

# Square lattice Ising model susceptibility: series expansion method and differential equation for $\chi^{(3)}$

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## Abstract

In a previous paper (2004 *J. Phys. A: Math. Gen.* **37** 9651–68) we have given the Fuchsian linear differential equation satisfied by  $\chi^{(3)}$ , the ‘three-particle’ contribution to the susceptibility of the isotropic square lattice Ising model. This paper gives the details of the calculations (with some useful tricks and tools) allowing one to obtain long series in polynomial time. The method is based on series expansion in the variables that appear in the  $(n-1)$ -dimensional integrals representing the  $n$ -particle contribution to the isotropic square lattice Ising model susceptibility  $\chi$ . The integration rules are straightforward due to remarkable formulae we derived for these variables. We obtain without any numerical approximation  $\chi^{(3)}$  as a fully integrated series in the variable  $w = s/2/(1+s^2)$ , where  $s = sh(2K)$ , with  $K = J/kT$  the conventional Ising model coupling constant. We also give some perspectives and comments on these results.

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## 1. Introduction

Since the formal expression for the magnetic susceptibility of a square lattice Ising model, derived by Wu, McCoy, Tracy and Barouch [1], and the exact expression of the Ising susceptibility written as an infinite sum

$$\chi(T) = \sum_{n=1}^{\infty} \chi^{(n)}(T) \quad (1)$$

of  $(n - 1)$ -dimensional integrals [2–7], the integration of the latter has become a long-standing problem in statistical physics. The above sum is restricted to odd (respectively even)  $n$  for the high- (respectively low-) temperature case. While  $\chi^{(1)}$  is obtained directly without integration, and  $\chi^{(2)}$  is given in terms of elliptic integrals, *no closed forms* for the higher terms are known. It is only recently that the differential equation for  $\chi^{(3)}$  has been found [8].

Recalling the particle physics terminology of Wu, McCoy, Tracy and Barouch, these  $(n - 1)$ -dimensional integrals are seen as successive ‘particle excitations’, the first one,  $\chi^{(1)}$ , appears to have been calculated by Syozi and Naya [9] for *anisotropic* Ising models (on the triangular lattice), and is actually a very good approximation to the susceptibility  $\chi$ , its *anisotropic* series expansion being also in remarkable agreement [10] with the anisotropic series expansion for  $\chi$ ,

$$\chi^{(1)}(t_1, t_2, t_3) = \frac{(1 - t_1^2)(1 - t_2^2)(1 - t_3^2)}{(1 - t_1 - t_2 - t_3 - t_1t_2 - t_2t_3 - t_1t_3 + t_1t_2t_3)^2} M^{*2}, \quad (2)$$

$$M^* = \left( 1 - \frac{16(1 + t_1t_2t_3)(t_1 + t_2t_3)(t_2 + t_1t_3)(t_3 + t_1t_2)}{(1 - t_1^2)^2(1 - t_2^2)^2(1 - t_3^2)^2} \right)^{1/8}$$

where  $t_1, t_2$  and  $t_3$  are the three standard high-temperature variables,  $t_i = th(K_i)$ , for the triangular Ising model, and where  $M^*$  is nothing but the magnetization of the triangular lattice Ising model for which the low-temperature variables have been replaced by the high-temperature ones [10].

For the square lattice Ising model,  $\chi^{(1)}$  is obtained as the  $t_3 = 0$  limit of (2) for the anisotropic case, and as the  $t_3 = 0$  and  $t_2 = t_1$  limit for the isotropic case. The two-particle contribution  $\chi^{(2)}$  is also known exactly and can be expressed in terms of the elliptic integrals  $E$  and  $K$  [1] (see also (E.6)). These are the only two exact results on the  $n$ -particle contributions  $\chi^{(n)}$ .

Besides these two exact results on the  $n$ -particle contributions  $\chi^{(n)}$ , the only two exact ‘global’ results known for the whole susceptibility  $\chi$ , correspond to the exact expression of the susceptibility satisfying the so-called *disorder conditions* [11], and the exact functional relation corresponding to the so-called *inversion relation* [12] for the susceptibility [10].

For one of the four disorder conditions of the checkerboard Ising model,  $t_1 + t_2t_3t_4 = 0$ , the susceptibility of the checkerboard Ising model reduces to the simple rational expression [11]

$$\chi(t_1 + t_2t_3t_4 = 0) = \frac{(1 + t_2)(1 + t_3)(1 + t_4)(1 + t_2t_3t_4)}{(1 - t_2t_3)(1 - t_3t_4)(1 - t_2t_4)} \quad (3)$$

or, more simply, on the anisotropic triangular lattice ( $t_4 = 1$  limit<sup>4</sup>):

$$\chi(t_1 + t_2t_3 = 0) = \frac{(1 + t_2)(1 + t_3)(1 + t_2t_3)}{(1 - t_3)(1 - t_2)(1 - t_2t_3)}. \quad (4)$$

Recall that the Syozi and Naya algebraic expression (2) for the anisotropic triangular Ising model reduces to the exact expression (4) when restricted to the disorder condition  $t_1 + t_2t_3 = 0$ . Therefore, one finds that all the  $\chi^{(n)}$  ( $n > 1$ ) of the anisotropic triangular<sup>5</sup> Ising model should vanish when restricted to the disorder condition.

The so-called *inversion relation* [12] for the susceptibility of the checkerboard Ising model and for the Ising model on the triangular lattice, read, respectively [10, 13],

<sup>4</sup> In this limit divide by a factor 2 to get the susceptibility per site.

<sup>5</sup> This is also true for the four disorder conditions on the checkerboard Ising model, namely,  $\chi^{(n)}(t_1 + t_2t_3t_4 = 0) = 0$ ,  $n > 1$ .

$$\chi(t_1, t_2, t_3, t_4) + \chi(-t_1, 1/t_2, -t_3, 1/t_4) = 0 \quad (5)$$

$$\chi(t_1, t_2, t_3) + \chi(-t_1, 1/t_2, -t_3) = 0 \quad (6)$$

to be combined with the obvious functional equations associated with the geometrical symmetries of the model ( $\chi(t_1, t_2, t_3) = \chi(t_2, t_1, t_3) = \dots$ ). It is straightforward to verify that the algebraic expression (2) actually satisfies the previous inverse functional relation (6), and deduce, order by order in the  $n$ -particle expansion (1), that all the  $n$ -particle contributions,  $\chi^{(n)}$ , should also satisfy equations (6), together with the obvious geometrical symmetries.

Of course all these ideas ( $\chi^{(1)}$  versus exact expressions of the susceptibility restricted to the disorder conditions, inversion relations together with geometrical functional equations, Kramers–Wannier duality, etc) can be worked out on the checkerboard Ising model (see, for instance, [10, 14, 15]). This kind of analysis underlines the crucial role played by the modulus<sup>6</sup> of the elliptic function parametrizing the checkerboard Ising model,

$$k^2 = \prod_{i=1}^4 \frac{t_i^*(t_i + t_j t_k t_l)(1 - t_i^{*2})}{t_i(t_i^* + t_j^* t_k^* t_l^*)(1 - t_i^2)} \rightarrow k^2 = \left( \frac{1}{\text{sh}(2K_1)\text{sh}(2K_2)} \right)^2 \quad (7)$$

where  $t_j^*$  denote the dual variables,  $t_j^* = (1 - t_j)/(1 + t_j)$ . For the *anisotropic* square Ising model, the inverse functional relation simply reads [10] ( $t_3 = 0$  limit of (6))

$$\chi(t_1, t_2) + \chi(1/t_1, -t_2) = 0 \quad (8)$$

which can be combined with the obvious symmetry  $\chi(t_1, t_2) = \chi(t_2, t_1)$ .

Using these last two exact identities, some re-summed high-temperature series expansions [18, 19] were performed for the susceptibility  $\chi$  of the anisotropic square lattice Ising model [10, 18, 19], showing the occurrence of  $(2k + 1)$ th root of unity poles [19],  $t_2^{2k+1} = 1$ , for the  $(2k + 1)$  particle excitations  $\chi^{(2k+1)}$ . This enabled Guttmann and Enting [19] to conclude that  $\chi(t_1, t_2)$ , as a function of  $t_2$ , for  $t_1$  fixed, has a *natural boundary* (the unit circle  $|t_2| = 1$ ), and, thus, cannot be expressed as a solution of a linear differential equation<sup>7</sup> of *finite* order  $N$  with polynomial coefficients of degree  $d$  (even with  $N$  and  $d$  very large). Solutions of such linear differential equations with polynomial coefficients are called *holonomic* or *D-finite* [20, 21]. Therefore, the susceptibility  $\chi$  is a ‘truly transcendental function’ (in  $t_2, t_1$  fixed) if one takes for the definition of transcendental<sup>8</sup> that it is not holonomic or *D-finite*. However, the  $\chi^{(n)}$ , being multiple integrals of simple holonomic (algebraic!) expressions, must be holonomic: *they are actually solutions of linear differential equations*. To sum up,  $\chi$  is *not* holonomic, but it is the sum of an infinite number of holonomic expressions. We have, here, a situation which is totally reminiscent of that encountered with *Feynman graphs* where all the individual Feynman contributions are holonomic, but the sum of all these contributions is not holonomic (see, for instance, all the papers on multi-loop Feynman integrals, nested sums and multiple polylogarithms, Euler–Zagier sums, and other ‘motives’ theory [22–25]). In this respect, the analysis of the susceptibility  $\chi$  should be seen as the simplest example of such nested sum calculations, and, beyond the legitimate interest one has for the Ising model, should be seen as a ‘laboratory’ for such calculations, hopefully displaying the emergence of structures and symmetries. In this respect,  $\chi$  being considered as an infinite sum of holonomic  $n$ -particle excitations  $\chi^{(n)}$ , a better knowledge of the analytical structure of the  $\chi^{(n)}$  is clearly a way to get a deeper understanding of the still mysterious analytic structure of  $\chi$  in the complex plane.

<sup>6</sup> Recall that the spontaneous magnetization of the two-dimensional Ising model reads [16, 17]  $M = (1 - k^2)^{1/8}$ .

<sup>7</sup> For instance, it cannot be expressed in terms of a linear combination of special functions of mathematical physics such as elliptic integrals or hypergeometric functions.

<sup>8</sup> For example, the gamma function is a transcendental function: it does not satisfy a linear differential equation, however it verifies finite-difference (linear and non-linear) functional equations.

Let us make here a few remarks. There are many ‘levels of complexity’ among transcendental functions. Here we mean by ‘transcendental’, non-holonomic, non- $D$ -finite. As far as  $\chi$  is concerned, being transcendental, but expressible as the infinite sum of holonomic terms, one could seek solutions of simple, but *non-linear*, differential equations. For instance, it is worth recalling some particular<sup>9</sup> non-linear differential equations, namely the so-called *Painlevé transcendentals* [28, 29] that are known to occur for some two-point correlation functions of the Ising models [1, 30] (Painlevé transcendentals do not have natural boundaries). As a consequence of the previously mentioned natural boundary, the susceptibility  $\chi$  cannot be a solution of a linear differential equation, but it may well be a solution of a *non-linear* differential equation, even a very simple one! Actually, it is also worth recalling the *Chazy equation* [31, 32]

$$\frac{d^3}{dw^3}y = 2y \frac{d^2}{dw^2}y - 3 \left( \frac{d}{dw}y \right)^2 \quad (9)$$

which arises in the study of third-order ordinary differential equations having the ‘Painlevé property’<sup>10</sup> [33]. This non-linear equation is probably the simplest example of an ordinary differential equation whose solutions *have a natural boundary*. For the Chazy equation (9), the boundary is a *movable circle*<sup>11</sup> (its position depends on the initial conditions). The whole susceptibility  $\chi$  being the sum of all the two-point correlation functions, one could, thus, perfectly imagine that  $\chi$ , *despite its unit circle natural boundary*<sup>12</sup>, could well be a solution of a simple *non-linear* differential equation related to Painlevé-like transcendentals.

