $x^{(2k-1)}_{>MN}$ in (W.2.14). Thus the 'graphical' rule to be observed is that with every loop of length ℓ is to be associated a weight of $-1/\ell$ where ℓ has its origins in the term $2n$ in the prefactor to the integral $F^{(2n)}_{>MN}$ in (W.2.16) and the -1 comes from the negative in the exponential in (W.2.14). From the exponential one also concludes that symmetry factors $1/m!$ must appear with each occurrence of an m-fold multiplicity in loops of the same length.

That the alternate expression (10) given in the introduction generates this same graphical expansion can be seen as follows. First, write for the first term in every bracket in (10) α and for the second term β so that schematically (10) is $(\alpha+\beta)^n$. Then note that in the expansion of the product (10), sequences such as $\alpha\alpha\beta\alpha\alpha\alpha\beta\beta\ldots$ are generated where it is understood that the order has been maintained. Reading from left to right, every occurrence of a factor β marks the termination of an open line and its conversion into a loop. The length of the loop is ℓ where $\ell/2-1$ is the number of preceding α factors. The anti-symmetry of each f_{ij} factor can be used to show a negative sign is generated with each loop. To verify the correct weight one must note the position of each factor β in the sequence; a β from the $(\ell/2)$th factor in (10) has weight $1/\ell$. Thus if, for example, successive loops are of length $\ell_1, \ell_2, \ell_3, \ldots$ the

† To generalize to a second moment calculation we need only include a factor M^2+N^2 in (20). By symmetry this is equivalent to $2N^2$ and leads to the replacement of (21) by $4\prod x(1+\prod x)/(1-\prod x)^3$, $\prod x = \prod_{m=1}^{2n+1} x_m$.

‡ The distinction between a line and loop, each a product of $2\ell f_{ij}$ factors and by definition of length 2ℓ, is that the line connects $2\ell+1$ distinct sites while the loop connects 2ℓ sites only.

β positions will determine the weight as $1/\ell_1/(\ell_1+\ell_2)/(\ell_1+\ell_2+\ell_3)/\ldots$ and to this must be added the weights of all sequences which differ only by a distinct permutation of the ℓ_i as these contribute to the same line/loop structure. If the ℓ_i are all different the correct weight follows immediately from the identify $\sum_{\mathrm{p}} 1/\ell_1/(\ell_1+\ell_2)/(\ell_1+\ell_2+\ell_3)/\ldots = 1/(\prod_i \ell_i)$. Otherwise the restriction on the permutation sum will automatically generate the correct $1/m!$ corrections for each m-fold multiplicity.

A quick sum rule check of the weights exclusive of sign can be obtained by noting that the generator for the weights defined by (W.2.14)–(W.2.16) is

$$g_w = (1+f^2+f^4+\cdots)\exp(f^2/2+f^4/4+f^6/6+\cdots) \tag{22}$$

where the exponential embodies the loop rules including their $1/\ell$ weight while the first factor ensures that a line appears only once with weight unity. The generator (22) has the expansion

$$g_w = (1-f^2)^{-3/2} = \sum f^{2n}(2n+1)!!/(2^n n!) \tag{23}$$

and the f^{2n} term in series (23) is exactly that given by (10), namely $\prod_{m=1}^{n} f^2(1+1/2m)$.

I know of no way to show the consistency of the key representations (6), (7) with the graphical rules above except by a detailed listing of cases. On the other hand, simple permutation and relabelling shows the equivalence of the two G forms in (6) so it is only necessary to use the simpler second, linear in G, form of (6) to verify correctness, i.e.

$$H^{(2n+1)} \stackrel{?}{\equiv} \left(\prod_{m=1}^{n} f_{2m-1,2m}\right) \sum_{\mathrm{p}} \delta_{\mathrm{p}} P\left(\prod_{m=1}^{n} g_{2m-1,2m}\right) \Big/ (2^n n!)^2. \tag{24}$$

The g_{ij} in (24) are identical to the f_{ij}; I introduce the notational difference here only to distinguish, for the following argument, those propagators (g) that come from the G factor as opposed to those (f) from the fixed prefactor. The sum in (24) as in (7) is over all permutations; therefore the total weight of all terms without regard to sign is $(2n+1)!/(2^n n!)^2 = (2n+1)!!/(2^n n!)$ and this is just the sum rule weight deduced from the generator (23). Also, in any of the products of $2n$ f_{ij} or g_{ij} propagators in (24) a site label k can appear at most twice, once in an f_{ik} and then once in g_{jk}. This implies that only loops or a single line together with loops can be generated. All loops are of even length; if ℓf_{ij} are involved there must be exactly ℓg_{ij} to join the first set into a loop. It is fairly straightforward to count the possible arrangements and show each particular loop structure comes with the correct weight, exclusive of sign.

To show the correctness of all sign factors it suffices to verify one particular configuration and then the relative sign between all pairs of configurations obtained by a transposition of neighbouring site labels, $i \leftrightarrow i+1$, $i = 1,\ldots,2n$. That is, these transpositions, if carried out enough times can generate any configuration from a given one and if all *relative* signs are correct then all signs are correct. The unpermuted configuration in (24) in combination with all $2^n n!$ redundant permutations serves as a starting point; it is $1/(2^n n!)\prod(f_{2i-1,2i}\, g_{2i-1,2i}) = (-1)^n/(2^n n!)\prod(f_{2i-1,2i}\, g_{2i,2i-1})$ which has the correct sign and weight for n loops of length 2.

To illustrate the sign proof I consider below two examples; the complete proof simply requires a listing of all cases which is not instructive. Consider first the case that a transposition occurs in a connected structure. To be specific, suppose f_{12} and f_{34} are connected by propagators and that we wish to compare with those configurations in G in which 2 and 3 have been transposed. Take as starting configuration $C_{\mathrm{start}} = f_{12}(g_{23}+g_{2k}f_{km}g_{m3}+\cdots)f_{34}$ with the central factor written as a sum to allow for different possible connections to be treated in a single analysis. Now note that terms in G that differ by nothing more than a $2 \leftrightarrow 3$ transposition also differ by a minus sign because G is anti-symmetric. It is these terms that constitute our comparison configuration $C_{\mathrm{comp}} = -f_{12}(g_{32}+g_{3k}f_{km}g_{m2}+\cdots)f_{34}$. The explicit anti-symmetry of the f, g factors allows us to rewrite this as $f_{12}(g_{23} + g_{2m} f_{mk} g_{k3} + \cdots) f_{34}$ and the sign change observed in the first few terms is common to all terms because the number of propagators in each product in the brackets is odd. The new configuration cannot yet be directly compared with the original because the fixed f_{ij} of equation (24) have changed. However, all the site labels are dummy variables of integration and so for purposes of *equivalence* we can relabel $k \leftrightarrow m$ and other labels as necessary to get $C_{\text{comp}} \equiv f_{12}(g_{23} + g_{2k} f_{km} g_{m3} + \cdots) f_{34}$ which is the original C_{start}.

