Experimental mathematics on the magnetic susceptibility of the square lattice Ising model

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Outline

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The Ising model: Definitions

Let $\sigma_{i,j} = \pm 1$ be the spin at lattice site (i,j) of the square lattice. The two-point correlation function is defined as

$$C(M,N) = \langle \sigma_{0,0}\sigma_{M,N} \rangle,$$

and the magnetic susceptibility is given by

$$kT \cdot \chi = \sum_M \sum_N (C(M,N) - \mathcal{M}^2).$$

The magnetisation $\mathcal{M}$ is zero at high temperatures ($T > T_c$) and $\mathcal{M} = (1 - s^{-4})^{1/8}$ for $T < T_c$, where $s = \sinh(2J/kT)$.

The susceptibility χ

Wu, McCoy, Tracy and Barouch [Phys. Rev. B **13**, 316 (1976)] showed that the susceptibility can be expressed as an infinite sum of n-particle contributions.
The high-temperature susceptibility is given by

$$kT \cdot \chi_H(w) = \sum \chi^{(2n+1)}(w) = \frac{1}{s}(1 - s^4)^{\frac{1}{4}} \sum \tilde{\chi}^{(2n+1)}(w)$$

and the low-temperature susceptibility is given by

$$kT \cdot \chi_L(w) = \sum \chi^{(2n)}(w) = (1 - 1/s^4)^{\frac{1}{4}} \sum \tilde{\chi}^{(2n)}(w)$$

in terms of the self-dual temperature variable $w = \frac{1}{2}s/(1 + s^2)$.

The n-particle contributions $\tilde{\chi}^{(n)}$

The n-particle contributions are given by $(n-1)$-dimensional integrals

$$\tilde{\chi}^{(n)}(w) \;=\; \frac{1}{n!} \cdot \Big(\prod_{j=1}^{n-1} \int_0^{2\pi} \frac{d\phi_j}{2\pi}\Big) \Big(\prod_{j=1}^{n} y_j\Big) \cdot R^{(n)} \cdot \; \Big(G^{(n)}\Big)^2$$

where the so-called Fermionic term $G^{(n)}$ is

$$G^{(n)} \;=\; \prod_{1 \le i < j \le n} h_{ij}, \quad h_{ij} \;=\; \frac{2 \sin\left((\phi_i - \phi_j)/2\right) \cdot \sqrt{x_i x_j}}{1 - x_i x_j},$$

and

$$R^{(n)} \;=\; \frac{1 + \prod_{i=1}^{n} x_i}{1 - \prod_{i=1}^{n} x_i},$$

The n-particle contributions $\tilde{\chi}^{(n)}$

The variables x_i and y_i are given by the expressions

$$x_i = \frac{2w}{1 - 2w\cos(\phi_i) + \sqrt{(1-2w\cos(\phi_i))^2 - 4w^2}},$$

$$y_i = \frac{2w}{\sqrt{(1-2w\cos(\phi_i))^2 - 4w^2}}, \qquad \sum_{j=1}^{n} \phi_j = 0$$

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Some properties of χ

Both the Ising free-energy and magnetisation are holonomic functions (i.e. *differentiably finite* or *D-finite* functions).

Guttmann and Enting [Phys. Rev. Lett. **76**, 344 (1996)] argued that the *anisotropic* Ising susceptibility is not D-finite.

Nickel [J. Phys. A **32** 3889 (1999), **33** 1693 (2000)] suggested that the *isotropic* susceptibility possessed a *natural boundary on the unit circle* $|s| = 1$.

He identified a set of singularities in $\tilde{\chi}^{(n)}$ which become dense on the unit circle.

Note that functions with a natural boundary cannot be D-finite.

Series expansion for χ

Orrick *et al* [J. Stat. Phys. **102**, 795 (2001)] used an algorithm of complexity $\mathrm{O}(N^6)$ to obtain the first 323 terms.

Quadratic partial difference equations are used to find $C(m,n)$ efficiently for high- and low-temperature series.