While there are *no algorithms* to find such *non-linear* differential equations, implementing an algorithm to seek for a linear differential equation reduces to solving a set of linear equations. One knows that each of the  $\chi^{(n)}$  is a solution of a linear differential equation, however, and unfortunately, the mathematical theorems that prove that the  $\chi^{(n)}$  are holonomic, because they are multiple integrals of holonomic expressions, do not give any upper bound on the order of the linear differential equation and no upper bound of the degree of the polynomials in front of the successive derivatives either [20, 21]. One can try to get enough coefficients of some high- (respectively low-) temperature series expansion to actually ‘guess’ the linear differential equation satisfied by a given  $\chi^{(n)}$ . Recalling the previous exact results that arise from a study of the anisotropic model, it might be tempting to generate *anisotropic* high-temperature series expansions in order to use these exact results to get severe exact constraints on the coefficients of the series expansion. This can be done in principle, however, the number of coefficients in the two variables, and the combinatorial complexity associated with the finding of these coefficients, is too large compared to the ‘advantage’ one gets from the previous exact constraints. Therefore, we will ignore the previous exact anisotropic results, and will generate more standard *isotropic* series expansions for  $\chi^{(n)}$ , and more specifically for  $\chi^{(3)}$ .

Recall that a huge amount of work had already been performed by Nickel [6, 7] to generate isotropic series coefficients for  $\chi^{(n)}$ . More recently, one should mention the generation by Orrick, Nickel, Guttmann and Perk [35], of coefficients of  $\chi$  using *non-linear Painlevé*

<sup>9</sup> They have fixed critical points [26] and are associated with some monodromy preserving property of some associated Schlesinger system [27].

<sup>10</sup> The solutions only have poles for movable singularities [26]. Movable means that the singularity’s position varies as a function of the initial values.

<sup>11</sup> Heuristically, this can be simply understood introducing exponentially small terms in the expansion of the solutions (see (3.37) in [34]), or as Chazy did [31, 32], by relating its solutions to those of a linear hypergeometric equation, performing an infinite process of analytic continuations yielding a tessellation of the interior (respectively exterior) of a circle.

<sup>12</sup> The susceptibility  $\chi$  of the *isotropic* Ising model has a unit circle natural boundary in the variable  $s = sh(2K)$ , see (10) below and [6, 7].

*difference equations*<sup>13</sup> for the correlation function [35–39]. This second method, because it uses an exact non-linear difference equation, was able to provide an algorithm for computing the successive coefficients in *polynomial* time [35] (namely  $O(N^6)$ ), instead of the exponential growth one expects at first sight. Roughly speaking, the first calculations by Nickel [6, 7] were actually performed using the multiple integral form of the  $\chi^{(n)}$  and were thus able to provide series expansions for the  $\chi^{(n)}$  *separately*. In contrast, the second method, which takes into account a fundamental non-linear symmetry, namely non-linear Painlevé difference equations [37–40], provides, as a consequence, a series expansion for the whole susceptibility  $\chi$ , where the various  $\chi^{(n)}$  are difficult to disentangle. To sum up roughly, the first standard method is holonomic, or linear, oriented (decomposition in the holonomic  $\chi^{(n)}$ ) while the second method is more non-holonomic, ‘non-linear oriented’ (transcendental Painlevé symmetries, etc).

As far as the singular behaviour near the dominant ferromagnetic point  $T = T_c$  is concerned, it is numerically extremely hard to disentangle the  $|T - T_c|^{9/4}$ ,  $|T - T_c|^{9/4} \log|T - T_c|$  and  $|T - T_c|^2 \log|T - T_c|$  contributions, and this was certainly a motivation to get longer series. This set of extensive results [6, 7, 35] (expansion up to order 116, then to order 257, and to order 323 for  $\chi$ ) already enabled one to get a better understanding of the various types of singular behaviour. The short-distance terms were shown to have the form  $(T - T_c)^p (\log|T - T_c|)^q$  with  $p \geq q^2$  [35, 36]. As far as the other singular points are concerned (non-physical singularities in the complex plane), Nickel [6] in a remarkable paper showed that  $\chi^{(2n+1)}$  is singular for the following values of  $s = sh(2J/kT)$  lying on the *unit circle* ( $k = m = 0$  excluded),

$$2 \left( s + \frac{1}{s} \right) = u^k + \frac{1}{u^k} + u^m + \frac{1}{u^m} \quad u^{2n+1} = 1, \quad -n \leq m, \quad k \leq n \quad (10)$$

the singularities being logarithmic branch points of order  $\epsilon^{2n(n+1)-1} \ln(\epsilon)$  with  $\epsilon = 1 - s/s_i$  where  $s_i$  is one of the solutions of (10). This confirms, this time for the *isotropic model*, the existence of a natural boundary for  $\chi(s)$ , namely  $|s| = 1$ , and that  $\chi(s)$  is a *transcendental* function: it is not  $D$ -finite (holonomic) as a function of  $s$ .

Our approach here is clearly of holonomic type, underlining the crucial role played by some well-suited *hypergeometric* functions. The emergence of these structures actually allows us to get extremely efficient *polynomial time* calculations (namely  $N^4$ , for  $\chi^{(3)}$ ), which enable us, in particular, to calculate the series coefficients *separately*, and *not from a recursion* that requires the storage of all the previous data. In what follows, we give a fully integrated expansion of the three-particle susceptibility contribution  $\chi^{(3)}$  as *multisums of hypergeometric functions*. This expression is used to generate a long series in the variable  $w = s/2/(1 + s^2)$ . With this long series, we succeeded [8] in obtaining the homogeneous seventh-order Fuchsian differential equation satisfied by  $\chi^{(3)}$ .

This paper is organized as follows. In section 2, we present the basic features of our expansion method that allow us to obtain the fully integrated  $\chi^{(3)}$  as a multisum of products of three hypergeometric functions, without any numerical approximation. The three-particle susceptibility  $\chi^{(3)}$  is written, for series generation purposes, as the sum of a closed, but involved, expression (sum of linear, quadratic and cubic products of elliptic integrals), of a second simple (non-closed, for the moment, but easy enough to compute) sum, and a last sum which is much harder to calculate, and which requires most of the computing time. The variable  $w$  being well suited to both high- and low-temperature regimes, the expansion method we use is generalizable to other  $\chi^{(n)}$  ( $n$  odd, or even). In section 3, we recall the homogeneous linear differential equation and discuss the new singularities discovered in [8]. In section 4, using a differential approximant method, we show how the new non-apparent singularities can

<sup>13</sup> More generically, this corresponds to the notion of the so-called Hirota bilinear equations.

be discovered even when the series are not long enough to obtain the exact linear differential equation. Finally, section 5 contains our conclusions.

**2. The fully integrated expansion of  $\chi^{(3)}$**

*2.1. The expansion method*

Let us focus on the third contribution to the susceptibility  $\chi$  defined by the double integral as given in [6],

$$\begin{aligned} \chi^{(3)}(s) &= (1 - s^4)^{1/4} / s \tilde{\chi}^{(3)}(s) \\ \tilde{\chi}^{(3)}(s) &= \frac{1}{4\pi^2} \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \tilde{y}_1 \tilde{y}_2 \tilde{y}_3 \left( \frac{1 + \tilde{x}_1 \tilde{x}_2 \tilde{x}_3}{1 - \tilde{x}_1 \tilde{x}_2 \tilde{x}_3} \right) H^{(3)} \end{aligned} \tag{11}$$

with

$$\begin{aligned} \tilde{x}_j &= \frac{s}{1 + s^2 - s \cos \phi_j + \sqrt{(1 + s^2 - s \cos \phi_j)^2 - s^2}}, \\ \tilde{y}_j &= \frac{s}{\sqrt{(1 + s^2 - s \cos \phi_j)^2 - s^2}}, \quad j = 1, 2, 3, \quad \phi_1 + \phi_2 + \phi_3 = 0. \end{aligned} \tag{12}$$

Many forms for  $H^{(3)}$  may be taken [6, 7] and are equivalent for integration purposes, e.g.,

$$H^{(3)} = f_{23} \left( f_{31} + \frac{f_{23}}{2} \right), \quad f_{ij} = (\sin \phi_i - \sin \phi_j) \frac{\tilde{x}_i \tilde{x}_j}{1 - \tilde{x}_i \tilde{x}_j}. \tag{13}$$

Instead of the variable  $s$ , we found it more suitable to use  $w = \frac{1}{2}s/(1 + s^2)$  where the unit circle  $|s| = 1$  becomes  $]-\infty, -1/4] \cup [1/4, \infty[$  in  $w$ . This variable allows us to deal with both limits (high and low  $s$ ) on an equal footing.

From now on, we will use the scaled variables

$$\begin{aligned} x_j &= \frac{\tilde{x}_j}{w} = \frac{2}{1 - 2w \cos \phi_j + \sqrt{(1 - 2w \cos \phi_j)^2 - 4w^2}}, \\ y_j &= \frac{\tilde{y}_j}{2w} = \frac{1}{\sqrt{(1 - 2w \cos \phi_j)^2 - 4w^2}} \end{aligned} \tag{14}$$

which behave like  $1 + O(w)$  at small  $w$ . These variables are related by

$$y_j(1 - w^2 x_j^2) = x_j. \tag{15}$$

Performing the integrals in (11) is highly non-trivial. For this, one may expand symbolically the integrand in (11) in the variable  $w$ , and integrate the angular part. This way one faces some 18 sums to carry out. These sums come from the expansion of the quantities  $x_j$  and  $y_j$ , and also of the denominators. The convoluted character of the integrand, and especially  $1/(1 - w^3 x_1 x_2 x_3)$ , makes the symbolic expansion in  $w$  almost intractable.

To overcome this difficulty we expand the integrand of  $\tilde{\chi}^{(3)}$  in various variables  $x_j$ . The expansion depends now only on combinations of the form

$$y_1 x_1^{n_1} y_2 x_2^{n_2} y_3 x_3^{n_3} P_{n_1, n_2, n_3}(\phi_1, \phi_2, \phi_3) \tag{16}$$

where  $P_{n_1, n_2, n_3}(\phi_1, \phi_2, \phi_3)$  is a polynomial in circular functions of the angles  $\phi_j$ . The structure (16) appearing in the integrand, after the expansion in the variables  $x_j$ , is independent of the particular form taken for  $H^{(3)}$ .

We succeeded in deriving a remarkable formula for  $y_j x_j^n$  that carries only *one summation index* and reads (we drop the indices)

$$y x^n = a(0, n) + 2 \sum_{k=1}^{\infty} w^k a(k, n) \cos k\phi \tag{17}$$

where  $a(k, n)$  is a *non-terminating* hypergeometric series that reads

$$a(k, n) = \binom{m}{k} {}_4F_3 \left( \frac{(1+m)}{2}, \frac{(1+m)}{2}, \frac{(2+m)}{2}, \frac{(2+m)}{2}; 1+k, 1+n, 1+m; 16w^2 \right) \quad (18)$$

where  $m = k + n$ . Note that  $a(k, n) = a(n, k)$ .

With this Fourier series, the angular integration of the form (16) becomes straightforward<sup>14</sup>.

The method described above being independent of the particular choice of  $H^{(3)}$ , let us consider the form (13). Noting that

$$\frac{\tilde{x}_i \tilde{x}_j}{1 - \tilde{x}_i \tilde{x}_j} = \frac{w}{2} \frac{x_i - x_j}{\cos \phi_i - \cos \phi_j} \quad (19)$$

the  $f_{ij}$  can be rewritten as

$$f_{ij} = -\frac{w}{2} (x_i - x_j) \cot(\phi_i/2 + \phi_j/2). \quad (20)$$

$H^{(3)}$  becomes simply a polynomial in the  $x_i$ :

$$H^{(3)} = \frac{w^2}{4} \left( \frac{1}{2} (x_2 - x_3)^2 \cot^2 \left( \frac{\phi_1}{2} \right) - (x_1 - x_3)(x_2 - x_3) \cot \left( \frac{\phi_1}{2} \right) \cot \left( \frac{\phi_2}{2} \right) \right). \quad (21)$$

Expanding the integrand of  $\tilde{\chi}^{(3)}$  in the variables  $x_j$ ,

$$\tilde{\chi}^{(3)}(w) = \frac{8w^3}{4\pi^2} \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \cdot y_1 y_2 y_3 \left( 1 + 2 \sum_{n=1}^{\infty} w^{3n} (x_1 x_2 x_3)^n \right) H^{(3)} \quad (22)$$

together with expression (21) for  $H^{(3)}$ , one notes that the integrand depends only on combinations of the form

$$y_1 x_1^{n_1} y_2 x_2^{n_2} y_3 x_3^{n_3} \cot^2(\phi_1/2) \quad (23)$$

$$y_1 x_1^{n_1} y_2 x_2^{n_2} y_3 x_3^{n_3} \cot(\phi_1/2) \cot(\phi_2/2) \quad (24)$$

which have straightforward integration rules.