The above example is to be contrasted with the case that transposition occurs between two disconnected structures. At least one of the structures must be a loop and we can take $C_{\text{start}} = (f_{12} g_{2j})(f_{34} g_{43} + f_{34} g_{4k} f_{km} g_{m3} + \cdots)$ where the second factor is the loop and whether the first factor $(f_{12} g_{2j})$ is part of a loop or line need not be specified. Again there will be a comparison configuration from terms in G that differ from the above by a $2 \leftrightarrow 3$ transposition. This configuration is $C_{\text{comp}} = -(f_{12} g_{3j})(f_{34} g_{42} + f_{34} g_{4k} f_{km} g_{m2} + \cdots)$ where the minus comes from the anti-symmetry of G as before. The key distinction with the previous case is that the number of propagators in each product term in the second bracket is even so that when we rewrite by explicit use of the f, g anti-symmetry we get $C_{\text{comp}} = -f_{12}(g_{24} f_{43} + g_{2m} f_{mk} g_{k4} f_{43} + \cdots) g_{3j}$ with terms conveniently rearranged to more clearly display the propagation sequence. The relabelling necessary to get the f_{ij} back to original form is $3 \leftrightarrow 4$, $k \leftrightarrow m, \ldots$ and with this relabelling one finds $C_{\text{comp}} = -f_{12}(g_{23} f_{34} + g_{2k} f_{km} g_{m3} f_{34} + \cdots) g_{4j}$. Besides the minus relative to C_{start} one should note the new structure is no longer disconnected and so involves a reduction of loop number by unity. Analysis of other cases shows the factor of $(-1)^{\text{loop number}}$ is general and equation (24) is verified.

4. High-temperature limits

The reduction of $G^{(2n+1)}$ in equation (7) that is useful for discussing both high-temperature series and the singularity structure of $\chi^{(2n+1)}$ starts with the observation that the anti-symmetric product satisfies a cumulant-like property, namely that any part of f_{ij} that depends on one of the variables ϕ_i independently of the other ϕ_j can be dropped. Specifically,

$$f_{ij} \equiv f_{ij} + \hat{f}_i - \hat{f}_j \qquad i < j \tag{25}$$

for any function $\hat{f}$. This result is obvious for $G^{(3)} = f_{12} - f_{13} + f_{23}$ and can be verified by induction in general. As an application, the f_{ij} of equation (4) is equivalent to

$$f_{ij} \equiv (\sin\phi_i - \sin\phi_j) x_i x_j / (1 - x_i x_j). \tag{26}$$

Since for small s, $x_i = s/2 + s^2/2 \cos\phi_i + \cdots$, the cumulant equivalent f_{ij} as written in (26) is $\mathrm{O}(s^2)$. However, a further subtraction of the leading $s^2/4(\sin\phi_i - \sin\phi_j)$ term reduces f_{ij} to $\mathrm{O}(s^3)$ and this is what appears in equation (11).

A surprising feature of the cumulant equivalent f_{ij} in (26) is that the last factor has the expansion

$$x_i x_j / (1 - x_i x_j) = \sum_{m=1}^{\infty} (s/2)^{m+1} B_m(s) (2^{m-1} (\cos^m \phi_i - \cos^m \phi_j) / (\cos\phi_i - \cos\phi_j)) \tag{27}$$

which was discovered with `Maple`† but can easily be proved by explicitly showing the cross derivative $\partial^2/\partial\phi_i \partial\phi_j (\cos\phi_i - \cos\phi_j) x_i x_j / (1 - x_i x_j)$ vanishes. The function $B_m(s)$, obtained by comparing series in the limit $\phi_i \to \phi_j$, is the hypergeometric function

$$B_m = F\left(\frac{m+1}{2}, \frac{m+2}{2}; 2; s^2/(1+s^2)^2\right) \Big/ (1+s^2)^{m+1}. \tag{28}$$

† `Maple V` software available from Waterloo Maple Software, 160 Columbia Street West, Waterloo, Ontario, Canada N2L 3L3.

The utility of the form (27) is that it enables us to derive a Laurent expansion for f_{ij} in $z_i = \exp(\mathrm{i}\phi_i)$ and $z_j = \exp(\mathrm{i}\phi_j)$, namely

$$
\begin{aligned}
f_{ij} &\equiv -\mathrm{i}\sum_{p=1}^{\infty}\sum_{q=1}^{\infty}(s/2)^{p+q+1}\left(z_i^p/z_j^q - z_j^p/z_i^q\right)A_{p+q} \qquad i < j \\
A_m &= {}_4F_3\left(\frac{m+1}{2},\frac{m+2}{2},\frac{m+2}{2},\frac{m+3}{2}; m+1, m+2, 2; 4s^2/(1+s^2)^2\right)\Big/(1+s^2)^{m+1}
\end{aligned}
\tag{29}
$$

and the fact that the coefficient of s^{2k} in the series expansion of A_m is a polynomial in m of degree $2k$ will be of importance below†. When the explicit f_{ij} from (29) is substituted into the $G^{(2n+1)}$ sum in (7), several simplifications can be made. First, the restriction $i < j$ on f_{ij} in (29), which is there to uniquely define the sign, can be dropped in the G sum since the correct sign is now obtained by the parity factor δ_{p}. Second, since the term $-z_j^p/z_i^q$ in the sum (29) will give the same contribution as z_i^p/z_j^q, it can be eliminated together with the 2^n in the normalization in (7). The result

$$
G^{(2n+1)} = (-\mathrm{i})^n \sum_{\{p,q\}}\sum_{\mathrm{p}}\delta_{\mathrm{p}} P\left(\frac{s}{2}\right)^{\sum p_i+\sum q_i+n}\left(\prod_{m=1}^{n} A_{p_m+q_m}(z_{2m-1})^{p_m}/(z_{2m})^{q_m}\right)\Big/ n! \tag{30}
$$

can be further reduced. Terms in the exponent set $\{p,q\}$ sum that maintain the pair sums $p_i + q_i$ but differ in ordering give the same contribution since a standard ordering can be achieved by even permutations involving only pairs z_{2i-1}, z_{2i}. Thus one can impose the ordering $p_1 < p_2 < \cdots < p_n$ and simultaneously drop the $n!$ in (30). The $n!$ terms that correspond to different q_i orderings involve products of different A_m amplitudes but these are the expansion of a determinant with the A_m as elements. The final result is

$$
G^{(2n+1)} = (-\mathrm{i})^n \sum_{\{p,q\}}^{\prime\prime}\left(\frac{s}{2}\right)^{\sum p_i+\sum q_i+n}\det|A\{p,q\}|\sum_{\mathrm{p}}\delta_{\mathrm{p}} P\left(\prod_{m=1}^{n}(z_{2m-1})^{p_m}/(z_{2m})^{q_m}\right) \tag{31}
$$

where the double prime on the $\{p,q\}$ set indicates the restriction to the ordering $p_1 < p_2 < \cdots < p_n$ and $q_1 < q_2 < \cdots < q_n$. Det$|A|$ is the determinant of an $n \times n$ matrix with the A_{ij} element equal to the A_m of equation (29) with $m = p_i + q_j$. Whether this result (31) for $G^{(2n+1)}$ is useful for numerical work in general is not clear but it does enable us to calculate easily the leading (few) terms in the series expansion of $\chi^{(2n+1)}$.