A series of N terms requires $C(m,n)$ for $m+n \leq 2N, m < n$. The diagonal $C(n,n)$ is the initial value data.

By using modular aritmetic (calculate series modulo several primes) and FFT to perform multiplications of polynomials we reduce the complexity to $\mathrm{O}(N^4 \log(N))$.

We calculated the first 2000 terms using just 240 CPU hours.

Series expansion for $\tilde{\chi}^{(5)}$ and $\tilde{\chi}^{(6)}$

In evaluating $\tilde{\chi}^{(n)}$ we convert to an n-fold ϕ_i integration with the explicit phase constraint $2\pi\delta(\sum \phi_i)$ now in the integrand.

By a Fourier transform we decouple all ϕ_i integrations at the expense of a sum over the Fourier integer k.

The end result is that we can replace the integration by a nested sum of products of hypergeometric functions.

Using a number of computational 'tricks' we finally arrive at an algorithm of complexity $\mathrm{O}(N^4 \log(N))$ per prime.

We calculated exact series for $\tilde{\chi}^{(5)}$ to order 2000 and for $\tilde{\chi}^{(6)}$ to order 1630 in $x = w^2$.

This took some 100000 CPU hours on a variety of machines.

Finally, for $\tilde{\chi}^{(5)}$ we calculated the first 10000 terms modulo a single prime. This took some 17000 CPU hours.

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Fuchsian ODEs for $\tilde{\chi}^{(n)}$

Zenine, Boukraa, Hassani and Maillard [J. Phys. A **37**, 9651 (2004)] made an important step towards the understanding of the three-particle contribution $\tilde{\chi}^{(3)}$.

They obtained the Fuchsian linear ODE for $\tilde{\chi}^{(3)}$.

In [J. Phys. A **38**, 4149 (2005)] they found the ODE for $\tilde{\chi}^{(4)}$.

An important observation coming out of the $\tilde{\chi}^{(3)}$ and $\tilde{\chi}^{(4)}$ work was that the $\tilde{\chi}^{(n)}$ were much more complicated functions than had been imagined.

This gives considerable urgency to finding new results for higher order $\tilde{\chi}^{(n)}$.

The form of our Fuchsian ODE

We consider only Fuchsian ODEs. So $x = 0$ and $x = \infty$ are regular singular points and we use operators of the form

$$L_{MD} = \sum_{m=0}^{M} \sum_{d=0}^{D} a_{md} \cdot x^d \cdot (x \frac{\mathrm{d}}{\mathrm{d}x})^m, \quad a_{M0} \neq 0, \; a_{MD} \neq 0. \quad (1)$$

$a_{M0} \neq 0$ makes $x = 0$ a regular singular point.

Use of the operator $x \frac{\mathrm{d}}{\mathrm{d}x}$ makes analysis around $x = \infty$ simple. $a_{MD} \neq 0$ makes $x = \infty$ ($y = 0$) a regular singular point.

The coefficients in the ODE are given by $L_{MD}(S(x)) = 0$. This yields a set of linear equations.

Finding the Fuchsian ODEs modulo a prime

There exists a non-trivial solution if the $N_{MD} \times N_{MD}$ determinant (with $N_{MD} = (M+1) \cdot (D+1)$) vanishes.

By Gaussian elimination we create an upper triangular matrix U. If $U(N,N) = 0$ for some N a non-trivial solution exists.

We set $a_{M0} = 1$ and determine the rest by back substitution.

The N for which $U(N,N) = 0$ is the minimum number of coefficients needed to find the ODE for a given M and D.

Henceforth, D will always refer to the minimum D for which a solution is found for a given M.

We define a unique non-negative deviation Δ by $N = N_{MD} - \Delta$.

A linear relationship for Fuchsian ODEs

A striking empirical observation arises from our work on $\tilde{\chi}^{(5)}$. For reasons we don't understand there is a linear relationship

$$N = A \cdot M + B \cdot D + C = (M+1) \cdot (D+1) - \Delta. \qquad (2)$$

A, B and C are *constants* depending on the particular series. For $\tilde{\chi}^{(5)}$ they are $A = 72$, $B = 33$, $C = -900$.

