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LETTER TO THE EDITOR

Analysis of a sum of modified remnant functions

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Abstract. The analysis of a sum of modified remnant functions, $P^{\alpha}_{\sigma,\tau}(z)=\frac{1}{2}\{R^{\alpha}_{\sigma,\tau}(z)+R^{-\alpha}_{\sigma,\tau}(z)\}$, where $\tau=0$, σ is half-odd integer, $0\leq\alpha<1$ and z complex, is presented. An analytical expression for $z\neq 0$ and $|\arg z|<\pi$ is obtained as well as a power expansion valid for all z. The behaviour of $P^{\alpha}_{\sigma,\tau}(z)$ as $|z|\to\infty$ and $z\to 0$ is also obtained.

The remnant functions, $R_{\sigma,\tau}(z)$, have been introduced and analysed in detail for arbitrary real σ and τ and for complex z by Fisher and Barber (1972). These functions arise, for example, in the analysis of the spherical constraint in the critical region of the d-dimensional spherical model (Barber and Fisher 1973). The remnant functions entering in this analysis arise as part of the scaling functions. They are of the form $R_{1/2(d-1),0}(z)$ with $d\geq 3$. The remnant function $R_{3/2,0}(z)$ also arises in the calculation of the scaling function of the two-dimensional Ising model in the extreme anisotropic quantum Hamiltonian limit (Hamer and Barber 1981). In these examples the quantity z, which is real, stands for the scaled fields. The behaviour of the scaling functions in the two limits of the scaled field, $z\to 0$ and $z\to\infty$, may be inferred from the behaviour of the remnant functions obtained by Fisher and Barber (1972). It has recently been shown that modified remnant functions, $R^{\alpha}_{\sigma,\tau}(z)$ (Fisher and Barber 1972), arise in the explicit calculation of the scaling function of the one-dimensional dimerised spin-$\frac{1}{2}$ XY model upon which arbitrary boundary conditions are imposed (Spronken and Kemp 1986). In fact, the relevant quantity involved in this calculation is

$$P^{\alpha}_{\sigma,\tau}(z)=\tfrac{1}{2}\{R^{\alpha}_{\sigma,\tau}(z)+R^{-\alpha}_{\sigma,\tau}(z)\} \tag{1}$$

where $\tau=0$, $\sigma=\frac{3}{2}$, $0\leq\alpha\leq\frac{1}{2}$ and z, which is real, stands for the scaled dimerisation parameter. To obtain the behaviour of the scaling function in the two limits, $z\to 0$ and $z\to\infty$, of the scaled field requires the analysis of $P^{\alpha}_{\sigma,\tau}(z)$ defined by (1). However, neither the modified remnant functions nor the sums of such functions have been analysed previously. It is the purpose of this letter to provide such an analysis of the function $P^{\alpha}_{\sigma,\tau}(z)$, defined by (1), in the simplest case, $\tau=0$. The quantity σ is restricted to half-odd integers and $0\leq\alpha<1$. The quantity z is assumed complex. The calculation is similar to the one performed by Fisher and Barber (1972). Many of the mathematical identities and definitions used here can be found in the table of Gradshteyn and Ryzhik (1980). These two references will be referred to here as FB and GR.

In the first part of this letter, an integral representation of $P^{\alpha}_{1/2,0}(z)$ is obtained. The use of the Mellin transform, the Hurwitz formula and the recursion relation for the function P, yield an explicit expression for $P^{\alpha}_{n+1/2,0}(z)$ for $n=0,1,2,\ldots$, $0\leq\alpha<1$, and $|\arg z|<\pi$. An asymptotic expansion for $|z|\to\infty$ is also obtained. A power expansion for $P^{\alpha}_{n+1/2,0}(z)$ is given in the second part.

The modified remnant functions involved in (1) are defined by FB (recalling that here, $\sigma = n + \frac{1}{2}$ with $n = 0, 1, 2, \ldots$):

$$R^{\delta}_{n+1/2,0}(z) = \frac{-2\sqrt{\pi}}{\Gamma(n+\frac{1}{2})} \sum_{k=1}^{\infty} [\![\{(k-\delta)^2 + z\}^{n-1/2}]\!]_{n+1} \qquad |\delta| < 1 \tag{2}$$

where

$$[\![g(z)]\!]_{n+1} = g(z) - \sum_{l=0}^{n} g_l\{z^l/l!\} \qquad g_l = \mathrm{d}^l g(z)/\mathrm{d}z^l|_{z=0}. \tag{3}$$

An empty sum in (3) is interpreted as zero. The recursion relations for the modified remnant functions are identical to those for the ordinary remnant functions (FB). These yield the following recursion relations for $P^{\alpha}_{n+1/2,0}(z)$:

$$P^{\alpha}_{n+1/2,0}(z) = \int_0^z \mathrm{d}w_1 \int_0^{w_1} \mathrm{d}w_2 \ldots \int_0^{w_{n-1}} \mathrm{d}w_n P^{\alpha}_{1/2,0}(w_n) \qquad n > 0. \tag{4}$$