Because of the way the elements A_{ij} of the matrix are constructed from the A_m above, different rows and columns, if restricted to some finite order in s, may be linearly dependent and in general we can expect a considerable amount of cancellation in the evaluation of the determinant. The terms that will be the last to cancel in det $|A|$ will be those with the strongest dependence on position within the matrix and for a calculation of the leading s dependence it is sufficient to keep only the dominant m dependence in A_m; this, from equation (29) is

$$
A_m \approx \sum_{k=0}^{\infty}(ms/2)^{2k}/(k!(k+1)!) \tag{32}
$$

and leads to

$$
\det|A\{p,q\}| = (s/2)^{n(n-1)}\left(\prod_{1\leqslant i<j\leqslant n}(p_j-p_i)(q_i-q_j)/(j-i)^2\right)(1+\mathrm{O}(s)). \tag{33}
$$

The conclusion from (33) is that for fixed n all determinants are of the same order in s and differ only in the numerical prefactor. To obtain the minimum power of s in $G^{(2n+1)}$ in (31) we

† Note that (29) is only equivalent to (26) with the substitution of (27), (28). Terms with $p = 0$ or $q = 0$ have been dropped in (29).

then simply need to set all adjacent $p_{i+1} - p_i = 1$ and similarly for the q_i. With this choice $(-\mathrm{i}\cdot s/2)^{n(n-1)}(1+\mathrm{O}(s))$ becomes the minimal determinant in (33). The corresponding minimal $G^{(2n+1)}$ is

$$G^{(2n+1)}(\min) = (-\mathrm{i})^{n^2}\left(\frac{s}{2}\right)^{n(2n+1)} \sum_{\mathrm{p}} \delta_{\mathrm{p}} P\left(\prod_{m=1}^{n} (z_{2m-1}/z_{2m})^m\right)(1 + \mathrm{O}(s)) \tag{34}$$

and the minimal $\chi^{(2n+1)}$ from equations (3), (6) is the simplified integral

$$\chi^{(2n+1)}(\min) = s^{2n}\left(\prod_{m=1}^{2n}\int \frac{\mathrm{d}\phi_m}{2\pi}\right)(G^{(2n+1)}(\min))^2/(2n+1)!(1+\mathrm{O}(s)). \tag{35}$$

We now make the trivial observation that $\int \mathrm{d}\phi_i z_i^p = 2\pi\delta_{\mathrm{p}0}$ so that to get a nonvanishing result in a product of two $G^{(2n+1)}(\min)$, every term in the second must be paired with that specific term in the first that is obtained by the inversion of all z_{2m-1}/z_{2m} ratios†. But this is just a permutation of all pairs $2m-1 \leftrightarrow 2m$ which has parity $(-1)^n$ and cancels the $(-1)^{n^2}$ from (34). All $(2n+1)!$ terms in one $G^{(2n+1)}(\min)$ will pair and give the identical contribution; the final result is that given in equation (8).

5. Singularities

From the definition of $x_m(s)$ in equations (4) one can show $|s| < 1$ implies $|x_m| < 1$ if the phase ϕ_m is real. This in turn implies that $\chi^{(2n+1)}$ as given by (3) is analytic for $|s| < 1$. Even on the boundary $|s| = 1$, $\chi^{(2n+1)}$ will not be singular wherever it is possible to deform the integration contours into the complex plane to avoid the integrand points where denominator factors such as $1 - \prod_{m=1}^{2n+1} x_m$ vanish for real ϕ_m. Such deformation is not possible at the stationary points of the integrand and of these the symmetry points $\phi_m = \phi^{(k)}$ and $x_m = \exp(\mathrm{i}\phi^{(\ell)})$ for all $m = 1, 2, \ldots, 2n+1$ are obvious candidates. Here $\phi^{(k)}, \phi^{(\ell)}$ and the associated singular points $s = s_{k\ell}$ are as given in equations (12). Note that $\cos(\theta_{k\ell})$ is invariant under the interchange $|k| \leftrightarrow |\ell|$ which is related to the horizontal $\leftrightarrow$ vertical bond symmetry of the original Ising lattice. This is because the x_m variable is the memory of the phase variable that was integrated out in deriving equation (3) from the integral $\chi^{(2n+1)}$ in W and (12) simply recovers the explicit symmetry lost in intermediate steps‡.

In connection with the breakdown of explicit symmetry in intermediate steps one should also note that in equations (4), (19), if $s = |s|\exp(\mathrm{i}\theta)$ with $|s| < 1$ and $0 < \theta < \pi$ then the variable x satisfies $\mathrm{Im}(x) > 0$. This in turn implies $0 < \theta_{k\ell} < \pi$ if $0 < \ell \leqslant n$ and $-\pi < \theta_{k\ell} < 0$ if $-n \leqslant \ell < 0$. However, the equation (19) identification $\exp(-\mathrm{i}\psi) \to x$ is based on an earlier arbitrary restriction $N \geqslant 0$ and $\mathrm{Im}(\psi) < 0$. Choosing $N \leqslant 0$ and $\mathrm{Im}(\psi) > 0$ would leave equation (3) unchanged but yield $\exp(\mathrm{i}\psi) \to x$; thus the sign of $\theta_{k\ell}$ depends on the prescription adopted. The only definitive conclusion is that for any specific choice there will be an equal number of positive and negative $\theta_{k\ell}$ in total as one scans through $\pm k$, $\pm\ell$ and this is the basis for the remarks following equations (12)–(14).

One can determine the singular part of $\chi^{(2n+1)}$ in the vicinity of the points $s_{k\ell}$, $0 < \ell \leqslant n$ as follows§. First, write

$$s = s_{k\ell}(1-\epsilon) = \exp(\mathrm{i}\theta_{k\ell})(1-\epsilon) \tag{36}$$

† This is not true in general. The phase constraint $\prod_{m=1}^{2n+1} z_m = 1$ allows for the possibility of extra z_m appearing so that the z_i from the two $G^{(2n+1)}$ factors alone need not cancel. This constraint will be crucial for getting correctly the first odd order contribution to $\chi^{(2n+1)}$ but is irrelevant here.

‡ For the invariance of $\chi^{(2n+1)}$ under ϕ, ψ interchange see the remarks following (W.4.87) ([1]).