The problem of integration is thus settled with a *limited number of sums*. In appendix A we give the integration rules used and show how the cancellation of the ‘artificial’ singularity introduced by taking the particular form (21) for  $H^{(3)}$  occurs.

The expansion of the integrand in the variables  $x_j$ , together with the remarkable formula (17), allows us to obtain  $\tilde{\chi}^{(3)}(w)$  as a fully integrated expansion (see appendices B and C), namely,

$$\tilde{\chi}^{(3)}(w) = 8w^9 (\tilde{\chi}_{cl}^{(3)}(w) + 2w^4 \Xi(w)) \quad (25)$$

where  $\Xi(w)$  are sums given in appendix B, and  $\tilde{\chi}_{cl}^{(3)}(w)$  is a *closed expression*,

$$\tilde{\chi}_{cl}^{(3)}(w) = \frac{1}{256(1-4w)^{3/2} w^{13}} \left( \sqrt{1-4w} \sum_{i=0}^3 \sum_{j=0}^i q_{j,i-j} \tilde{K}^j \tilde{E}^{i-j} + \sum_{i=0}^2 \sum_{j=0}^i p_{j,i-j} \tilde{K}^j \tilde{E}^{i-j} \right) \quad (26)$$

<sup>14</sup> Note that we can deduce from the Fourier series (17) that  $yx^n$  also has an expansion in the variable  $w$  (respectively  $\sin^2(\phi/2)$ ) with coefficients as *hypergeometric functions* of the variable  $\sin^2(\phi/2)$  (respectively  $w$ ). Actually, the expansion (17) is more suitable for angular integration purposes.

with  $\tilde{K}$  and  $\tilde{E}$  being functions of  $w$  related to elliptic integrals  $K$  and  $E$ ,

$$\begin{aligned} \tilde{K} &= {}_2F_1(1/2, 1/2; 1; 16w^2) = 2K(4w)/\pi, \\ \tilde{E} &= {}_2F_1(-1/2, 1/2; 1; 16w^2) = 2E(4w)/\pi, \end{aligned} \tag{27}$$

and where the  $q_{i,j}$  and  $p_{i,j}$  are polynomials in  $w$  given in appendix D. One should note that this closed expression (26) is not ‘natural’: the separation in (25) is not unique. It comes from our ability to evaluate some sums, and is only made for series generation purposes (see appendices B and C for details). In fact,  $\tilde{\chi}^{(3)}$  in (25) can be written as a multisum of the product of three hypergeometric functions  $a(k, n)$ , as can be clearly seen<sup>15</sup> in (16).

One recalls that the key ingredient in obtaining (25) is the Fourier expansion of  $yx^n$ , a quantity appearing in any  $\chi^{(n)}$ . The method is thus generalizable, independent of whether  $n$  is even or odd, since the variable  $w$  has, by construction, Kramers–Wannier duality invariance ( $s \leftrightarrow 1/s$ ). Appendices E and F show how the known result [1] for  $\chi^{(2)}$  appears, in this framework, as a sum of products of two hypergeometric functions merging into a *single* hypergeometric function.

For the  $\tilde{\chi}^{(3)}$  case, we see that the mechanism of *fusion relations* on hypergeometric functions that we saw previously for  $\tilde{\chi}^{(2)}$ , may also hold similarly. However, we have not discovered a similar fusion mechanism for  $\tilde{\chi}^{(3)}$ .

### 2.2. Series generation

From our integrated forms of  $\tilde{\chi}^{(3)}$ , the generation of series coefficients becomes straightforward. Recall that (25) is already integrated, and, thus, the computing time to obtain the series coefficients comes from the evaluation of the sums. For the forms used, this time<sup>16</sup> is of order  $N^4$ .

We have been able to generate a long series of coefficients from expression (25) up to order 490. More precisely, the series expansion for  $\Xi$  in (25), was, in fact, obtained as the sum of two series, a ‘hard to compute’ series up to order 490,  $\Xi_h$ , requiring most of the computing time<sup>17</sup>, and a simpler one,  $\Xi_s$ , requiring much less computing time, but of course, more time than the closed expression  $\tilde{\chi}_{cl}^{(3)}$ . They read, respectively,

$$2w^4\Xi_h(w) = 16w^4 + 88w^5 + 1008w^6 + 5144w^7 + \dots \tag{28}$$

$$2w^4\Xi_s(w) = 4w^4 - 4w^5 + 6w^6 - 1628w^7 - 11\,738w^8 + \dots \tag{29}$$

and<sup>18</sup>

$$\tilde{\chi}_{cl}^{(3)}(w) = 1 + 36w^2 + 4w^3 + 864w^4 + 112w^5 + 17\,518w^6 + \dots \tag{30}$$

The expansion of  $\tilde{\chi}^{(3)}$  thus reads

$$\begin{aligned} \frac{\tilde{\chi}^{(3)}(w)}{8w^9} &= 1 + 36w^2 + 4w^3 + 884w^4 + 196w^5 + 18\,532w^6 + \dots \tag{31} \\ &430\,990\,415\,607\,244\,903\,400\,516\,891\,368\,318\,213\,367\,308\,330\,575\,817\,905 \\ &813\,380\,442\,285\,066\,457\,219\,428\,362\,271\,319\,439\,164\,276\,111\,839\,658\,488 \end{aligned}$$

<sup>15</sup> For  $\Xi(w)$  this multisum of the product of three hypergeometric functions can be seen in the definition of the auxiliary functions (see appendices A–C) in terms of  $a(k, n)$ .

<sup>16</sup> The overall computing time can be reduced by using the inhomogeneous recurrences on, and relations between the coefficients of the functions introduced (see appendix G).

<sup>17</sup> Expression  $\Xi_h$  actually corresponds to the true limitation in our series expansion. It corresponds to the third term on the right-hand side of (B.11), see appendix B.

<sup>18</sup> This sum is actually analytic near  $w = 0$ , while the expansions of the various cubic sums, quadratic sums and linear sums in  $K$  and  $E$  in the closed form (26) exhibit  $1/w^{13}$ ,  $1/w^{12}$ , ... poles.

$$\begin{aligned}
&820\ 854\ 328\ 108\ 563\ 517\ 776\ 050\ 668\ 285\ 313\ 206\ 447\ 166\ 513\ 353\ 732\ 686 \\
&903\ 643\ 836\ 043\ 378\ 474\ 616\ 173\ 307\ 206\ 177\ 943\ 565\ 786\ 520\ 352\ 551\ 853 \\
&500\ 345\ 493\ 340\ 110\ 011\ 396\ 345\ 698\ 876\ 727\ 619\ 330\ 445\ 413\ 593\ 141\ 923 \\
&791\ 195\ 381\ 220\ 947\ 969\ 620w^{481} + \dots
\end{aligned}$$

in agreement with the coefficients obtained by Nickel [7] and those obtained by Guttmann *et al*<sup>19</sup>, these last expansions being, in fact, written in terms of the  $u = s/2$  variable [7]:

$$\frac{\tilde{\chi}^{(3)}(u)}{4u^8} = 1 + 4u^3 + 16u^4 + 4u^5 + 20u^6 + 84u^7 + 247u^8 + \dots \quad (32)$$

For large values of  $N$ , the coefficients  $C_N$ , on the right-hand side of (31) and (32), grow, in the variable  $w$  as

$$C_N \simeq 13.5 \times 4^N, \quad N \text{ even}, \quad C_N \simeq 11 \times 4^N, \quad N \text{ odd} \quad (33)$$

and in the variable  $u = s/2$ , as  $C_N^{(u)} \simeq 15 \times 2^N$ .

Our long series is obtained as the sum of three contributions of different algorithmic complexity. The contribution (30) being given by an exact closed form, we were tempted to seek a linear differential equation satisfied by  $\tilde{\chi}_{cl}^{(3)}$ . Appendix H contains a report on this matter, which suggests that seeking for the differential equation for  $\tilde{\chi}^{(3)}$ , seen as the sum (25), is in fact much simpler than seeking the differential equation for each constituent. The whole sum (25) is, thus, a better candidate for seeking for a linear differential equation.

### 3. The Fuchsian differential equation satisfied by $\tilde{\chi}^{(3)}$

With our long series, and with a dedicated program, we have succeeded in obtaining the differential equation for  $\tilde{\chi}^{(3)}$  that is given in [8] and recalled here,

$$\sum_{n=0}^7 a_n(w) \frac{d^n}{dw^n} F(w) = 0 \quad (34)$$

with

$$\begin{aligned}
a_7 &= w^7(1-w)(1+2w)(1-4w)^5(1+4w)^3(1+3w+4w^2)P_7(w), \\
a_6 &= w^6(1-4w)^4(1+4w)^2P_6(w), \quad a_5 = w^5(1-4w)^3(1+4w)P_5(w), \\
a_4 &= w^4(1-4w)^2P_4(w), \quad a_3 = w^3(1-4w)P_3(w), \\
a_2 &= w^2P_2(w), \quad a_1 = wP_1(w), \quad a_0 = P_0(w).
\end{aligned} \quad (35)$$

where  $P_7(w)$ ,  $P_6(w)$ ,  $\dots$ ,  $P_0(w)$  are polynomials of degree respectively 28, 34, 36, 38, 39, 40, 40 and 36 given in [8].

The differential equation (34) is an equation of the Fuchsian type since there are no singular points, finite or infinite, other than regular singular points. The singularities correspond to the roots of the polynomial in front of the highest derivative in (34). The ferromagnetic ( $w = 1/4$  or  $s = 1$ ), antiferromagnetic ( $w = -1/4$  or  $s = -1$ ), zero or infinite temperature ( $w = 0$  or  $s = 0, \infty$ ), non-physical ( $w = \infty$  or  $s = \pm i$ ) and Nickel singularities ( $w = 1, -1/2$  or  $2 - s + 2s^2 = 0, 1 + s + s^2 = 0$ ) are indeed regular singular points of the differential equation. The last two are given by Nickel's relation (10) for  $n = 1$ . Besides the known singularities mentioned above, we note the occurrence of the roots of the polynomial  $P_7(w)$  of degree 28 in  $w$ , and of the two *quadratic numbers*  $1 + 3w + 4w^2 = 0$  which *are not* of Nickel's form (10).

<sup>19</sup> Private communication: Orrick and Guttmann obtained the series up to 250 coefficients, in agreement with our 490 coefficients.

**Table 1.** Critical exponents for each regular singular point.  $N_F$  and  $P$  are, respectively, the number of solutions in Frobenius form, and the maximum power of the logarithmic terms for each singularity of (34).  $w_P$  is any of the 28 roots of  $P_7(w)$ . We have also shown the corresponding roots in the  $s$  variable. In the variable  $s$  the local exponents for  $w = \pm 1/4$  are twice those given.

$w$ -singularity	$s$ -singularity	Critical exponents in $w$	$N_F$	$P$
0	$0, \infty$	9, 3, 2, 2, 1, 1, 1	4	2
$-1/4$	$-1$	3, 2, 1, 0, 0, 0, $-1/2$	4	2
$1/4$	1	1, 0, 0, 0, $-1, -1, -3/2$	4	2
$-1/2$	$\frac{-1 \pm i\sqrt{3}}{2}$	5, 4, 3, 3, 2, 1, 0	6	1
1	$\frac{1 \pm i\sqrt{15}}{4}$	5, 4, 3, 3, 2, 1, 0	6	1
$\frac{-3 \pm i\sqrt{7}}{8}$	$\frac{-1 \pm i\sqrt{7}}{4}, \frac{-1 \pm i\sqrt{7}}{2}$	5, 4, 3, 2, 1, 1, 0	6	1
$\infty$	$\pm i$	3, 2, 1, 1, 1, 0, 0	4	2
$w_P, 28$ roots	$s_P, 56$ roots	7, 5, 4, 3, 2, 1, 0	7	0

Applying Frobenius's method [26], we give in table 1, for each regular singular point, the critical exponents, the number of solutions in Frobenius form, and the maximum power of the logarithmic terms. One sees that only log and  $\log^2$  terms appear in the local solutions of (34).