This relationship also holds for many other problems.

Eq. (2) has no (positive) solution for D if $M < B$. Thus $B = M_0$ is the minimum order possible for the linear differential operator that annihilates the original series.

Similarly, $A = D_0$ is the minimum possible degree.

The Fuchsian ODE for $\tilde{\chi}^{(5)}$

M is the order of the ODE, D the degree of the polynomials, $N_{MD} = (M+1)(D+1)$, N is the number of terms predicted by (2), and Δ is the difference $N_{MD} - N$.

Terms needed to find $\tilde{\chi}^{(5)}$				
M	D	N_{MD}	N	Δ
52	141	7526	7497	29
53	137	7452	7437	15
54	134	7425	7410	15
55	132	7448	7416	32
56	129	7410	7389	21
57	127	7424	7395	29
58	125	7434	7401	33
59	123	7440	7407	33
60	121	7442	7413	29

Exact ODEs from the modular ODEs

Procedure for finding the exact minimum order ODE.

- Generate a long series modulo a single prime.

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- Find the minimal order ODE mod these primes.

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Procedure for finding the exact minimum order ODE.

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- Find the ODE requiring the least number of terms.
- Generate series for more primes p_i and find the ODEs.
- Turn ODE into recurrence and generate longer series.
- Find the minimal order ODE mod these primes.
- Combine to find the exact minimal order ODE:
  Use Chinese Remainder Theorem to get coefficients a_{ij}.
  This gives us $Q = a_{ij} \bmod P$, where $P = \prod p_i$.
  Find the exact rational coefficients say by using the Maple call $a_{ij} = \mathrm{iratrecon}(Q, P)$.

Some properties of ODE for $\tilde{\chi}^{(5)}$

In earlier work [ZBHM, J. Phys A, **38**, 1875 and 4149 (2005)] we observed a "Russian-doll" structure for the linear differential equations for $\tilde{\chi}^{(3)}$ and $\tilde{\chi}^{(4)}$.

We conjecture for arbitrary $\tilde{\chi}^{(n)}$ that differential operator for $\tilde{\chi}^{(n)}$ right-divides the differential operator for $\tilde{\chi}^{(n+2)}$.

We have verified this conjecture on $\tilde{\chi}^{(5)}$.

A stronger property amounts to saying that in the differential operator for $\tilde{\chi}^{(n+2)}$ the differential operator for $\tilde{\chi}^{(n)}$ occurs as part of a *direct sum*.

Such a reduction was found for $6\tilde{\chi}^{(n+2)} - n\tilde{\chi}^{(n)}$, $n = 1$ or 2, and we now *verify this conjecture for the case* $n = 3$.

The Fuchsian ODE for $2\tilde{\chi}^{(5)} - \tilde{\chi}^{(3)}$

M is the order of the ODE, D the degree of the polynomials, $N_{MD} = (M+1)(D+1)$, N is the number of terms predicted by (2), and Δ is the difference $N_{MD} - N$.

Terms needed to find $2\tilde{\chi}^{(5)} - \tilde{\chi}^{(3)}$

M	D	N_{MD}	N	Δ
48	131	6468	6450	18
49	128	6450	6428	22
50	125	6426	6406	20
51	123	6448	6414	34
52	120	6413	6392	21
53	118	6426	6400	26
54	116	6435	6408	27
55	114	6440	6416	24
56	112	6441	6424	17

Further reductions of the ODE for $2\tilde{\chi}^{(5)} - \tilde{\chi}^{(3)}$

Simple solutions of the $2\tilde{\chi}^{(5)} - \tilde{\chi}^{(3)}$ ODE/operator can be used to further reduce the number of term required.