§ The singular points $s = \pm 1, \pm\mathrm{i}$ require a different treatment and will not be discussed (the ferromagnetic point $s = 1$ has of course been analysed in great detail in W). The contributions for $-n \leqslant \ell < 0$ follow by complex conjugation since χ is a real function. The case $\ell = 0$ can be avoided by using the $|k| \leftrightarrow |\ell|$ symmetry.

with $0 < \theta_{k\ell} < \pi$ as discussed above and for now take ϵ as infinitesimal real and positive. Then x_m is unambiguously in the upper half complex plane and to first order is

$$\begin{aligned} x_m &\simeq \exp(\mathrm{i}\phi^{(\ell)} - (2\epsilon\sin(\theta_{k\ell}) + \mathrm{i}\delta_m\sin(\phi^{(k)}) + \mathrm{i}\delta_m^2 A_{k\ell})/\sin(\phi^{(\ell)})) \\ A_{k\ell} &= (\cos(\phi^{(k)}) + \sin^2(\phi^{(k)})\cos(\phi^{(\ell)})/\sin^2(\phi^{(\ell)})/2 \end{aligned} \tag{37}$$

where the deviation $\delta_m = \phi_m - \phi^{(k)}$ is appropriately considered $\mathrm{O}(\sqrt{\epsilon})$ for power counting purposes. Because of the constraint $\sum\delta_m = 0$, the product $\prod_{m=1}^{2n+1} x_m$ simplifies and results in the divergent factor in the integrand for $\chi^{(2n+1)}$ becoming the single variable Lorentzian

$$1\bigg/\left(1 - \prod_{m=1}^{2n+1} x_m\right) \simeq \sin(\phi^{(\ell)})/(2\epsilon(2n+1)\sin(\theta_{k\ell}) + \mathrm{i}\delta^2 A_{k\ell}) \tag{38}$$

with $\delta^2 = \sum_{m=1}^{2n+1}\delta_m^2$ defined as the 'radial' deviation from the singularity. The only other important variation in the integrand in equation (3) is in the H factor because it vanishes at the symmetry point. Indeed, from equations (6), (7) one can conclude that to leading order one can set $\epsilon = 0$ and

$$H^{(2n+1)}\{f_{ij}\} \simeq (-1)^n B_{k\ell}^{(2n+1)} \prod_{1\leqslant i<j\leqslant 2n+1} (\delta_i - \delta_j)^2 \tag{39}$$

where $B_{k\ell}^{(2n+1)}$ is a constant I will determine below. One can elsewhere also set δ to zero; for example, $sy_m \simeq \mathrm{i}/\sin(\phi^{(\ell)})$. The leading singular contribution to the susceptibility near the point $s_{k\ell}$ is now given by the simpler

$$\begin{aligned} \chi_{k\ell}^{(2n+1)}/(1 - s_{k\ell}^4)^{1/4} &\simeq (2\mathrm{i}/s_{k\ell}) B_{k\ell}^{(2n+1)} \sin^{-2n}(\phi^{(\ell)}) \\ &\times\left(\prod_{m=1}^{2n}\int\frac{\mathrm{d}\delta_m}{2\pi}\right)\left(\prod_{i<j}^{2n+1}(\delta_i - \delta_j)^2\right)\bigg/(2\epsilon(2n+1)\sin(\theta_{k\ell}) + \mathrm{i}\delta^2 A_{k\ell}) \end{aligned} \tag{40}$$

and the integral in (40) can be reduced by using the result† that for any function of the radial coordinate only, $f(\delta^2)$,

$$\begin{aligned} &\left(\prod_{m=1}^{2n}\int\frac{\mathrm{d}\delta_m}{2\pi}\right)\left(\prod_{i<j}^{2n+1}(\delta_i - \delta_j)^2\right) f(\delta^2) = K_{2n+1}\int_{\delta>0}\mathrm{d}\delta\,\delta^{4n(n+1)-1} f(\delta^2) \\ &K_{2n+1} = 4/(\pi^n\Gamma(2n(n+1))\sqrt{(2n+1)}) \prod_{m=1}^{2n+1}(m!/2^m). \end{aligned} \tag{41}$$

The integral (40) combined with (41) is of course highly divergent at large δ but this is not singular as $\epsilon \to 0$. For the correct singular part one need only keep the nonpolynomial (in ϵ) part of the partial fraction reduction of the ratio $\delta^{4n(n+1)-1}/(2\epsilon(2n+1)\sin(\theta_{k\ell}) + \mathrm{i}\delta^2 A_{k\ell})$ which is $\delta/(2\epsilon(2n+1)\sin(\theta_{k\ell}) + \mathrm{i}\delta^2 A_{k\ell})$ multiplied by the factor $(2\mathrm{i}\epsilon(2n+1)\sin(\theta_{k\ell})/A_{k\ell})^{2n(n+1)-1}$. The result of the remaining elementary integral for the singular contribution is then

$$\begin{aligned} \chi_{k\ell}^{(2n+1)}/(1 - s_{k\ell}^4)^{1/4} &\simeq (\mathrm{i}/s_{k\ell}) K_{2n+1} B_{k\ell}^{(2n+1)} \sin^{-2n}(\phi^{(\ell)}) \\ &\times (2\epsilon(2n+1)\sin(\theta_{k\ell})/A_{k\ell})^{2n(n+1)-1}\ln(\epsilon)/A_{k\ell}. \end{aligned} \tag{42}$$

† The functional form follows by power counting; the constant K_{2n+1} can then be determined by choosing $f(\delta^2) = \exp(-\delta^2)$. However, the following tricks still appear to be essential. First, one can make the implicit constraint explicit by supplying the redundant factor $\int \mathrm{d}\delta_{2n+1}\delta(\sum\delta_m)$; second, one can show that a $(2n+1)$-dimensional integral without $\delta(\sum\delta_m)$ in the integrand is larger than one with $\delta(\sum\delta_m)$ by the factor $\sqrt{(\pi(2n+1))}$. This is done by transforming to Jacobi coordinates and performing the 'centre of mass' integrals explicitly while leaving the relative coordinate integrals unevaluated. The final step (this is apparently a very old problem. See [17] for the solution in the context of random matrices: the authors give references dating to 1883.) involves recognizing that the unconstrained $(2n+1)$-dimensional integral is an integral over the square of a Vandermonde determinant which can be converted to a Slater determinant in an orthogonal Hermite polynomial basis. The integral is then a textbook exercise in wavefunction normalization in quantum mechanics.

This completes the proof of the order of the singularity as $\epsilon^{2n(n+1)-1}\ln(\epsilon)$ and I turn now to the explicit evaluation of the constant $B^{(2n+1)}_{k\ell}$.

As an intermediate step to determining $B^{(2n+1)}_{k\ell}$ it is necessary to determine the expansion of f_{ij} given in equations (4). One can define, in addition to the above $\delta_m = \delta_m^{(k)} = \phi_m - \phi^{(k)}$, the deviation $\delta_m^{(\ell)}$ where $x_m = \exp(\mathrm{i}\phi^{(\ell)} + \mathrm{i}\delta_m^{(\ell)})$. Since $\epsilon = 0$, these deviations are symmetrically related by the constraint $\cos(\phi^{(k)} + \delta_m^{(k)}) + \cos(\phi^{(\ell)} + \delta_m^{(\ell)}) = \cos(\phi^{(k)}) + \cos(\phi^{(\ell)}) = 2\cos(\theta_{k\ell})$ and one finds that $f_{ij} = (\mathrm{i}/2)(\sin(\phi^{(k)} + \delta_i^{(k)}) - \sin(\phi^{(k)} + \delta_j^{(k)}))\cot(\phi^{(\ell)} + (\delta_i^{(\ell)} + \delta_j^{(\ell)})/2)$. A direct expansion of f_{ij} in the δ is possible but it is hard to see in this case how the very simple final result for $B^{(2n+1)}_{k\ell}$ obtains. A simpler algebraic expansion can be obtained by using as variables $t = \tan(\delta/2)$ in which case the constraint and the cumulant equivalent† f_{ij} become