One can see that the roots of  $P_7$  are *apparent singularities*, the local solutions carry *no logarithmic terms* and *are analytic* since the exponents are *all positive integers*. Consider the apparent singularity effect from the series expansion  $\tilde{\chi}^{(3)}$  viewpoint of this paper. If the roots of  $P_7$  were not apparent and were singularities of  $\tilde{\chi}^{(3)}$ , the coefficients of (31), instead of being dominated by the  $w = \pm 1/4$  singularities, yielding a  $4^N$  growth of the coefficients, would be dominated by the smallest (in modulus) root of  $P_7$ , namely  $w \simeq -0.0424$ , yielding a growth  $\simeq (23.553)^N$  of the coefficients. We have checked this on many (slight) deformations of (34), keeping all but one of the  $P_n$  unchanged (in particular  $P_7$ ), and slightly modifying one  $P_n$  ( $n \neq 7$ ). One immediately sees a change in the growth of the coefficients, with the  $4^N$  growth changing drastically into a  $\simeq (23.553)^N$  growth. It is thus crucial that the roots of  $P_7$  are *apparent singularities*, which require some very specific 'alchemical tuning' between the various  $P_n$ . In other words, the Fuchsian equation (34) corresponds to a rather *rigid structure*, since the apparent singularity character of  $P_7$  is an *unstable property*.

The two quadratic numbers,  $w = (-3 \pm i\sqrt{7})/8$  (or  $1 + 3w + 4w^2 = 0$ ), which read in the  $s$  variable

$$(2s^2 + s + 1)(s^2 + s + 2) = 0 \quad (36)$$

have their roots lying, respectively, on the circles  $|s| = 1/\sqrt{2}$  and  $|s| = \sqrt{2}$ . Near these points, one of the solutions of (34) has weak singular behaviour (a log singularity). Note, however, that some of these logarithmic terms, occurring in the general solution of (34) and shown in table 1, *may not exist*<sup>20</sup> in the particular solution  $\tilde{\chi}^{(3)}$ . Actually, the two unexpected quadratic numbers correspond to singularities of solutions of (34) which behave locally like  $(1 + 3w + 4w^2) \ln(1 + 3w + 4w^2)q_1 + q_2$ , where  $q_1$  and  $q_2$  are analytic functions near the two quadratic roots  $1 + 3w + 4w^2 = 0$ . This weak singularity<sup>21</sup> gives a  $2^N$  contribution to the growth of the  $w$ -coefficients. However, this does not mean that each solution<sup>22</sup> of (34) has

<sup>20</sup> See, for instance, the two simple rational and algebraic solutions  $S_1$  and  $S_2$  below (see (37)) which are free of the  $1 - w = 0$ ,  $1 + 2w = 0$ ,  $w = 0$  and  $1 + 3w + 4w^2 = 0$  singularities.

<sup>21</sup> This 'weakly' singular behaviour can also be seen in the monodromy matrix (see [8]) associated with these two roots, where one finds a nilpotent matrix of order 2 (no  $\log^2$  term).

<sup>22</sup> A solution of (34) can exhibit *only a restricted set of the whole set of singularities* of the Fuchsian equation: this is very clear with  $S_1$  or  $S_2$  (see (37) below).

such  $(1 + 3w + 4w^2) \ln(1 + 3w + 4w^2)$  singular behaviour near the two roots  $1 + 3w + 4w^2 = 0$ . Actually, as far as the ‘physical’ solution  $\tilde{\chi}^{(3)}$  is concerned, and as far as the series analysis viewpoint developed in this paper is concerned, this  $(1 + 3w + 4w^2) \ln(1 + 3w + 4w^2)$  singular behaviour should be excluded: in the  $s$  variable, instead of the  $w$  variable, it would give (beyond other terms) a  $(1 + s + 2s^2) \ln(1 + s + 2s^2)$  term, yielding a  $\sqrt{2}^N$  growth, which would be in contradiction with the growth of the coefficients of  $\tilde{\chi}^{(3)}$  in the  $s$  variable. This requires further investigations that we will address in a forthcoming publication.

To end this section and to be complete, we will recall the pertinent algebraic properties of the Fuchsian differential equation whose analysis was sketched in [8]. The Fuchsian differential equation (34) has two remarkable rational and algebraic solutions, namely,

$$S_1(w) = \frac{w}{1 - 4w}, \quad S_2(w) = \frac{w^2}{(1 - 4w)\sqrt{1 - 16w^2}}. \quad (37)$$

This results in very important factorization properties for  $L_7$ , the seventh-order linear differential operator, corresponding to the Fuchsian differential equation (34):

$$L_7 = \frac{d^7}{dw^7} + \frac{1}{a_7} \sum_{k=0}^6 a_k \frac{d^k}{dw^k}. \quad (38)$$

The adjoint differential operator  $L_7^*$  has the following rational solution<sup>23</sup>

$$S_1^*(w) = \frac{f(w)Q_6(w)}{w^3 P_7(w)} \quad (39)$$

where  $f(w) = (1 - w)(1 + 2w)(1 - 4w)^5(1 + 4w)^3(1 + 3w + 4w^2)$  and  $Q_6$  is a polynomial of degree 28 given in [8].

All these findings imply the following factorization of  $L_7$ ,

$$L_7 = M_6 L_1, \quad L_7 = N_6 N_1 \quad (40)$$

$$L_7 = M_1 L_6, \quad L_6 = L_5 N_1 \quad (41)$$

where  $M_6$ ,  $N_6$  and  $L_5$  are operators of order respectively 6, 6 and 5, and where the order-1 operators  $L_1$ ,  $N_1$  and  $M_1$  are such that  $L_1(S_1) = 0$ ,  $N_1(S_2) = 0$  and  $M_1^*(S_1^*) = 0$ . The operators  $L_6$ ,  $M_6$ ,  $N_6$  and  $L_5$  can easily be calculated from the previous factorization relations, by right or left division by the first-order operators  $L_1$ ,  $N_1$  and  $M_1$  defined above. The decompositions (40), (41) imply that the general solution of (34) is a linear combination of  $S_1$  and a solution,  $S(L_6)$ , of the sixth-order linear homogeneous differential equation associated with  $L_6$ . The particular ‘physical’ solution of  $L_7$ ,  $\tilde{\chi}^{(3)}$ , can be written as  $\tilde{\chi}^{(3)} = \alpha S_1 + S(L_6)$ , where  $\alpha$  is deduced from  $L_6(\tilde{\chi}^{(3)} - \alpha S_1) = 0$  and has the remarkably simple value  $\alpha = 1/3$ . The homogeneous operator  $L_6$  has the polynomial  $w^6 f(w) Q_6(w)$  in front of the highest derivative. The roots of the polynomial  $Q_6(w)$  are also *apparent singularities* of the linear homogeneous differential equation associated with  $L_6$ .

#### 4. Towards the new non-apparent singularities: a Diff-Padé method

From the ideas developed in section 2, we were able to obtain a very long series expansion for  $\tilde{\chi}^{(3)}$ , sufficiently long to actually identify the Fuchsian equation for  $\tilde{\chi}^{(3)}$ . However, when considering further similar calculations on the next  $\chi^{(n)}$  ( $\chi^{(4)}$ ,  $\chi^{(5)}$ , ...), we may not be able to obtain large enough series to identify the corresponding Fuchsian equations. One may ask

<sup>23</sup> We thank Jacques-Arthur Weil for the remarkable results (39) and (41).

the following question: What kind of results can one get from the analysis of long series, but not long enough to find the exact Fuchsian equation? This obviously supposes taking into account some of the ideas previously encountered, namely the homogeneous character of the linear differential equation, the Fuchsian character of some known singularities (such as  $s = \pm i$  and Nickel's singularities, see (10)), the possible occurrence of unexpected, but simple, regular singularities (such as the quadratic numbers  $1 + 3w + 4w^2 = 0$ ), and above all, the possible occurrence of quite a large set of apparent singularities<sup>24</sup> (such as the 28 roots of polynomial  $P_7$ ).

In fact, the preliminary studies we performed before finding the Fuchsian equation (34) give some hint as to the kind of results one might expect<sup>25</sup>.

One knows that  $\tilde{\chi}^{(3)}$  satisfies a linear differential equation. For a given number of terms  $N$  in the  $\tilde{\chi}^{(3)}/w^9$  series, there is a linear differential equation of order  $q$  that reproduces the first  $N - q$  terms but may fail for subsequent coefficients. Let us show what kind of information arises from the differential equations obtained for increasing order  $q$ , and increasing degrees of the polynomials in front of the derivatives. We will consider the following form:

$$\sum_{n=0}^q p_n(w) \frac{d^n F(w)}{dw^n} = 0. \quad (42)$$

There are various ways to choose the degrees of the polynomials  $p_n(w)$ . One may take

$$\deg(p_n) = \deg(p_{n-1}) + 1, \quad \deg(p_n) = \mu + n. \quad (43)$$

The differential equation (42) then has  $1/2(q + 1)(q + 2\mu + 2)$  unknowns. The number  $N$  of terms in the  $\tilde{\chi}^{(3)}/w^9$  series used is

$$N = \frac{1}{2}(q + 1)(q + 2\mu + 2) - 1 - q. \quad (44)$$

One should note that the results below are not dependent on the form (43) we took, and are also obtained when the degrees of the polynomials  $p_n(w)$  are taken to be equal<sup>26</sup>.

We systematically considered linear homogeneous differential equations with polynomial coefficients (in  $w$ ) of increasing order. The degrees of the various polynomial coefficients are taken as large as possible. With such a strategy, the order of the homogeneous linear differential equation and the degrees of the polynomials are not on the same footing (the order is much smaller than the degrees and the order of a differential equation is a much more fundamental character of the differential equation). For  $N$  terms in the series, one then explores all the linear differential equations reproducing these terms with  $(q, \mu)$  staying on the hyperbola (44).

Let us fix  $q = 4$  and compute the linear differential equation for increasing values of  $\mu$ . The polynomial in front of the highest derivative is solved for the variable  $w$ . For  $\mu = 6$ , one gets  $w = -1/2$  with three correct digits,  $w = -1/4$  (double) with five digits,  $w = +1/4$  (double) with four digits, and  $w = 1$  with two digits. With these values of  $w$ , we get four other solutions. As  $\mu$  increases, the number of correct digits of the roots  $w = -1/2$ ,  $w = -1/4$ ,  $w = 1/4$  and  $w = 1$  increases. For  $\mu = 15$ , the values become correct to, respectively, 8, 13, 14 and 6 digits. For  $\mu = 28$ , they are correct to 14, 20, 26 and 13 digits. The roots  $w = \pm 1/4$  still have multiplicity 2. One observes that for  $q = 4$  and  $\mu = 28$ , the number of series coefficients used is just 150 terms. Further, as  $\mu$  increases, the other solutions

<sup>24</sup> This suggests considering Fuchsian equations with quite large degrees for the polynomial coefficients, compared to the order of the homogeneous linear differential equation.

<sup>25</sup> At this step, one can certainly consider using the differential-Padé approximation calculations developed by Rehr, Joyce and Guttman [41], or similar differential-Padé approximations considered by other authors [42].

<sup>26</sup> The form (43) assures  $w = \infty$  as a regular singularity of the differential equation.

increase in number ( $p_q(w)$  has  $q + \mu$  roots) and do not converge to stable values. At around  $\mu \sim 19$  a root oscillating around  $-1/4$  appears. One can imagine that the root  $w = -1/4$  is going to be of multiplicity 3. For the root  $w = +1/4$ , one has to wait until  $\mu = 28$  to see this happen.