There are 2 order 1 operators whose solutions also occured in the analysis of the differential operator for $\tilde{\chi}^{(3)}$

$$S_1 \;=\; w/(1-4w) \quad \text{and} \quad S_2 \;=\; w^2/((1-4w)\sqrt{1-16w^2}).$$

We have also found an order 1 operator whose solution

$$S_3 \;=\; w^2/(1-4w)^2$$

is a solution of the differential operator for $2\tilde{\chi}^{(5)} - \tilde{\chi}^{(3)}$, but not a solution of the differential operator for $\tilde{\chi}^{(3)}$.

Further reductions of the ODE for $\tilde{\chi}^{(5)}$

Let L_2 be the differential operator annihilating both S_1 and S_2, and L_3 the differential operator annilating S_3 as well. When these act on the series $2\tilde{\chi}^{(5)} - \tilde{\chi}^{(3)}$ the reductions are

Series	$N = D_0M + M_0D + C$	M	D	N_{MD}	N
$\tilde{\chi}^{(5)}$	$72M + 33D - 900$	56	129	7410	7389
$2\tilde{\chi}^{(5)} - \tilde{\chi}^{(3)}$	$68M + 30D - 744$	52	120	6413	6392
L_2	$65M + 28D - 526$	50	117	6018	6000
L_3	$64M + 27D - 409$	49	117	5900	5886

So 5900 terms are enough to get the ODE for $\tilde{\chi}^{(5)}$.

We believe we have found more complicated operators as well. Using these we think 5100 terms should suffice.

Singularities of the ODE for $\tilde{\chi}^{(5)}$

In [J. Phys A **40**, 11713 (2007)] BHMZ performed a detailed analysis of the integrals $\Phi_H^{(n)}$ obtained by removing $(G^{(n)})^2$

$$\Phi_H^{(n)}(w) \;=\; \frac{1}{n!} \cdot \Big(\prod_{j=1}^{n-1} \int_0^{2\pi} \frac{d\phi_j}{2\pi}\Big)\Big(\prod_{j=1}^{n} y_j\Big) \cdot \frac{1+\prod_{i=1}^{n} x_i}{1-\prod_{i=1}^{n} x_i}.$$

They obtained the following polynomial factors for the head polynomial expressed in terms of Chebyshev polynomials of the first and second kind:

$$\begin{aligned} T_{2p_1}(1/2w+1) \;&=\; T_{n-2p_1-2p_2}(1/2w-1)\,, \\ 0 \le p_1 \le [n/2], \quad &\quad 0 \le p_2 \le [n/2] - p_1, \end{aligned}$$

Singularities of the ODE for $\tilde{\chi}^{(5)}$

and the polynomial arising from the elimination of z in:

$$\begin{aligned}
T_{n_1}(z) \; - T_{n_2}\Big(\frac{4w-z}{1-4w\,z}\Big) \;&=\; 0, \\
T_{n_1}\left(\frac{1}{2w}-z\right) \; - T_{n_2}\Big(\frac{1}{2w}-\frac{4w-z}{1-4w\,z}\Big) \;&=\; 0, \\
U_{n_2-1}(z)\cdot U_{n_1-1}\Big(\frac{1}{2w}-\frac{4w-z}{1-4w\,z}\Big)& \\
-U_{n_2-1}\left(\frac{1}{2w}-z\right)\cdot U_{n_1-1}\Big(\frac{4w-z}{1-4w\,z}\Big) \;&=\; 0,
\end{aligned}$$

$$n_1 \;=\; p_1, \qquad\qquad n_2 \;=\; n\;-p_1\;-2p_2,$$

$$0\;\le\; p_1 \;\le\; n, \qquad\qquad 0\;\le\; p_2 \;\le\; [(n-p_1)/2].$$

Singularities of the ODE for $\tilde{\chi}^{(5)}$

From the linear ODE for $\tilde{\chi}^{(5)}$ obtained modulo a prime, one can easily reconstruct the singularity polynomials of the ODE as they appear at the highest derivative. These polynomials read

$$
\begin{aligned}
& w^{33} \cdot (1-4w)^{22}(1+4w)^{16}(1-w)^4(1+2w)^4(1+3w+4w^2)^4 \\
& (1+w)(1-3w+w^2)(1+2w-4w^2)(1-w-3w^2+4w^3) \\
& (1+8w+20w^2+15w^3+4w^4)(1-7w+5w^2-4w^3) \\
& (1+4w+8w^2)(1-2w).
\end{aligned}
$$

All these singularities, except $(1-2w)$, are predicted by the model integrals.