$$\begin{aligned}
&t^{(k)}\sigma^{(k)}/(1+t^{(k)2}) + t^{(\ell)}\sigma^{(\ell)}/(1+t^{(\ell)2}) = 0 \qquad \sigma = \sin(\phi) + t\cdot\cos(\phi)\\
&f_{ij} \equiv \mathrm{i}\cdot\sin(\phi^{(\ell)})(t_j^{(k)} - t_i^{(k)})t_i^{(\ell)}t_j^{(\ell)}/(\sigma_i^{(k)}\sigma_j^{(k)}(\sigma_i^{(\ell)}\sigma_j^{(\ell)} - t_i^{(\ell)}t_j^{(\ell)})).
\end{aligned} \tag{43}$$

It is not apparent in (43) but can be shown by somewhat involved trigonometric manipulation that f_{ij} is anti-symmetric in k, ℓ, i.e. $f_{ij}(k,\ell) = -f_{ij}(\ell,k)$. Expansion in either $t^{(k)}$ or $t^{(\ell)}$ breaks this symmetry and it is better to use as expansion variable τ where

$$\tau^2 = -t^{(k)}t^{(\ell)}/(\sigma^{(k)}\sigma^{(\ell)}) \tag{44}$$

and where the sign of τ is made definite by $2\tau \simeq \delta^{(k)}/\sin(\phi^{(\ell)}) \simeq -\delta^{(\ell)}/\sin(\phi^{(k)})$ for small δ. Other symmetric variables are obviously possible but this particular choice has been motivated by the form of f_{ij} in equation (43). Specifically, with the definition (44), $f_{ij} \equiv \mathrm{i}(\tau_j - \tau_i)\tau_i\tau_j$ + terms $\propto \tau_i^p\tau_j^q$ with $p, q \geqslant 2$, which is to say that all linear terms $\tau_i\tau_j^q$ and $\tau_j\tau_i^p$ are eliminated for $p, q > 2$. What this argument does not predict is the remarkably simple general expansion

$$\begin{aligned}
f_{ij} &\equiv \mathrm{i}\tau_i\tau_j/(1-\tau_i\tau_j)\Bigg\{(\tau_j - \tau_i) + \tau_i\tau_j/(1+\tau_i\tau_j)\\
&\qquad\times\sum_{n=0}^{\infty}(\tau_j^{2n+1} - \tau_i^{2n+1})(P_{n+1}(-\cos(2\theta_{k\ell})) - P_{n-1}(-\cos(2\theta_{k\ell})))/(2n+1)\Bigg\}\\
&= \mathrm{i}\sum_{p=1}^{\infty}\sum_{q=1}^{\infty} b_{k\ell}^{(p,q)}\tau_i^p\tau_j^q
\end{aligned} \tag{45}$$

where the P_n are Legendre polynomials with the convention $P_{-1} = P_0 = 1$ and the last line defines the coefficient array $b_{k\ell}^{(p,q)}$ to be used in the discussion below. Just as in the case of the expansion (27), equation (45) was discovered with `Maple` and can be proved along similar lines. Multiplying both equations (43) and (45) for f_{ij} by $1 - 1/(\tau_i^2\tau_j^2)$ results in difference functions $f_i - f_j$ and thus equation (45) is proved if the single variable identity‡

$$\begin{aligned}
&\sum_{n=0}^{\infty}\tau^{2n+1}(P_{n+1}(-\cos(2\theta_{k\ell})) - P_{n-1}(-\cos(2\theta_{k\ell})))/(2n+1)\\
&\qquad\stackrel{?}{=} 1/\tau - \tau + \sin(\phi^{(k)})/t^{(\ell)} - (\sin(\phi^{(\ell)})/\sin(\phi^{(k)}))(\cos(\phi^{(k)}) - t^{(k)}/\sigma^{(k)})
\end{aligned} \tag{46}$$

is true. Now the constraint equations in (43) combined with the definition (44) lead to a quadratic equation for $t^{(k)}/\sigma^{(k)} = -\tau^2\sigma^{(\ell)}/t^{(\ell)}$ whose solution substituted into the right-hand side (RHS) of (46) gives

$$\mathrm{RHS}(46) = -\tau + (1/\tau)(1 - \sqrt{(1 + 2\tau^2\cos(2\theta_{k\ell}) + \tau^4)}). \tag{47}$$

† As discussed in section 3 (cf equation (25)), terms of the form $f(t_i)$ or $f(t_j)$ will not contribute to f_{ij} and can be dropped.

‡ The equality of the differences only defines the functions to within an additive constant. An explicit low-order calculation has been used to determine the constant which is included in equation (46).

Hence the result (45) is proved.

To complete the discussion of the derivation of $B^{(2n+1)}_{k\ell}$ I note that although $G^{(2n+1)}$ in equation (7) is given as a sum of products of f_{ij}, it is also an anti-symmetric function and in the neighbourhood of the symmetry point where all $\tau_i = 0$, its lowest order nonvanishing term must be proportional to the product $\prod_{i<j}(\tau_i - \tau_j)$. For the coefficient of proportionality it is only necessary to compare, for example, the specific term $\tau_1^{2n}\tau_2^{2n-1}\cdots\tau_{2n-1}^2\tau_{2n}$ with the result

$$G^{(2n+1)} \simeq \mathrm{i}^n \left\{ \sum_{\mathrm{P}} \delta_{\mathrm{P}} P \left(\prod_{m=1}^{n} b^{(2m,2m-1)}_{k\ell} \right) \Big/ (2^n n!) \right\} \left(\prod_{i<j}^{2n+1} (\tau_i - \tau_j) \right) \tag{48}$$

where P is the permutation operator on the indices $1 \leqslant p, q \leqslant 2n$ so that the { } expression in equation (48) is a Pfaffian [16]. Finally, from $H^{(2n+1)} = (G^{(2n+1)})^2/(2n+1)!$ in equation (6) one obtains

$$\begin{aligned}(-1)^n H^{(2n+1)}_{k\ell}(2n+1)! &\simeq \left\{ \sum_{\mathrm{P}} \delta_{\mathrm{P}} P \left(\prod_{m=1}^{n} b^{(2m,2m-1)}_{k\ell} \right) \Big/ (2^n n!) \right\}^2 \prod_{i<j}^{2n+1} (\tau_i - \tau_j)^2 \\ &\simeq \det |b^{(i,j)}_{k\ell}| \prod_{i<j}^{2n+1} (\tau_i - \tau_j)^2 \end{aligned} \tag{49}$$

with the last line based on the general connection between Pfaffians and determinants [16] and where it is to be understood that $b^{(i,j)}_{k\ell}$ is restricted to a truncated $2n \times 2n$ array. From the specific form of the expansion of f_{ij} in equation (45) it follows $\det |b^{(i,j)}_{k\ell}| = 1$ for all n.