The differential equations we obtain are quite cumbersome and carry as much information (in the number of unknowns) as the  $N$  terms used. This is, then, just another way to *encode* the information contained in the  $N$  terms. What is remarkable in this procedure is the appearance of the singularities with increasingly correct digits and the fact that they converge to the correct multiplicity as  $\mu$  increases. What is more remarkable is *the appearance of the other unexpected singularities*  $1 + 3w + 4w^2 = 0$  which were obtained with three digits at ( $q = 4, \mu = 2$ ), and with nine correct digits at ( $q = 6, \mu = 35$ ).

Within this systematic approximation scheme, we actually discovered, at smaller orders than the actual one (namely order 7), the existence of the unexpected quadratic numbers singularities  $1 + 3w + 4w^2 = 0$ , with an extremely good level of confidence. This indicates that such a systematic procedure was probably converging towards some exact result, which we actually found with the next orders. This method is obviously applicable to any series that satisfies a linear homogeneous differential equation. Actually we will show, in a forthcoming publication, that we can actually find the singularities of the successive  $\chi^{(n)}$  even when we are not able to find the ODEs satisfied by the  $\chi^{(n)}$ .

## 5. Conclusion

Considering the isotropic Ising square lattice model susceptibility, we focused on the third-order component  $\chi^{(3)}$  in the form given by Nickel [6]. We used an expansion in the variables  $x_j$  that appear in the integrand of the double integral defining  $\chi^{(3)}$  instead of the variable  $w$  (or  $s$ ). The angular integration becomes straightforward thanks to the remarkable formula we derived for the quantity  $y_j x_j^n$ . This formula is a Fourier series carrying one summation index and where the coefficients are *non-terminating*  ${}_4F_3$  hypergeometric functions. We succeeded, in this way, in writing  $\tilde{\chi}^{(3)}$  as a fully integrated expansion, containing a few sums of products of three such hypergeometric functions. For  $\tilde{\chi}^{(2)}$ , the sums bear on products of two hypergeometric functions but due to remarkable identities, they ‘fuse’ into a *single hypergeometric function* giving the known result (see appendices E and F). We note that these *fusion identities* on hypergeometric functions occurring for  $\tilde{\chi}^{(2)}$ , may be the sign of deep structures and symmetries. We have not yet recognized a similar mechanism for  $\tilde{\chi}^{(3)}$ , but it seems plausible.

We used the fully integrated multisum giving  $\chi^{(3)}$  to generate a long series of coefficients with a *polynomial time* ( $N^4$ ) algorithm. We recall that the series coefficients are obtained *without any numerical approximation*. We were able to obtain the series up to order 490 in the variable  $w$ , and used it to find the seventh-order linear differential equation (34) satisfied by  $\chi^{(3)}$ . This limitation to 490 terms is a reflection of the minimal computer resources used. Much longer series can readily be obtained. This differential equation, which is of Fuchsian type, is highly non-trivial and structured. This result shows that quite involved sums of products of three hypergeometric functions can be solutions of quite simple linear differential equations.

The ferromagnetic, antiferromagnetic, zero or infinite temperature points, the non-physical and Nickel singularities are all regular singular points of the differential equation. The Fuchsian differential equation shows other simple singularities, which are not of Nickel’s form (10), and are lying on the circles  $|s| = \sqrt{2}$  and  $|s| = \frac{1}{\sqrt{2}}$ . We also note the occurrence of a polynomial of degree 28 in  $w$  whose roots are *apparent singularities* of the Fuchsian

differential equation. We also saw that any slight deformation of the Fuchsian differential equation drastically modifies the growth of the coefficients in the series expansions of the solutions, confirming the highly selective character of this ordinary differential equation.

The behaviour of the local solutions of the Fuchsian differential equation at each regular singular point is sketched and shows the occurrence of logarithmic terms up to  $\log^2$ . The question of whether these terms occur in the physical solution  $\tilde{\chi}^{(3)}$  is of the utmost importance and, particularly, for the new singularities  $1 + 3w + 4w^2 = 0$  not previously known<sup>27</sup>. We will report on the integration constants corresponding to the physical solution  $\tilde{\chi}^{(3)}$  in a forthcoming publication.

The Fuchsian differential equation has two simple rational, and algebraic, solutions enabling one to give the factorization of the differential operator corresponding to the Fuchsian differential equation. The solution is a linear combination of a rational solution, namely  $w/(1 - 4w)$ , and of a solution of a sixth-order homogeneous linear differential equation.

Recall that the variable  $w$  we used deals with both high- and low-temperature cases on an equal footing. Furthermore, the key ingredient in obtaining (25), and finally (34), is the Fourier expansion of  $yx^n$ , a quantity appearing in any  $\chi^{(n)}$ . So the expansion method we used is not specific to the third contribution  $\chi^{(3)}$  and can be generalized *mutatis mutandis* to the other  $\chi^{(n)}$ , and in particular those with  $n$  even, associated with the *low-temperature* susceptibility (in appendix E we discuss the form of  $\chi^{(2)}$  in this variable). The next step is clearly the evaluation of  $\chi^{(4)}$  which can be seen [6, 7] to be a function of  $s^2$ , and, in fact, a function of  $w^2$ . This gives some hope of finding the corresponding Fuchsian differential equation.

The Fuchsian differential equation, satisfied by  $\chi^{(3)}$ , is certainly an important step towards the understanding of the analytical structure of isotropic Ising square lattice model susceptibility. Along these lines, one can easily imagine finding the Fuchsian differential equation satisfied by  $\chi^{(3)}$  for the *isotropic triangular* Ising model. However, recalling the nice and simple exact results we displayed in the introduction on the *anisotropic* square Ising model, on the anisotropic triangular Ising model and on the checkerboard Ising model, it is tempting for such *anisotropic* models to seek for the homogeneous ‘Fuchsian partial differential equation’ (generalizing our Fuchsian differential equation restricted to isotropic models) in the corresponding two, three or four, high-temperature variables  $t_1, t_2, t_3$  and  $t_4$ . No doubt the modulus  $k$  of the elliptic functions parametrizing the Ising model (see (7)) should play a special role in writing down a simple enough expression for this ‘Fuchsian PDE’. In this anisotropic, partial differential, framework one can also imagine that generalizations of hypergeometric functions to *several variables* could occur [43–45]. Having such a homogeneous ‘Fuchsian PDE’, it will be extremely interesting to see how this Fuchsian PDE can be invariant<sup>28</sup> (or covariant since it is homogeneous) under the whole set of *birational transformations* [48–50] generated by the inversion relation symmetries (5), (6) or (8), combined with the geometrical symmetries.

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<sup>27</sup> For  $1 + 3w + 4w^2 = 0$  singularities, in section 3, we gave arguments in favour of its absence in  $\tilde{\chi}^{(3)}$ .

<sup>28</sup> See, for instance, section 5 in [45], or section 5 in [46], or section 3 in [47], for birational transformations preserving partial differential equations or systems.

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## Appendix A

In this appendix, we give the various formulae used to obtain (25). We use  $\langle \cdot \cdot \cdot \rangle$  to mean the normalized angular integrations  $\prod_i \frac{d\phi_i}{2\pi}$ . The variables  $x$  and  $y$  are defined as in (14). From (17), one gets

$$\langle yx^n \cos(p\phi) \rangle = w^p a(n, p) = w^p a(p, n). \quad (\text{A.1})$$

Recall that  $a(n, p)$  is defined in (18) in terms of  ${}_4F_3$  hypergeometric functions.

Define the following functions:

$$\begin{aligned} g(n, p) &= \sum_{i=0}^{\infty} (i+1) w^i a(n+i+1, p) = w^{-p} \left\langle \frac{yx^{n+1}}{(1-wx)^2} \cos(p\phi) \right\rangle, \\ v(n, p) &= \sum_{i=0}^{\infty} w^i a(n+i+1, p) = w^{-p} \left\langle \frac{yx^{n+1}}{1-wx} \cos(p\phi) \right\rangle. \end{aligned} \quad (\text{A.2})$$

From the integral representations, one has

$$\begin{aligned} a(n+1, p) &= v(n, p) - wv(n+1, p), \\ v(n, p) &= g(n, p) - wg(n+1, p). \end{aligned}$$

The following integrals can, then, be computed,

$$\begin{aligned} \langle yx^n \cot(\phi/2) \sin(k\phi) \rangle &= y_0 x_0^n - w^k (a(k, n) + 2wv(k, n)), \\ \langle yx^n \cot(\phi/2)^2 \cos(k\phi) \rangle &= -2ky_0 x_0^n - w^k (a(k, n) + 4wg(k, n)) + y_0 x_0^n \left\langle \frac{1}{\sin(\phi/2)^2} \right\rangle. \end{aligned} \quad (\text{A.3})$$

where  $x_0$  and  $y_0$  are the variables defined in (14) and taken at  $\phi = 0$ .

Some integrals appearing in the intermediate steps are ( $k \geq 1$ )

$$\left\langle \frac{1 - \cos(k\phi)}{\sin(\phi/2)^2} \cos(p\phi) \right\rangle = \begin{cases} 2(k-p), & k > p \\ 0, & k \leq p \end{cases} \quad (\text{A.4})$$

$$\langle \cot(\phi/2) \sin(k\phi) \cos(p\phi) \rangle = \begin{cases} 1, & k > p \\ 1/2, & k = p \\ 0, & k < p. \end{cases} \quad (\text{A.5})$$

We now turn to the ‘artificial’ singularity appearing on the right-hand side of (A.3). This term contributes to the total integrand (11) as

$$\left\langle \frac{1}{\sin(\phi/2)^2} \right\rangle \left( d(0) + 2 \sum_{p=1}^{\infty} w^{3p} d(p) \right) \quad \text{with} \quad (\text{A.6})$$

$$\begin{aligned} d(p) &= y_0 x_0^p (S(p+2, p) - S(p+1, p+1)), \\ S(p, q) &= a(p, 0)a(q, 0) + 2 \sum_{k=1}^{\infty} w^{2k} a(p, k)a(q, k). \end{aligned} \quad (\text{A.7})$$

Noting that

$$S(p, q) = \langle y^2 x^{p+q} \rangle = \langle yx^p yx^q \rangle \quad (\text{A.8})$$

it is straightforward to see the cancellation of  $d(p)$ , and thus of (A.6) as it should.

Note that formula (17) has been used extensively in the following appendices, and each time we have an expression similar to (A.8), we manage to write it in terms of (17). Another trick used throughout the appendices is the technique of switching to and fro between the sums and the integral representation, and the judicious selection of the correct place to use (15).