Exponents of the ODE for $\tilde{\chi}^{(5)}$

Singularity	Exponents
w^{33}	$1^5, 2^4, 3^4, 4^3, 5^3, 6^3, 7^2, 8^2, 9^2,$ $10, 12^2, 15, 25$
$(1-4w)^{22}$	$-2, -7/4, -3/2, -5/4, -1^3, -1/2, 0^4,$ $1/2, 1^2, 2^2, 3, 4, 5, 6, 7$
$(1+4w)^{16}$	$-1, -1/2, 0^4, 1/2, 1^2, 3/2, 2^2, 3^2, 4, 5$
$1/w^{19}$	$0^3, 1^4, 2^2, 3^3, 4^2, 5^2, 6, 7, 8$
$(1+2w)^4$	$2, 5/2, 3^2$
$(1-w)^4$	$2, 3^2, 4$
$(1+3w+4w^2)^4$	$0, 1^2, 2$
$(1+w)$	11
$(1+2w-4w^2)$	11
$(1-3w+w^2)$	11
$(1+8w+20w^2+15w^3+4w^4)$	7
$(1-7w+5w^2-4w^3)$	5
$(1-w-3w^2+4w^3)$	7
$(1+4w+8w^2)$	5
$(1-2w)$	$7/2$

Diff-Padé analysis: Introduction

A diff-Padé or differential approximant analysis consists of finding an ODE of order M with polynomials of degree D reproducing the first $N = (M+1)(D+1)$ terms of the series.

If not the exact ODE it will fail for subsequent coefficients.

By varying M and D many approximate ODEs can be analysed.

We analyse the 2000 term exact series for $\tilde{\chi}^{(5)}$.

The 1600 (non-zero) tems of $\tilde{\chi}^{(5)}$.

Various combinations such as $\tilde{\chi} - \tilde{\chi}^{(1)} - \tilde{\chi}^{(3)} - \tilde{\chi}^{(5)}$ which will tell us something about $\tilde{\chi}^{(n)}$, $n \geq 7$.

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Diff-Padé analysis: General procedure

Analyzing very long exact series is computionally expensive.

We start by looking at ODEs using only a few hundred terms.

We locate the dominant singularities and explicitly add these to the head polynomial(s).

To find the multiplicity of a root we repeat our analysis until the singularity no longer occurs.

We then repeat the analysis using more and more terms, keeping some of the already found singularities in the head polynomial.

Results for $\tilde{\chi}^{(5)}$

Since we have obtained the exact linear ODE for $\tilde{\chi}^{(5)}$ this case provides a valuable test of our diff-Padé analysis.

The main conclusion is that a diff-Padé analysis can provide accurate information about the exact ODE.

The comparison with the exact ODE results shows that the diff-Padé analysis on only 2000 terms is able to correctly give all the singularities together with the correct multiplicity.

The indicial exponents are accurate enough to “guess” their exact values in agreement with the exact ODE results.

These results give us confidence that our analysis of $\tilde{\chi}^{(6)}$ and of higher order susceptibility components is correct.

Results for $\tilde{\chi}^{(5)}$

The number of significant digits found from our diff-Padé analysis of series of length 400, 1250 and 1980 terms.

Singularity polynomial	400	1250	1980
$(1+w)$	36		
$(1+2w-4w^2)$	36		
$(1-3w+w^2)$	36		
$(1+8w+20w^2+15w^3+4w^4)$	12	15	67
$(1-7w+5w^2-4w^3)$	12	15	67
$(1-w-3w^2+4w^3)$	4	15	51
$(1+4w+8w^2)$	-	8	17
$(1+2w)$	3	5	7
$(1-w)$	3	3	5
$(1+3w+4w^2)$	-	-	4
$(1-2w)$	-	12	27

Results for $\tilde{\chi}^{(6)}$

In a diff-Padé analysis, increasing the order of the linear ODE and the degree of the polynomials, the singularities predicted by the $\Phi_H^{(6)}$ model integral are obtained with increasing accuracy.