Finally, because we are working to leading order only, we can replace $2\tau \to \delta^{(k)}/\sin(\phi^{(\ell)})$ in equation (49) and make the identification for the required constant in (39) as

$$B^{(2n+1)}_{k\ell}(2n+1)! = 1/(2\sin(\phi^{(\ell)}))^{2n(2n+1)}. \tag{50}$$

The combined result of all the calculations above is the general formula quoted in the introduction equation (14) which has the expected invariance under $|k| \leftrightarrow |\ell|$ interchange. Additional evidence for the correctness of this result rests with the numerical series analysis presented in appendix B.

Acknowledgments

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Appendix A. Numerical generation of series

A key observation from the explicit formulae (4) for $x(\phi)$ and $y(\phi)$ and (11) for f_{ij} is that in a high-temperature expansion of the integrand for $\chi^{(2n+1)}$ in equation (3), no Fourier component more rapidly varying than $\sin((N-4n)\phi)$ can occur at order s^N. This means that if the expansion in powers of s is generated as a numerical series, the exact coefficient of s^N can be recovered by a numerical integration over ϕ using at most $N-4n$ uniformly spaced points on the interval $-\pi \leqslant \phi \leqslant \pi$. In fact this is a substantial overestimate. I find empirically that integration on $N-2(n+1)(2n-1)$ uniformly spaced points will give exact results to order s^N (with N even).

The high-temperature expansion is completely straightforward. Expand $x(\phi)$ and $y(\phi)$ and store as series in s at the points $\phi^{(k)} = \pi k/M$, $k = -M, -M+1, \ldots, M$, where

$M = N/2 - (n+1)(2n-1)$. Since $\chi^{(2n+1)}$ is order s^{8n} if one uses the equivalent f_{ij} from equation (11), each series can be restricted to a length of $N + 1 - 8n$ terms. Standard routines for series multiplication and division can be used to generate and accumulate the integrand in (3) as numerical series.

A crude operation count for the total procedure is $(N - 8n)^2/2$ scalar multiplies for each series multiplication/division. The number of integration points is $(N - 2(n+1)(2n-1))^{2n}$ if one invokes no symmetries. However, there is the obvious inversion symmetry that all $\phi \to -\phi$ leaves the integrand in (3) invariant. The complete permutation symmetry is probably not useful as the potential $(2n)!$ gain comes at the expense of having to evaluate all distinct $(2n+1)!!$ products in $G^{(2n+1)}$ in equation (7). The better route seems to be to use symmetrized versions of equations (9), (10). These are, for the two lowest nontrivial orders

$$H^{(3)} \equiv \tfrac{1}{2} f_{12}(f_{23} - f_{13} + f_{12}) \qquad H^{(5)} \equiv \tfrac{1}{4} f_{12}(f_{23}f_{14} - f_{13}f_{24} + f_{12}f_{34})(f_{45} - f_{35} + \tfrac{1}{2} f_{34}) \tag{51}$$

and in general each central two-term factor in (10) is replaced by the three-term $\frac{1}{2}(f_{2m,2m+1}f_{2m-1,2m+2} - f_{2m-1,2m+1}f_{2m,2m+2} + f_{2m-1,2m}f_{2m+1,2m+2}/m)$. The use of inversion plus this pairwise symmetry reduces the number of integration points by 2^{n+1} and requires only a marginal increase in the number of series operations. I find about 20 series multiplication/divisions are required in the innermost loop of the integration routine. Thus a rough timing estimate is

$$T \simeq 20\tau((N - 8n)^2/2)((N - 2(n+1)(2n-1))^{2n}/2^{n+1}) \tag{52}$$

with τ the time for a scalar multiply. Improvements can be made by the usual trade-off of data storage in place of repeated function evaluation.

A remaining issue is that of round-off error. The advantage of using s as expansion variable is that the radius of convergence of the series is unity and so all numerical coefficients are sensibly normalized. I find that no serious round-off errors develop and the accuracy of the final series is only one or two digits less than the computer word size. The only place one does have to be careful is in the generation of the initial series for $x(\phi)$ and $y(\phi)$. From equation (4) for y it follows that

$$\begin{aligned} \mathrm{d}y/\mathrm{d}s(1 - 2s\cdot\cos\phi + s^2(\cos^2\phi + 1) - 2s^3\cdot\cos\phi + s^4) \\ = y(\cos\phi - s(\cos^2\phi + 1) + 3s^2\cdot\cos\phi - 2s^3) \end{aligned} \tag{53}$$

and on substituting $y = \sum s^n g_n$ into (53) one can obtain the recursion relation

$$(n+1)g_{n+1} = (2n+1)\cos\phi\cdot g_n - n(\cos^2\phi + 1)g_{n-1} + (2n-1)\cos\phi\cdot g_{n-2} - (n-1)g_{n-3} \tag{54}$$

which is stable for forward recursion. Appropriate for $x(\phi)$ is

$$x = sy/(1 + (1 + s^2 - s\cdot\cos\phi)y) \tag{55}$$

which follows directly from (4) and eliminates the need for a second recursion formula.

The series in s for $\chi^{(2n+1)}$ are summarized below. The reader can convert to other representations as desired; I have converted to $v = \tanh(K)$ the few terms in the published series [3, 15] that need to be corrected by the addition of $\chi^{(7)}$. These are, for the total χ, $36912183772984768028v^{48}$, $22164947092555461057 2v^{50}$, $13294400774247125168 84v^{52}$ and $79654880659404636792 68v^{54}$.

$$\chi^{(1)} = (1 - s^4)^{1/4}/(1 - s)^2$$

$$\begin{aligned} \chi^{(3)} = 4(s/2)^8[&1, 0, 0, 4, 16, 4, 20, 84, 247, 188, 536, 1524, 4140, 4584, 11164, 27884, \\ &70128, 93456, 217124, 500996, 1190728, 1788648, 4019068, 8857404, \end{aligned}$$

20337695, 32855320, 72136120, 155198996, 347003020, 588148504, 1272754780, 2692201900, 5902536420, 10366753636, 22160925180, 46307647436, 100154617112, 180464969656, 382047574868, 791824710548, 1693712632332, 3110849108804, 6539936949172, 13467369401316, 28548267779720, 53233613340744, 111268207398460, 227997121825148, 479923398673972, 905331036961540, 1883299812962700, 3845474171869468, 8046864612290488, 15318087259999576, 31744377825521284, 64634781151767236, 134589216372542043, 258119734021734396, 533133709272235624, 1083018464018398996, 2246234877571466748, 4333906525071598248, 8925651535203772188, 18099334772981593516, 37410856536526302308, 72539370174918149828, 149036477928584673980, 301753056841850788236, 621874438456997865688, 1210879527614829677816, 2482595317106536689172, 5020039987360235170644, 10319715684451678215008, 20164132636961510005880, 41265182381709135449804, 83356862902542086879468, 170978340515589313718120] + O(s^{85})

where every nth term in [ ] is understood to be multiplied by $(s/2)^{n-1}$. In the same notation,