## Appendix B

Expansion of (11) in terms of  $y_j x_j^n$ , using (17) and the integration rules given in appendix A, gives for  $\tilde{\chi}^{(3)}$ ,

$$\tilde{\chi}^{(3)} = 8w^5 \left( I(0) + 2 \sum_{p=1}^{\infty} w^{3p} I(p) \right), \quad (\text{B.1})$$

with

$$\begin{aligned} I(p) &= \frac{1}{w^2} \langle y_1 y_2 y_3 (x_1 x_2 x_3)^p H^{(3)} \rangle \\ &= C(p) + w^2 F(0, p) + 2w^2 \sum_{k=1}^{\infty} w^{3k} F(k, p), \end{aligned} \quad (\text{B.2})$$

where  $H^{(3)}$  is taken in the form (21).  $F(k, p)$  consists of sums of cubic terms of the hypergeometric function (18), and can be written in terms of this hypergeometric function and the auxiliary functions  $g(k, p)$  and  $v(k, p)$  defined in appendix A, as

$$\begin{aligned} F(k, p) &= g(k+1, p)(a(k, p+1)^2 - a(k, p+2)a(k, p)) + a(k, p+2)v(k, p)^2 \\ &\quad + a(k, p)v(k, p+1)^2 - 2a(k, p+1)v(k, p)v(k, p+1). \end{aligned} \quad (\text{B.3})$$

The function  $C(p)$ , written as

$$C(p) = -\frac{1}{2}y_0^2 x_0^{2p} C_1(p) + y_0 x_0^p C_2(p), \quad (\text{B.4})$$

consists of a linear term in the  $a$ ,

$$C_1(p) = a(0, p+2) + x_0^2 a(0, p) - 2x_0 a(0, p+1),$$

and a quadratic term in the  $a$ ,

$$C_2(p) = \sigma_0(p) + 2w\sigma_1(p) + 2wx_0\sigma_2(p), \quad (\text{B.5})$$

where the sums  $\sigma_i(p)$  ( $i = 0, 1, 2$ ) are given by

$$\begin{aligned} \sigma_0(p) &= \sum_{k=1}^{\infty} (k+1)w^{2k}(a(k, p+1)^2 - a(k, p+2)a(k, p)), \\ \sigma_1(p) &= \sum_{k=1}^{\infty} w^{2k}(a(k, p+1)v(k, p+1) - a(k, p+2)v(k, p)), \\ \sigma_2(p) &= \sum_{k=1}^{\infty} w^{2k}(a(k, p+1)v(k, p) - a(k, p)v(k, p+1)). \end{aligned}$$

To get the final form of  $\tilde{\chi}^{(3)}$ , further manipulations are made on that part of  $I(0)$  and  $I(p)$  in (B.1) containing the  $C$ . The aim is to get *only one summation* instead of two. We show in appendix C how to obtain the part of (B.1) containing the  $C$ . It reads

$$C(0) + 2 \sum_{p=1}^{\infty} w^{3p} C(p) = \xi_1 + \sigma_C \quad (\text{B.6})$$

where

$$\begin{aligned}\xi_1 &= y_0 C(0) + \frac{y_0^3}{w} (J_0(0) - a(1, 0)) \\ \sigma_C &= 2y_0^3 \sum_{n=1}^{\infty} w^{3n-2} x_0^{n-1} (J_0(n) - w(1 - wx_0)J_1(n))\end{aligned}\quad (\text{B.7})$$

where

$$\begin{aligned}J_0(n) &= a(0, n)^2 - w^2 a(1, n)^2, \\ J_1(n) &= (a(0, n) + wa(1, n))(a(0, n+1) - x_0 a(0, n)).\end{aligned}\quad (\text{B.8})$$

We have decomposed the term  $\sigma_C$  as

$$\sigma_C = \xi_2 + 2w^8 \sigma$$

with

$$\begin{aligned}\xi_2 &= 2y_0^3 (w(J_0(1) - w(1 - wx_0)J_1(1)) \\ &\quad + x_0 w^4 (J_0(2) - w(1 - wx_0)J_1(2)) + x_0^2 w^7 a(0, 3)^2),\end{aligned}$$

and

$$\sigma = y_0^3 \sum_{p=0}^{\infty} w^{3p} x_0^{p+2} ((wx_0 - 1)J_1(p+3) - wa(1, p+3)^2 + w^2 x_0 a(0, p+4)^2). \quad (\text{B.9})$$

Collecting all previous results, and after some manipulations,  $\tilde{\chi}^{(3)}$  can then be written as

$$\tilde{\chi}^{(3)} = 8w^9 (\tilde{\chi}_{cl}^{(3)} + 2w^4 \Xi),$$

where

$$\tilde{\chi}_{cl}^{(3)} = \frac{1}{w^4} (\xi_1 + \xi_2) + \frac{F(0, 0)}{w^2} + 2w(F(1, 0) + F(0, 1)), \quad (\text{B.10})$$

and

$$\Xi = \sigma + \sum_{p=0}^{\infty} w^{3p} (F(0, p+2) + F(p+2, 0)) + 2 \sum_{k=0}^{\infty} \sum_{p=0}^{\infty} w^{3k+3p} F(k+1, p+1). \quad (\text{B.11})$$

Appendix D gives the detailed derivation of the closed form (27) from (B.10).

### Appendix C

The purpose in this appendix is to derive relation (B.6). From the definition of the variables  $x_n$  and  $Z_n = \exp(i\phi_n)$ , one can deduce the following identity:

$$(Z_1 - Z_2) \frac{w^2 x_1 x_2}{1 - w^2 x_1 x_2} = w(x_2 - x_1) \frac{Z_1 Z_2}{1 - Z_1 Z_2}. \quad (\text{C.1})$$

The first step is to simplify the expression of  $C_2(p)$  defined in (B.5). Taking the integral representation of  $a(k, n)$  and  $v(k, n)$  ( $n = p, p+1, p+2$ ), and summing on the index  $k$ , the sums  $\sigma_i(p)$  become

$$\begin{aligned}\sigma_0(p) &= w^{-2p} \left\langle y_1 y_2 \frac{x_1 x_2}{1 - w^2 x_1 x_2} \frac{2 - w^2 x_1 x_2}{1 - w^2 x_1 x_2} (Z_1 Z_2)^p (Z_1 Z_2 - Z_1^2) \right\rangle, \\ \sigma_1(p) &= w^{-2p} \left\langle y_1 y_2 \frac{x_1 x_2}{1 - w^2 x_1 x_2} \frac{x_2}{1 - wx_2} (Z_1 Z_2)^p (Z_1 Z_2 - Z_1^2) \right\rangle, \\ \sigma_2(p) &= \frac{1}{2} w^{-2p} \left\langle y_1 y_2 \frac{x_1 x_2}{1 - w^2 x_1 x_2} \frac{1 + wx_2}{1 - wx_2} (Z_1 Z_2)^p (Z_1 - Z_2) \right\rangle.\end{aligned}$$

The sum  $C_2(p)$  (sum of the  $\sigma$ ) becomes

$$C_2(p) = w^{-2p} \left( \left\langle y_1 y_2 \frac{x_1 x_2}{(1 - w^2 x_1 x_2)^2} (Z_1 Z_2)^p \left( -\frac{1}{2} (Z_2 - Z_1)^2 \right) \right\rangle + \left\langle y_1 y_2 \frac{1 + w x_2}{1 - w x_2} \frac{x_1 x_2}{(1 - w^2 x_1 x_2)} (Z_1 Z_2)^p (Z_1 - w x_0) (Z_2 - Z_1) \right\rangle \right), \quad (\text{C.2})$$

where, for the first term in the brackets on the right-hand side of (C.2), the quantity  $Z_1 Z_2 - Z_1^2$  has been replaced by  $-\frac{1}{2}(Z_2 - Z_1)^2$  due to the symmetry of the rest of the integrand in the integration variables. Using (C.1) and the following relation,

$$\left\langle \frac{y}{x} Z^{n+1} \right\rangle = w^{n+3} a(1, n+1), \quad n \geq 0$$

then expanding in the  $Z$  variables, working out the integration over the angles and making use of the identities

$$\left\langle y \frac{1 + w x}{1 - w x} \cos(p\phi) \right\rangle = \left\langle y \frac{1 + w x}{1 - w x} Z^p \right\rangle = y_0 x_0^p w^p, \quad (\text{C.3})$$

$$v(0, p) = \frac{1}{2w} (y_0 x_0^p - a(0, p)), \quad (\text{C.4})$$

one obtains

$$C_2(p) = S_0(p) + S_1(p) + \sum_{j=1}^{\infty} w^{2j-1} y_0 x_0^{j+p} J_2(j+p), \quad (\text{C.5})$$

with

$$S_0(p) = \sum_{j=1}^{\infty} j w^{2j} J_0(j+p+1), \quad S_1(p) = \sum_{j=1}^{\infty} w^{2j-1} J_1(j+p).$$

$J_0$  and  $J_1$  are defined in (B.8), while  $J_2$  reads

$$J_2(n) = x_0(a(0, n) - w a(1, n)) - (a(0, n+1) - w a(1, n+1)).$$

$C_2(p)$  is now written as a sum of contributions quadratic in  $a$  and linear in  $a$  (the last term). The latter will be shown to cancel  $C_1(p)$  identically in (B.4). Using the following relation,

$$2w^2 a(1, n) = a(0, n) - a(0, n-1) - w^2 a(0, n+1) \quad (\text{C.6})$$

one obtains the identity

$$J_2(n) = \frac{1}{2w x_0} (C_1(n-1) - w^2 x_0 C_1(n)).$$

The last sum in (C.5) simply reads

$$\sum_{j=1}^{\infty} w^{2j-1} y_0 x_0^{j+p} J_2(j+p) = \frac{1}{2} y_0 x_0^p C_1(p).$$

Collecting terms in (B.4), one gets

$$C(p) = y_0 x_0^p (S_0(p) + S_1(p)) \quad (\text{C.7})$$

Some manipulations, such as shifts in the indices of the sums, allow us to evaluate two summations and to cast the quantity of interest (B.6) as

$$C(0) + 2 \sum_{p=1}^{\infty} w^{3p} C(p) = y_0 C(0) - 2w y_0^3 \xi_0 + \sigma_C. \quad (\text{C.8})$$

Here  $\xi_0$  is a sum that can be worked out using (15), (17), (A.7) and (A.8):

$$\xi_0 = \sum_{n=0}^{\infty} w^{2n} J_0(n+1) = \frac{1}{2w^2} (a(1, 0) - J_0(0)). \quad (\text{C.9})$$

This ends the derivation of (B.6) given in appendix B.

## Appendix D

In the closed part (B.10), there is still a summation to be done in the term  $\xi_1$  defined in (B.7), namely the evaluation of  $C(0)$ . For this purpose, we consider  $C(p)$  in the form (C.7).

To evaluate  $S_0(0)$ , one shifts the index of summation to cast it as

$$S_0(0) = \sum_{n=1}^{\infty} (n-1)w^{2n-2} J_0(n) = \widehat{S}_0(0) - \xi_0, \quad (\text{D.1})$$

with

$$\widehat{S}_0(0) = \sum_{n=1}^{\infty} n w^{2n-2} J_0(n).$$

At this point, note that  $x^n$  has the following Fourier expansion,

$$x^n = b(n, 0) + 2 \sum_{k=1}^{\infty} w^k b(n, k) \cos k\phi,$$

where  $b(k, n)$  reads (with  $m = k + n$ ):

$$b(k, n) = \binom{m-1}{k} {}_4F_3 \left( \frac{(1+m)}{2}, \frac{(1+m)}{2}, \frac{(2+m)}{2}, \frac{m}{2}; 1+k, 1+n, 1+m; 16w^2 \right) \quad (\text{D.2})$$

and satisfies

$$\begin{aligned} b(i, p) &= a(i-1, p) - w^2 a(i+1, p), & i \geq 1 \\ nb(1, n) &= b(n, 1). \end{aligned} \quad (\text{D.3})$$

Using (D.3) and the symmetry of  $a(k, p)$  in  $k$  and  $p$ ,  $\widehat{S}_0(0)$  becomes

$$\widehat{S}_0(0) = \frac{1}{2} \sum_{n=1}^{\infty} w^{2n-2} (a(n, 0)b(n, 1) - 2nw^2 a(n, 1)^2 + na(n, 0)(a(n, 0) + w^2 a(n, 2))),$$

and, in integral form, we obtain

$$\begin{aligned} \widehat{S}_0(0) &= \frac{1}{2w^2} \left\langle y_1 \frac{wx_1x_2}{1-w^2x_1x_2} \cos(\phi_2) \right\rangle \\ &\quad + \frac{1}{2w^2} \left\langle y_1y_2 \frac{w^2x_1x_2}{(1-w^2x_1x_2)^2} 2 \cos(\phi_2) (\cos(\phi_2) - \cos(\phi_1)) \right\rangle. \end{aligned}$$

Using the identity (C.1) and relation (15),  $\widehat{S}_0(0)$  simply becomes

$$\widehat{S}_0(0) = \frac{1}{2w} \langle y_1y_2x_2 \cos(\phi_2) \rangle = \frac{1}{2} a(0, 0)a(1, 1).$$

For the evaluation of  $S_1(p)$ , we make use of (C.6) to get

$$\begin{aligned} S_1(0) &= -\frac{1}{2} \sum_{n=1}^{\infty} w^{2n-2} (a(0, n+1)(a(0, n-1) + w^2 a(0, n+1)) \\ &\quad + a(0, n)(2x_0w(a(0, n) + wa(1, n)) - (1+2w)a(0, n+1))). \end{aligned}$$