Our calculations show the existence of a new singularity at $x = 1/8$. So the factor $1 - 8w^2 = 0$ must appear in the head polynomial of the true ODE. Note that these new singularities lie on the unit circle $|s| = 1$.

The singularities and corresponding exponents for $\tilde{\chi}^{(6)}$ are summarised in the next slides.

Results for $\tilde{\chi}^{(6)}$

The number of significant digits found from a diff-Padé analysis.

Singularity Polynomial	387 terms, order 12	387 terms, order 16	997 terms, order 31
$1 - x$	28	29	
$1 - 4x$	30	30	
$1 - 9x$	30	30	
$1 - 25x$	13	14	
$1 - x + 16x^2$	8	10	
$1 - 10x + 29x^2$	10	12	
$1 - 8x$	3	4	26

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Exponents for $\tilde{\chi}^{(6)}$

Exponents for $\tilde{\chi}^{(6)}$ found by the diff-Padé analysis.

Singularity Polynomial	Exponents (diff-Padé)
x	$0, -1^2, -1/2$
$1-16x$	$-3/2, -1, 0^5, 1$
$1/x$	$-1^2, 0^2, -1/2^2, 1/2^6$
$1-x$	33/2
$1-4x$	$11/2, 13/2^2, 15/2, 33/2$
$1-9x$	33/2
$1-25x$	17/2
$1-x+16x^2$	17/2
$1-10x+29x^2$	23/2
$1-8x$	7

Main results for $\tilde{\chi}^{(n)}$, $n \geq 7$

We know the first 2000 (1630) coefficients for $\tilde{\chi}^{(5)}$ ($\tilde{\chi}^{(6)}$), and the series for $\tilde{\chi}^{(n)}$, $n \leq 4$, up to an arbitrary number of coefficients.

We examine if the total $\tilde{\chi}$ with the lower $\tilde{\chi}^{(n)}$ terms removed, can yield any information about the singularities of the linear ODE of $\tilde{\chi}^{(n)}$, $n \geq 7$.

From the “limited" analysis done here for $\tilde{\chi}^{(n)}$, $n \geq 7$, our main conclusion is that there are no new singularities that are not in the “known" sets from the model integrals.

The high-temperature series $\tilde{\chi} - \tilde{\chi}^{(1)} - \tilde{\chi}^{(3)} - \tilde{\chi}^{(5)}$

		500 terms		900 terms		1956 terms	
n	Singularity polynomial	Digits	Order	Digits	Order	Digits	Order
7	$1 - 5w + 6w^2 - w^3$	18	12	33	19	50	18
7	$1 + 2w - w^2 - w^3$	16	11	28	15	58	18
7	$1 + 2w - 8w^2 - 8w^3$	18	11	34	15	58	18
9	$1 - w$	-		-		15	14
9	$1 + 2w$	-		6	13	30	16
9	$1 + 3w - w^2$	5	11	16	15	45	15
9	$1 - 6w + 9w^2 - w^3$	7	12	20	13	45	18
9	$1 - 3w^2 - w^3$	-		8	15	30	18
9	$1 - 12w^2 + 8w^3$	-		14	14	40	20
11	$1 - 9w + 28w^2 - 35w^3 + 15w^4 - w^5$	-		7	13	30	18
11	$1 + 2w - 5w^2 - 2w^3 + 4w^4 - w^5$	-		-		23	17
11	$1 + 2w - 16w^2 - 24w^3 + 48w^4 + 32w^5$	-		-		20	20
13	$1 - 11w + \cdots + w^6$	-		-		16	16
13	$1 + 2w - 20w^2 + \cdots - 64w^6$	-		-		7	18
15	$1 + 2w - 4w^2$	-		-		5	14
15	$1 - 9w + \cdots + w^4$	-		-		5	14
7	$1 + 12w + 54w^2 + \cdots + 4w^6$	-		6	13	12	17
7	$1 - 3w - 10w^2 + \cdots - 16w^8$	-		-		4	12
9	$1 + 16w + 104w^2 + \cdots + 4w^8$	-		-		7	17