$\chi^{(5)} = 16(s/2)^{24}$[1, 0, 0, 0, 48, 4, 0, 4, 1463, 228, 28, 248, 36304, 7972, 1864, 9468, 801661, 221532, 74112, 286404, 16438116, 5382792, 2295212, 7530952, 320482495, 119856148, 61188256, 180246140, 6026865364, 2511621784, 1476355096, 4032689592, 110347180596, 50356068440, 33187060312, 85779335560, 1979543921484, 976496522740, 707837755996, 1754683199016, 34949776971561, 18452824614036, 14501021397972, 34798435456904, 609270636967496, 341626213259368, 287796156305644, 673040682652176, 10512702107247313, 6220763534246424, 5567911455434816, 12752092161432520, 179869321769052280, 111744680073378996, 105495627686468404, 237503860512867456, 3056036718790296147, 1984676379219429672, 1964487397269198000, 4359903276200726968, 51618661720552233864] + O(s^{85})

$\chi^{(7)} = 64(s/2)^{48}$[1, 0, 0, 0, 96, 0, 0, 4, 5231, 4, 0, 436, 213136, 456, 36, 26588, 7232113, 28952, 4408, 1198004, 216135776, 1353328, 298448, 44506752, 5882815986, 52005072, 14783296, 1444017180, 149044674900, 1741004728, 598685156, 42361975404, 3568323690294, 52589908552, 21020411728, 1149599078568, 81610343951508] + O(s^{85})

$\chi^{(9)} = 256(s/2)^{80}$[1, 0, 0, 0, 160] + O($s^{88}$).

As a check of transcription errors, note the sum of all coefficients in each [ ] grouping is 336016104447651492568810 for $\chi^{(3)}$, 63655452600073075449 for $\chi^{(5)}$, 86603288006141 for $\chi^{(7)}$ and 161 for $\chi^{(9)}$.

Appendix B. Series analysis

The contributions to the series coefficients in $\chi^{(2n+1)}/(1-s^4)^{1/4} = \sum K_N^{(2n+1)} s^N$ from singularities on the unit circle $|s|=1$ exclusive of $s=\pm 1, \pm\mathrm{i}$ are given in (15) as $\Delta K_N^{(3)}$ for $n=1$. The corresponding reduction of equations (12), (14) for $n=2$ gives

$$\begin{aligned}
&\Delta K_N^{(5)} = N^{-12}(18\sqrt{5}/\pi^2)(\tfrac{5}{2})^{10}\sum_{m=1}^{5} a_m \sin((N+1)\theta_m)/\sin(\theta_m) \\
&\{a_m,\theta_m\} = (4-4/\sqrt{5})^6, 4\pi/5;\ 2(\tfrac{24}{5})^6, \arccos(-\tfrac{1}{4}); \\
&\qquad (9+17/\sqrt{5})^6, \arccos((3-\sqrt{5})/8);\ (4+4/\sqrt{5})^6, 2\pi/5; \\
&\qquad (9-17/\sqrt{5})^6, \arccos((3+\sqrt{5})/8)
\end{aligned} \tag{56}$$

and the latter series contribution is particularly small relative to, say, the $s=1$ ferromagnetic contribution which is $\mathrm{O}(N)$†. The challenge of a series analysis method to verify these contributions is to eliminate to high precision the uninteresting but dominant terms. I use below a technique that works well when the location of the singularities is known as is the case here; the method can be viewed either as a variant of Neville–Aitken extrapolation, series smoothing, or simply numerical differentiation.

A trivial observation that is the basis of many series analysis methods is that if a series coefficient of s^N varies as, say, $f_N \propto 1/N^p$, then this contribution can be eliminated by the differentiation $\mathrm{d}g_N/\mathrm{d}N \simeq g_{N+1}-g_N$, $g_N = N^p f_N$. If $g_N \propto (-1)^N$ one would use instead $g_{N+1}+g_N$—an example of series smoothing. In either case the process is equivalent to multiplying the series $\sum g_N s^N$ by $s-\bar{s}$ where $\bar{s}$ is the location of the singularity. Thus in the case of a complex pair at $\bar{s}_\pm = \exp(\pm\mathrm{i}\theta)$ one can multiply by $(s-\bar{s}_+)(s-\bar{s}_-)/s$ or form the combination $D_\theta g_N = g_{N+1} - 2\cos(\theta) g_N + g_{N-1}$. It is this process I use below to eliminate known terms and enhance, relatively, any possible residual singularity contributions.

The dominant contributions to the series coefficients $K_N^{(3)}$ after subtraction of the ferromagnetic term ${}^F\Delta K_N^{(3)}$ appear to be $\propto (\pm 1)^N \ln(N)/N$ and $(\pm\mathrm{i})^N/N$ which, together with some subdominant terms, are eliminated by the transformations

$$ {}_0g_N = (D_c^2 N^2)^2 (K_N^{(3)} - {}^F\Delta K_N^{(3)}) \qquad D_c g_N = g_{N+2} - g_{N-2} \tag{57}$$

where the composite derivative operator D_c corresponds to fourfold differentiation or, equivalently, series multiplication by $(s-1)(s+1)(s-\mathrm{i})(s+\mathrm{i})/s^2$. Oscillations in ${}_0g_N$ of period three and constant amplitude at large N corresponding to $\bar{s}_\pm = \exp(\pm\mathrm{i}2\pi/3)$ from the first term of equation (15) are clearly apparent and when these are reduced by forming $D_{2\pi/3}\, {}_0g_N = {}_0g_{N+1} + {}_0g_N + {}_0g_{N-1}$ the oscillations from the second term $\bar{s}_\pm = \frac{1}{4} \pm \mathrm{i}\sqrt{\frac{15}{4}}$ are unambiguous‡. Having thus established the existence of the predicted complex s singularities I now modify the above procedure to suppress these also so as to improve the chance of finding

† W have shown the ferromagnetic singularity is a double pole, i.e. $\chi/(1-s^4)^{1/4} \propto 1/(1-s)^2$, with corrections $\mathrm{o}(1)$. This means the leading *two* ferromagnetic contributions to the series coefficients are given by ${}^F\Delta K_N^{(3)} \simeq 0.8144625656625044393912171285627 22 \times 10^{-3}(N+1)$ and ${}^F\Delta K_N^{(5)} \simeq 0.797091208314753855633583588577 \times 10^{-6}(N+1)$. The constants above are numerically improved versions of (W.7.13–W.7.14) and combined with higher-order terms must satisfy the sum rule $1 + 0.814\ldots \times 10^{-3} + 0.797\ldots \times 10^{-6} + \cdots = 2^{3/8}\ln(1+\sqrt{2})^{7/4} C_{0+} = 1.000815260440212647119476363047210236937 5$. Also $2^{3/8}\ln(1+\sqrt{2})^{7/4} C_{0-} = 1.000960328725262189480934955172097320572 5/12\pi$. These accurate values for the susceptibility amplitudes $C_{0\pm}$ have been obtained by integrating the Painlevé equation (W.2.36) by predictor/corrector methods of high orders $P \leqslant 15$. I find that if the variable θ in (W.2.36) is first replaced by $x = \ln(\mathrm{e}^\theta - 1)$, a uniform stepsize h is appropriate in the numerical work and yields $C_{0\pm}$ accurate to $\approx (2h)^P$.