Using (17), (A.7), (A.8) and the useful identities

$$\begin{aligned} \langle y^2 \cos(\phi) \rangle &= 2wa(0, 0)a(0, 1) + 2 \sum_{n=1}^{\infty} w^{2n+1} a(0, n)a(0, n+1), \\ \langle y^2 \cos(2\phi) \rangle &= w^2 a(0, 1)^2 + 2 \sum_{n=1}^{\infty} w^{2n} a(0, n-1)a(0, n+1), \end{aligned}$$

we obtain

$$S_1(0) = \frac{x_0}{2w}((a(0, 0) + wa(1, 0))a(0, 0) - \langle y^2(1 + wx) \rangle) \\ + \frac{1}{4w^3} \langle y^2 \cos(\phi)(1 - 2w \cos(\phi) + 2w) \rangle \\ + \frac{1}{4w^2} (3w^2 a(0, 1)^2 + a(0, 0)^2 - 2(1 + 2w)a(0, 0)a(0, 1)).$$

With relation (15) and using (C.4), we obtain

$$\langle y^2(1 + wx) \rangle = v(0, 0) = \frac{y_0 - a(0, 0)}{2w}.$$

With the following relation,

$$1 - 2w \cos(\phi) = \frac{1}{x} + w^2 x,$$

and using (C.3), we get

$$\langle y^2 \cos(\phi)(1 - 2w \cos(\phi) + 2w) \rangle = wy_0 x_0$$

and finally,

$$S_1(0) = \frac{1}{4w^2} (x_0 a(0, 0) + (1 + 2wx_0)a(0, 0)^2 + 3w^2 a(0, 1)^2 \\ + 2(w^2 x_0 - 1 - 2w)a(0, 0)a(0, 1)). \tag{D.4}$$

The last step in calculating the closed form (B.10) is to explicitly evaluate the terms  $F(0, 0)$ ,  $F(1, 0)$  and  $F(0, 1)$ . This can be done with the help of appendix A. Note that  $g(1, 1)$  and  $g(0, 0)$  can be written as

$$g(1, 1) = \frac{1}{2w^2} (g(1, 0) - 2g(0, 0) + 2v(0, 0) - a(1, 0)), \\ g(0, 0) = \frac{1}{4w} \left( \frac{\tilde{E}}{1 - 4w} - \tilde{K} \right),$$

with  $\tilde{E}$  and  $\tilde{K}$  being defined in (27).

Collecting all the previous results, expanding in the basis of  $\tilde{E}$  and  $\tilde{K}$  functions, one obtains relation (27), where the polynomials  $q_{i,j}$  and  $p_{i,j}$  are given by

$$q_{00} = -96w^6 + 276w^5 - 120w^4 + 144w^3 - 64w^2 + 32w - 16, \\ q_{10} = 128w^7 - 832w^6 - 792w^5 + 740w^4 - 680w^3 + 295w^2 + 32w - 16, \\ q_{01} = 68w^5 - 212w^4 - 120w^3 + 89w^2 - 96w + 48, \\ q_{20} = 960w^7 - 416w^6 + 1924w^5 - 1048w^4 - 170w^3 + 98w^2 + 3w - 2, \\ q_{11} = 584w^5 - 256w^4 + 744w^3 - 386w^2 - 38w + 20, \\ q_{02} = 82w^3 - 32w^2 + 67w - 34, \\ q_{30} = (4w - 1)^2(4w + 1)^2(2w - 1)(2w + 1)w^2, \\ q_{21} = -(4w - 1)(4w + 1)(4w^3 - 28w^2 - 2w + 5)w^2, \\ q_{12} = -8(6w^3 - 9w^2 - w + 1)w^2, \\ q_{03} = -2(3w - 2)w^2, \\ p_{00} = 528w^6 - 464w^5 + 248w^4 - 272w^3 + 96w^2 - 64w + 16, \\ p_{10} = -1280w^7 + 352w^6 + 1984w^5 - 1504w^4 + 1284w^3 - 264w^2 - 64w + 16,$$

$$\begin{aligned}
p_{01} &= -320w^5 + 208w^4 + 284w^3 - 184w^2 + 192w - 48, \\
p_{20} &= 256w^8 - 1280w^7 + 2320w^6 - 4144w^5 + 928w^4 + 372w^3 - 98w^2 - 7w + 2, \\
p_{11} &= 384w^6 - 896w^5 + 960w^4 - 1548w^3 + 356w^2 + 78w - 20, \\
p_{02} &= 56w^4 - 120w^3 + 94w^2 - 135w + 34.
\end{aligned}$$

## Appendix E

This appendix contains the details of evaluation of  $\chi^{(2)}$  using the  $yx^n$  expansion method. One should note, however, that  $\chi^{(2)}$  can be obtained in a straightforward manner by direct integration.

One writes  $\chi^{(2)}$  as [7]

$$\chi^{(2)} = (1 - s^{-4})^{1/4} \tilde{\chi}^{(2)} \quad (\text{E.1})$$

where

$$\tilde{\chi}^{(2)} = 4w^4 \left\langle y^2 x^2 \frac{1 + w^2 x^2}{(1 - w^2 x^2)^3} (1 - \cos(2\phi)) \right\rangle.$$

One defines

$$A(k, n) = A(-k, n) = w^{|k|} a(|k|, n).$$

With the variable  $Z = \exp(i\phi)$ , the expansion of  $yx^n$  is written as

$$yx^n = \sum_{k=-\infty}^{\infty} A(k, n) Z^k = \sum_{k=-\infty}^{\infty} A(k, n) Z^{-k}.$$

Expanding in  $x$ ,  $\tilde{\chi}^{(2)}$  becomes

$$\tilde{\chi}^{(2)} = 4w^4 \sum_{n=0}^{\infty} (n+1)^2 w^{2n} \langle y^2 x^{2n+2} (1 - \cos(2\phi)) \rangle. \quad (\text{E.2})$$

Now write  $\langle y^2 x^{2n+2} (1 - \cos(2\phi)) \rangle$  as  $\langle yx^{n_1} yx^{n_2} (1 - \cos(2\phi)) \rangle$  with  $n_1 + n_2 = 2n + 2$ . One has

$$\begin{aligned}
\langle yx^{n_1} yx^{n_2} (1 - \cos(2\phi)) \rangle &= \sum_{k_1, k_2=-\infty}^{\infty} A(k_1, n_1) A(k_2, n_2) \langle (1 - Z^2/2 - Z^{-2}/2) Z^{k_1+k_2} \rangle \\
&= \sum_{k=-\infty}^{\infty} A(k, n_1) (A(k, n_2) - A(k+2, n_2)/2 - A(k-2, n_2)/2).
\end{aligned} \quad (\text{E.3})$$

Some manipulations give

$$\langle yx^{n_1} yx^{n_2} (1 - \cos(2\phi)) \rangle = \sum_{k=1}^{\infty} (A(k-1, n_1) - A(k+1, n_1)) (A(k-1, n_2) - A(k+1, n_2)). \quad (\text{E.4})$$

Coming back to the definition (E.2) of  $A(k, n)$ , one recognizes in (E.4) the function  $b(k, n)$  defined in (D.2).  $\tilde{\chi}^{(2)}$  then becomes (recall that  $n_1 + n_2 = 2n + 2$ )

$$\tilde{\chi}^{(2)} = 4w^4 \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} (n+1)^2 w^{2n+2k} b(k+1, n_1) b(k+1, n_2).$$

One thus has many equivalent forms for  $\tilde{\chi}^{(2)}$  depending on the partition  $n_1 + n_2 = 2n + 2$ . The above sums merge into a *single* hypergeometric function,

$$\tilde{\chi}^{(2)} = 4w^4 {}_2F_1\left(\frac{5}{2}, \frac{3}{2}; 3; 16w^2\right), \tag{E.5}$$

which is the well-known result [1]:

$$\tilde{\chi}^{(2)} = \frac{1}{6\pi} \left( \frac{1 - 8w^2}{1 - 16w^2} E(4w) - K(4w) \right). \tag{E.6}$$

**Appendix F**

Here we give an alternative derivation of (E.5), performed this time with another expansion of the quantity  $yx^n$ , which underlines the role played by some *fusion relations* on hypergeometric functions.

$yx^n$  can be written as

$$yx^n = \sum_{j=0}^{\infty} (-4w)^j \binom{n+j}{n} \sin\left(\frac{\phi}{2}\right)^{2j} {}_2F_1(n+1/2, n+j+1; 2n+1; 4w). \tag{F.1}$$

Taking  $\tilde{\chi}^{(2)}$  in the form (E.2), writing  $y^2x^{2n+2}$  as  $yx^{n+1}yx^{n+1}$ , using the expansion (F.1) for each  $yx^n$ , the angular integration gives

$$\begin{aligned} \tilde{\chi}^{(2)} = 4w^4 \sum_{n, k_1, k_2=0}^{\infty} C(n, k_1, k_2) {}_2F_1\left(n + \frac{3}{2}, n + 2 + k_1; 2n + 3; 4w\right) \\ \times {}_2F_1\left(n + \frac{3}{2}, n + 2 + k_2; 2n + 3; 4w\right) \end{aligned} \tag{F.2}$$

where

$$C(n, k_1, k_2) = w^{2n+k_1+k_2} (-4)^{k_1+k_2} (n+1)^2 \frac{(3/2)_{k_1+k_2}}{(3)_{k_1+k_2}} \binom{n+1+k_1}{k_1} \binom{n+1+k_2}{k_2}$$

and  $(N)_m$  are the usual Pochhammer symbols. It is worth comparing (E.5) with (F.2). One sees, with this alternative expression for  $\chi^{(2)}$ , that the complexity of  $\chi^{(2)}$  has now been encapsulated in a single hypergeometric expression  ${}_2F_1(5/2, 3/2; 3; 16w^2)$ . In the holonomic approach developed in this paper, the occurrence of the prototype of holonomic functions, namely hypergeometric functions, is quite natural. These calculations also underline the important role the fusion identities [51] (see relation (1.9) in [51]) on hypergeometric functions, such as  $F = \sum CFF$ , can play in such calculations. This is probably the sign of quite deep structures, and symmetries, like the *fusion relations* encountered in CFT, or integrable models, and deeply connected with Yang–Baxter relations [52, 53].

At this point it is worth recalling that the fusion relation (F.2) is totally reminiscent of, for instance, the fusion relation (1.9) in [51],

$$\begin{aligned} {}_{r+t}F_{s+u} \left[ \begin{matrix} a_r, c_t \\ b_s, d_u \end{matrix} ; xw \right] = \sum_{n=0}^{\infty} \frac{(c_t)_n (e_k)_n (-x)^n}{(d_u)_n (f_m)_n (n+\gamma)_n n!} \\ \times {}_{k+t}F_{m+u+1} \left[ \begin{matrix} n + c_t, n + e_k \\ 2n + 1 + \gamma, n + d_u, n + f_m \end{matrix} ; x \right] \\ \times {}_{m+r+2}F_{k+s} \left[ \begin{matrix} -n, n + \gamma, a_r, f_m \\ b_s, e_k \end{matrix} ; w \right] \end{aligned}$$

where  $\gamma, e$  and  $f$  are arbitrary and  $a_r, c_t, \dots$  are  $r, t, \dots$  upper and lower parameters.

This fusion relation, of the type  $F(uv) = \sum CF(u)F(v)$ , gives a representation of a hypergeometric function of the product  $uv$ , as a sum of products of hypergeometric functions of  $u$  and hypergeometric functions of  $v$ . In this respect, relation (F.2) corresponds to particular cases of fusion relations  $F(uv) = \sum CF(u)F(v)$ , with  $u = v = 4w$ .

## Appendix G

To evaluate the sums in (25) in order to obtain our long series for  $\tilde{\chi}^{(3)}$ , substantial computing time is spent in the computation of the coefficients of the various functions  $a(k, p)$ ,  $g(k, p)$ ,  $v(k, p)$  and  $y_0x_0^p$ . While the series expansion of  $a(k, p)$  and  $y_0x_0^p$  simply read

$$a(k, p) = \sum_{j=0}^{\infty} w^{2j} \binom{k+p+2j}{j} \binom{k+p+2j}{j+k} \quad (\text{G.1})$$

$$y_0x_0^p = \sum_{j=0}^{\infty} w^j \binom{2p+2j}{j} \quad (\text{G.2})$$

the coefficients of the auxiliary function  $g(k, p)$  are given by recurrences of depth 3 with huge polynomials in  $k$ ,  $p$  and  $j$ . For series generation purposes, we have found it more efficient to use the following inhomogeneous recurrences between the coefficients of  $g(k, n)$  and  $a(k, n)$ .