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The low-temperature series $\tilde{\chi} - \tilde{\chi}^{(2)} - \tilde{\chi}^{(4)} - \tilde{\chi}^{(6)}$

n	Singularity polynomial	Order 14	Order 20
8, 12, 16	$1-4x$	69	72
8, 16	$1-2x$	51	52
8, 16	$1-8x$	74	75
8, 16	$1-12x+4x^2$	73	79
10, 12	$1-x$	21	24
10	$1-5x$	43	46
10	$1-7x+x^2$	42	44
10	$1-12x+16x^2$	49	53
10	$1-15x+25x^2$	55	59
12	$1-9x$	12	16
12	$1-3x$	10	12
12	$1-12x$	9	13
12	$1-14x+x^2$	35	40
12	$1-8x+4x^2$	6	6
14	$1-21x+98x^2-49x^3$	21	24
16	$1-24x+148x^2-176x^3+4x^4$	10	12
8	$1-20x+16x^2-16x^3$	8	7
8	$1-26x+242x^2-960x^3+1685x^4-1138x^5$	6	6
10	$1-24x+128x^2-289x^3$	-	4
10	$1-46x+866x^2+\cdots-56642x^9$	-	6

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Notes on the full susceptibility χ

In our paper we also extend the Landau singularity analysis of Boukraa, Hassani, Maillard and Zenine [J. Phys A **40**, 2583 and 11713 (2007)] and Nickel [J. Phys. A **38**, 4517 (2005)] of $\tilde{\chi}^{(n)}$.

We show that in the absence of the "Fermionic factor", the singularities found by Boukraa *et al* are exhaustive.

We also show that none of these singularities, beyond those found by Nickel [J. Phys. A **32**, 3889 (1999)], can lie on the principal s-plane unit circle.

This dispels any hope of singularity cancellation. As a result the unit circle must be a natural boundary.

Some final remarks

The exact $\tilde{\chi}^{(5)}$ ODE confirms that the singularities are the ones of $\Phi_H^{(5)}$ together with the new factor $1 - 2w$.

The diff-Padé calculations confirmed that the singularities of the as yet unknown ODE for $\tilde{\chi}^{(6)}$ are (at least) the ones of $\Phi_H^{(6)}$ together with the roots of a new polynomial $1 - 8w^2$.

For $\tilde{\chi}^{(n)}$ with $n \geq 7$ we found no evidence of singularities other than those predicted by $\Phi_H^{(n)}$.

We do not know whether or not these extra singularities of the $\tilde{\chi}^{(n)}$ ODEs are singularities of the actual integrals.

The most common case is that in which all the singularities of the ODE and the integral are the same.

Some final remarks

This is the case for $\tilde{\chi}^{(3)}$ if one takes into account analytical continuations. For example both the Landau analysis and the ODE for $\tilde{\chi}^{(3)}$ predict a singularity at $s = (-1 + \mathrm{i}\sqrt{7})/4$ for which $|s| < 1$. So $\tilde{\chi}^{(3)}$ on the principal disc is not singular at this point, but there exists an analytic continuation of $\tilde{\chi}^{(3)}$ that is.

Our analysis of certain “toy” integrals provides an example of a difference between the singularities of the ODE and those of the integral. The ODE for the toy analog of $\tilde{\chi}^{(5)}$ has singularities at $w = 1/2$ and $w^2 = 1/8$ but our Landau analysis of the toy integral fails to find singularities at these points.

This may be a genuine distinction, or it may be that we missed something in the Landau analysis, or that the Landau analysis can't be guaranteed to give all singularities.