‡ Although the amplitudes of the two terms in equation (15) are comparable, the 'multiplication' by $(s^4-1)^4/s^8$ to generate ${}_0g_N$ reduces the amplitude of the second relative to the first by the factor $\frac{25}{256}$ to leading order in N.

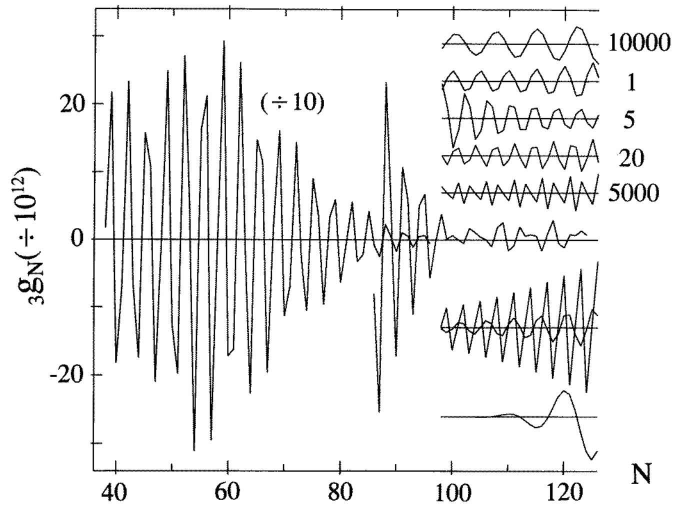

Figure B1. Series amplitude $_3g_N/10^{13}$ (left) and $_3g_N/10^{12}$ (right) versus order N from equations (58). The curves on the upper right, shifted vertically for clarity, are the extra contributions to $_3g_N/10^{12}$ that would result if $K_N^{(3)}$ contained the $\Delta K_N^{(5)}$ terms in equation (56) but scaled *down* as indicated. The curves on the lower right are the changes in $_3g_N/10^{12}$ that would result from modifications of existing contributions: for the lowest curve increasing $K_{125}^{(3)}$ by one part in 10^{22}; for the two overlapping curves decreasing the amplitudes in $\Delta K_N^{(3)}$ in equation (15) by one part in 10^6.

yet other $|s| = 1$ singularities. Specifically I subtract out the $\Delta K_N^{(3)}$ contribution from (15) and define the transformations

$$\begin{aligned} {}_1g_N &= N^5 D^5_{\arccos(1/4)} D^5_{2\pi/3} D_c^4 N^4 D_c^5 N^5 (K_N^{(3)} - {}^F\Delta K_N^{(3)} - \Delta K_N^{(3)}) \\ {}_3g_N &= D_{2\pi/3}\, {}_2g_N \qquad {}_2g_N = N({}_1g_{N+1} - {}_1g_{N-1}). \end{aligned} \tag{58}$$

The choice of operations in (58) is such that if all series coefficients $K_N^{(3)} - {}^F\Delta K_N^{(3)} - \Delta K_N^{(3)}$ are of the form $(\pm 1)^N \ln(N)/N^p$, $(\pm \mathrm{i})^N/N^p$, $p \geqslant 1$ and $\exp(\pm \mathrm{i}\theta)/N^p$, $p \geqslant 5$ then ${}_3g_N = \mathrm{O}(1)$ as $N \to \infty$. This assumption may not be strictly correct (e.g. there could be extra $\ln(N)$ factors in the series coefficients) but that does not affect the qualitative argument that, because the cumulative N product in (58) reaches to a final N^{15}, ${}_3g_N$ is very sensitive to small contributions in the initial $K_N^{(3)}$. Significant changes are observed in ${}_3g_N$ for $N \gtrsim 100$ for changes in the amplitudes in $\Delta K_N^{(3)}$ in equation (15) as small as one part in 10^6; this confirms precisely equation (14) for the leading singular behaviour of $\chi_{k\ell}^{(3)}$.

A comparison of ${}_3g_N$ with contributions of the form of those in equation (56) for $\Delta K_N^{(5)}$ with variously scaled amplitudes is shown in figure B1. There is no evidence that $\chi^{(3)}$ contains any of the complex s, $|s| = 1$, singularities in $\chi^{(5)}$ from equation (56). Even if these singularities were present in $\chi^{(3)}$, four of the five pairs could not possibly have sufficiently large amplitude to cancel those in $\chi^{(5)}$. The argument for the pair at $|\theta| = 2\pi/5$ is not as convincing because this angle is too close to the singularity angle $|\theta| = \arccos(\frac{1}{4}) \simeq 75.5^\circ$ in $\chi^{(3)}$. Finally, to complete the cancellation argument I have checked that $\chi^{(5)}$ does not have singularities that might cancel those in $\chi^{(3)}$.

To deduce the nature of the singularities in $\chi^{(5)}$ I have calculated

$${}_1h_N = N^3 (D_c^3 N^3)^3 ({}_0h_{N+1} + {}_0h_N + {}_0h_{N-1} + {}_0h_{N-2}) \qquad {}_0h_N = K_N^{(5)} - {}^F\Delta K_N^{(5)} \tag{59}$$

to eliminate terms such as $\ln^2(N)/N$ in analogy with equation (57). The sequence ${}_1h_N$, as the maximum available $N = 127$ is approached, is oscillatory with approximate period 5 and amplitude 5×10^9. On the basis of this result one can conclude that any contribution to ${}_0h_N$ of the form of the two terms in $\Delta K_N^{(3)}$ must have amplitudes smaller than those given in equation (15) by factors 10^{10} and 10^8, respectively.

Furthermore, if $K_N^{(5)}$ has the structure indicated in equation (56), then the sequence ${}_1h_N$ should asymptotically approach

$${}_1h_N \simeq \sum_{m=1}^{5} b_m \cos((N+1/2)\theta_m) \qquad \{b_m/10^9\} \simeq 2.52, 0.450, 0.0384, 6.60, 0.485. \tag{60}$$

The observations are reasonably consistent with the first and fourth terms above although it is also clear that one has not yet reached the asymptotic limit $N \to \infty$ at the available $N \leqslant 127$. Subtracting the corresponding two $\Delta K_N^{(5)}$ terms in equation (56) from ${}_0h_N$ in (59) and then reducing the residuals further by the transformation to

$${}_2h_N = ((N+3)\,{}_1h_{N+3} - (N-2)\,{}_1h_{N-2})/N \tag{61}$$

should relatively enhance the remaining terms. The behaviour of ${}_2h_N$ in equation (61) can plausibly be interpreted in terms of the second and fifth terms in (60) but this result is by no means definitive and the contribution from the third term is too small to be demonstrated at all. On the other hand the numerical analysis above is entirely consistent with the assumption that the only singularities in $\chi^{(2n+1)}$ on the circle $|s| = 1$ are those that have been described analytically in this paper.

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