Noting by  $C_g(k, p, i)$  the coefficient of  $w^i$  in the expansion of  $g(k, p)$  (and similarly for  $a(k, p)$  and  $v(k, p)$ ), the inhomogeneous recurrences read

$$0 = C_g(n+2, p, i) - 2C_g(n+1, p, i+1) + C_g(n, p, i+2) - \begin{cases} C_a(n+1, p, i/2+1), & i \text{ even} \\ 0, & i \text{ odd.} \end{cases} \quad (\text{G.3})$$

Once the coefficients of  $g(k, p)$  are found, those of  $v(k, p)$  are given by

$$C_v(n, p, i) = C_g(n, p, i) - C_g(n+1, p, i-1).$$

The following identities are useful for (G.3),

$$C_g(k, p, 0) = C_a(k+1, p, 0), \quad C_g(k, p, 1) = 2C_a(k+2, p, 0), \quad (\text{G.4})$$

$$C_g(1, p, i) = C_g(0, p, i+1) - \frac{1}{2} \binom{2p+2i+4}{i+2} + \begin{cases} \frac{1}{2}C_a(0, p, i/2+1), & i \text{ even} \\ 0, & i \text{ odd} \end{cases} \quad (\text{G.5})$$

where (G.5) is deduced from (C.4).

## Appendix H

Recall that the separation of  $\tilde{\chi}^{(3)}$  into a relatively simple closed form (26), a ‘hard to compute’ series  $\Xi_h$ , and a simpler one  $\Xi_s$ , is made for algorithmic considerations. Although this separation is not ‘natural’, it is tempting to seek immediately, as a first step, a linear differential equation for (26) which should be ‘simpler’ than  $\tilde{\chi}^{(3)}$ . Having two functions,  $f$  and  $g$ , satisfying two homogeneous linear differential equations (like the second-order differential equations satisfied by  $\tilde{K}$  and  $\tilde{E}$  (see (27)), there are some formal computer programs (gfun or others [54]) which enable one to build the homogeneous linear differential equation satisfied by the product  $f \cdot g$  or the sum  $f + g$ , and of course step-by-step, a (cubic) sum of products

like (26). For instance, from the two order-2 differential equations for  $\tilde{K}$  and  $\tilde{E}$ , one builds the order-4 differential equation of the product  $\tilde{K} \cdot \tilde{E}$  and the order-6 differential equation of the cubic term  $\tilde{K} \cdot \tilde{E}^2$ . The latter term (with a polynomial multiplying the highest derivative of degree 17), combined with its associated algebraic expression, gives an order-6 differential equation with a polynomial multiplying the highest derivative of degree 38. This step-by-step procedure gives more and more complicated linear differential equations. It seems pointless to give these extremely involved, and cumbersome, expressions. Just note the linear differential equations corresponding to the sum of the strictly cubic terms in  $\tilde{E}$  and  $\tilde{K}$  will be of order 20, the one for the strictly quadratic terms in  $\tilde{E}$  and  $\tilde{K}$  will be of order 18, of order 8 for the linear terms in  $\tilde{E}$  and  $\tilde{K}$ , and, of course, of order 1 for the algebraic part in (26), yielding a linear differential equation for (26) of order 47 and an *extremely large degree* 267 as a lower bound<sup>29</sup> This means that using a brute force approach based on series expansions, instead of using the closed form, would have required more than 12 500 coefficients for finding this homogeneous linear differential equation! As a consequence, it might look hopeless, at first sight, to seek a homogeneous linear differential equation for  $\tilde{\chi}^{(3)}$ .

From the series point of view, let us focus on the growth of the coefficients of the three series comprising  $\tilde{\chi}^{(3)}$ . The integer coefficients of  $w^{481}$  read, respectively, for the ‘closed’, ‘simple’, ‘hard’ and  $\tilde{\chi}^{(3)}/8w^9$  series,

$$\begin{aligned} C_{cl} &\simeq 24\,752.108 \times 4^{481}, & C_s &\simeq -25\,012.475 \times 4^{481}, \\ C_h &\simeq 271.423 \times 4^{481}, & C &\simeq 11.056 \times 4^{481}. \end{aligned}$$

One thus sees that the coefficients for  $\tilde{\chi}^{(3)}$  are actually obtained from mutual cancellations of much larger integers: the coefficients of  $\tilde{\chi}_{cl}^{(3)}$  and  $\Xi_s(w)$  are of the same order but of opposite signs, their sum,  $C_{cl} + C_s \simeq -260.366 \times 4^{481}$ , is of the same order as the coefficient of  $\Xi_h(w)$ , but of opposite sign, the total sum becoming the coefficient of  $\tilde{\chi}^{(3)}$ . The coefficient of  $w^{481}$  for the closed form  $\tilde{\chi}_{cl}^{(3)}$  is  $\simeq 2238.72$  times larger than the corresponding coefficient for  $\tilde{\chi}^{(3)}$ !

These points show that  $\tilde{\chi}^{(3)}$  seen as the sum (25) should be much simpler than the sum of its constituents. This is indeed what was discovered.

## References

- [1] Wu T T, McCoy B M, Tracy C A and Barouch E 1976 *Phys. Rev. B* **13** 316–74
- [2] Nappi C R 1978 *Nuovo Cimento A* **44** 392
- [3] Palmer J and Tracy C 1981 *Adv. Appl. Math.* **2** 329
- [4] Yamada K 1984 *Prog. Theor. Phys.* **71** 1416
- [5] Yamada K 1985 *Phys. Lett. A* **112** 456–8
- [6] Nickel B 1999 *J. Phys. A: Math. Gen.* **32** 3889–906
- [7] Nickel B 2000 *J. Phys. A: Math. Gen.* **33** 1693–711
- [8] Zenine N, Boukraa S, Hassani S and Maillard J M 2004 *J. Phys. A: Math. Gen.* **37** 9651–68 (*Preprint math-ph/0407060*)
- [9] Syozi I and Naya S 1960 *Prog. Theor. Phys.* **24** 829
- [10] Hansel D and Maillard J-M 1988 *J. Phys. A: Math. Gen.* **21** 213–25
- [11] Dhar D and Maillard J-M 1985 *J. Phys. A: Math. Gen.* **18** L383–8
- [12] Baxter R J 1982 *J. Stat. Phys.* **28** 1–41
- [13] Jaekel M T and Maillard J-M 1985 *J. Phys. A: Math. Gen.* **18** 641, 1229, 2271
- [14] Hansel D and Maillard J-M 1987 *Mod. Phys. Lett. B* **1** 145–53
- [15] Hansel D and Maillard J-M 1988 *Int. J. Mod. Phys. B* **2** 1447–62
- [16] Yang C N 1952 *Phys. Rev.* **85** 808–16
- [17] Chang C H 1952 *Phys. Rev.* **88** 1422

<sup>29</sup> Much larger than in the seventh-order Fuchsian equation given in [8] for  $\tilde{\chi}^{(3)}$  and recalled in the following (see (34)).

- [18] Hansel D, Maillard J M, Oitmaa J and Vergakis M J 1987 *J. Stat. Phys.* **48** 69–80
- [19] Guttman A J and Enting I G 1996 *Phys. Rev. Lett.* **76** 344–7
- [20] Lipshitz L 1989 *J. Algebra* **122** 354
- [21] Zeilberger D 1990 *J. Comput. Appl. Math.* **32** 321
- [22] Cartier P 2002 Fonctions polylogarithmes, nombres polyzétas et groupes pro-unipotents *Astérisque* **282** 137–73 (Sém. Bourbaki no 885)
- [23] Terasoma T 2002 *Invent. Math.* **149** 339–69 (Preprint AG/0104231)
- [24] Hoffman M E and Ohno Y 2003 *J. Algebra* **262** 332–47 (Preprint QA/0010140)
- [25] Oi S 2004 Representation of the Gauss hypergeometric function by multiple polylogarithms and relations of multiple zeta values Preprint NT/0405162
- [26] Ince H K 1927/1956 *Ordinary Differential Equations* (London/New York: Longmans/Dover)
- [27] Mugan U and Sakka A 1995 *J. Math. Phys.* **36** 1284–98
- [28] Painlevé P 1900 *Bull. Soc. Math. Phys. France* **28** 201–61
- [29] Kitaev A V 2001 Special functions of the isomonodromy type, rational transformations of spectral parameter, and algebraic solutions of the sixth Painlevé equation Preprint nlin/0102020
- [30] Barouch E, McCoy B M and Wu T T 1973 *Phys. Rev. Lett.* **31** 1409–11
- [31] Chazy J 1910 *C. R. Acad. Sci., Paris* **150** 456–8
- [32] Chazy J 1911 *Acta Math.* **34** 317–85
- [33] Conte R *The Painlevé Property, One Century Later (CRM Series in Mathematical Physics)* ed R Conte (Berlin: Springer)
- [34] Kruskal M D, Joshi N and Halburd R 1997 Analytic and asymptotic methods for nonlinear singularity analysis: a review and extensions of tests for the Painlevé property *Integrability of Nonlinear Systems (Pondicherry, India) (Lecture Notes in Physics vol 495)* ed B Grammaticos and K Tamizhmani (Berlin: Springer) pp 171–205
- [35] Orrick W P, Nickel B G, Guttman A J and Perk J H H 2001 *J. Stat. Phys.* **102** 795–841
- [36] Orrick W P, Nickel B G, Guttman A J and Perk J H H 2001 *Phys. Rev. Lett.* **86** 4120–3
- [37] McCoy B M and Wu T T 1980 *Phys. Rev. Lett.* **45** 675–8
- [38] Perk J H H 1980 *Phys. Lett. A* **79** 3–5
- [39] Jimbo M and Miwa T 1980 *Proc. Japan Acad. A* **56** 405  
Jimbo M and Miwa T 1981 *Proc. Japan Acad. A* **57** 347
- [40] McCoy B M and Wu T T 1981 *Nucl. Phys. B* **180** 89
- [41] Rehr J J, Joyce G S and Guttman A J 1980 *J. Phys. A: Math. Gen.* **13** 1587–602
- [42] Khan M H 2002 *J. Comput. Appl. Math.* **149** 457–68
- [43] Sasaki T 2001 *Kyushu J. Math.* **55** 1–21
- [44] Higashi K and Sasaki T 2004 *Kyushu J. Math.* **58** 105–20
- [45] Sasaki T and Yoshida M 2001 *J. Phys. A: Math. Gen.* **34** 2319–28
- [46] Sasaki T and Yoshida M 1999 *Proc. Japan Acad.* **75** 129–33
- [47] Sasaki T and Yoshida M 2000 *Kobe J. Math.* **17** 29–57
- [48] Maillard J M 1995 *Math. Comput. Modelling* **26** 169–225
- [49] Boukraa S, Maillard J-M and Rollet G 1995 *J. Stat. Phys.* **78** 1195–251
- [50] Boukraa S and Maillard J-M 2001 *J. Stat. Phys.* **102** 641–700 (Preprint hep-th/0003212)
- [51] Gasper G 1990 Using symbolic computer algebraic systems to derive formulae involving orthogonal polynomials and other special functions *Orthogonal Polynomials: Theory and Practice* ed P Nevai (Boston, MA: Kluwer) pp 163–79
- [52] Avan J, Maillard J-M, Talon M and Viallet C-M 1990 *Int. J. Mod. Phys. B* **4** 1895–912
- [53] Gomez C, Ruiz-Altaba M and Sierra G 1996 Duality in conformal field theories *Quantum Groups in Two-dimensional Physics (Cambridge Monographs on Mathematical Physics)* (Cambridge: Cambridge University Press) chapter 9
- [54] Mgfuns's project: <http://algo.inria.fr/chyzak/mgfun.html>; gfun (generating functions package): <http://algo.inria.fr/libraries>