Accordingly, one needs only to consider the function $P^{\alpha}_{1/2,0}(z)$, the recursion relation (4) allowing the determination of $P^{\alpha}_{n+1/2,0}(z)$ for all $n > 0$. From (1), (2) and (3), one obtains

$$P^{\alpha}_{1/2,0}(z) = \tfrac{1}{2} \sum_{k=1}^{\infty} [h(k-\alpha, z) + h(k+\alpha, z)] \tag{5}$$

where the auxiliary function $h(y, z)$ is defined by

$$h(y, z) = -2[(y^2 + z)^{-1/2} - y^{-1}]. \tag{6}$$

The integral representation for the function $P^{\alpha}_{1/2,0}(z)$ is obtained using the Mellin transform (Magnus *et al* 1966). The Mellin transform, $M(p, z)$, of the function $h(y, z)$ is (FB)

$$M(p, z) = \int_0^{\infty} \mathrm{d}y\, h(y, z) y^{p-1} = -\pi^{-1/2} z^{(p-1)/2} \Gamma(p/2) \Gamma[(1-p)/2] \tag{7}$$

where $\Gamma(s)$ is the gamma function (GR). The inverse Mellin transform is

$$h(y, z) = \frac{1}{2\pi \mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \mathrm{d}p\, M(p, z) y^{-p} \tag{8}$$

from which one obtains, using (5) and (6), the following representation for $P^{\alpha}_{1/2,0}(z)$:

$$P^{\alpha}_{1/2,0}(z) = \frac{1}{4\pi \mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \mathrm{d}p\, M(p, z)[\zeta(p, 1-\alpha) + \zeta(p, 1+\alpha)] \tag{9}$$

where $\zeta(s, a)$ is the Riemann generalised zeta function (GR). In (9), the strip $1 < c = \mathrm{Re}(p) < 3$ is chosen such that the defining integral (7) converges as $y \to \infty$ and $y \to 0$ and that the pole at $\mathrm{Re}(p) = 1$ of the generalised zeta function is excluded. This ensures that (9) correctly represents the absolutely convergent sum (5) (FB). In order to use the Hurwitz formula for the function $\zeta(s, a)$, we shall first modify the integral representation (9).

From the definition of the generalised zeta function (GR) one has $\zeta(p, 1+\alpha) = \zeta(p, \alpha) - \alpha^{-p} (\alpha \neq 0)$. Using this, (9) reads, after a change of variable,

$$P^{\alpha}_{1/2,0}(z) = \frac{1}{2\pi i} \int_{c'-i\infty}^{c'+i\infty} dp\, M(1-2p, z)[\zeta(1-2p, 1-\alpha) + \zeta(1-2p, \alpha)] - \frac{1}{4\pi i} \int_{c-i\infty}^{c+i\infty} dp\, M(p, z)\alpha^{-p} \tag{10}$$

where $c' = \frac{1}{2}(1-c) (-1 < c' < 0)$. The last term on the RHS of (10) is $-\frac{1}{2}h(\alpha, z)$ (cf (8)) while the first term is evaluated using the fact that the function $M(s, z)$ decreases exponentially to zero as $|\mathrm{Im}(s)| \to \infty$ when $|\arg z| < \pi$ (BF). Let C be a closed rectangular contour whose sides parallel to the imaginary axis extend from $-i\infty$ to $i\infty$. These sides intercept the real axis at c' and c'' respectively. Applying the residue theorem, one obtains

$$P^{\alpha}_{1/2,0}(z) = \{\alpha^2 + z\}^{-1/2} - \alpha^{-1} + \sum \mathrm{res} + \frac{1}{2\pi i} \int_{c''-i\infty}^{c''+i\infty} dp\, M(1-2p, z)[\zeta(1-2p, 1-\alpha) + \zeta(1-2p, \alpha)]. \tag{11}$$

Choosing $c'' > \frac{1}{2}$ enables us to use the Hurwitz formula for the generalised zeta function (GR). For clarity, let us quote this formula:

$$\zeta(s, a) = 2(2\pi)^{s-1}\Gamma(1-s) \sum_{m=1}^{\infty} m^{s-1} \sin(2\pi m a + \tfrac{1}{2}\pi s) \tag{12}$$

where $\mathrm{Re}(s) < 0$ and $0 < a \leqslant 1$. Using (12), one obtains

$$\zeta(1-2p, 1-\alpha) + \zeta(1-2p, \alpha) = 4(2\pi)^{-2p}\Gamma(2p)\cos(p\pi) \sum_{m=1}^{\infty} m^{-2p} \cos(2\pi\alpha m). \tag{13}$$

In addition one has, from the Legendre duplication formula for $\Gamma(2p)$ and from the relation $\Gamma(\frac{1}{2}+p)\Gamma(\frac{1}{2}-p)\cos(p\pi) = \pi$ (GR),

$$\Gamma(2p)\Gamma(\tfrac{1}{2}-p)\cos(p\pi) = \sqrt{\pi}\, 2^{2p-1}\Gamma(p). \tag{14}$$

Regrouping (7), (13) and (14), it is easily shown that (11) reduces to

$$P^{\alpha}_{1/2,0}(z) = \{\alpha^2 + z\}^{-1/2} - \alpha^{-1} + \sum \mathrm{res} - \frac{1}{\pi i} \sum_{m=1}^{\infty} \cos(2\pi\alpha m) \int_{c''-i\infty}^{c''+i\infty} dp\, \Gamma^2(2p)(\pi^2 m^2 z)^{-p}. \tag{15}$$

The contribution from the residues is now obtained. The integrand of the first term on the RHS of (10) is, using (7),

$$(2\pi i\sqrt{\pi})^{-1} z^{-p}\Gamma(\tfrac{1}{2}-p)\Gamma(p)[\zeta(1-2p, 1-\alpha) + \zeta(1-2p, \alpha)] \tag{16}$$

which has a simple pole at $p = \frac{1}{2}$ with a vanishing residue (i.e. $\zeta(0, a) = \frac{1}{2} - a$; Erdélyi (1953a)) and a double pole at $p = 0$ as can be seen from (GR and FB)

$$\lim_{p\to 0} \zeta(1-2p, a) = -(2p)^{-1} - \psi(a) \tag{17a}$$

$$\lim_{p\to 0} \Gamma(p) = p^{-1} + \psi(1) \tag{17b}$$

where $\psi(a)$ is the digamma or psi function and $-\psi(1)=C_{\mathrm{E}}$ which is the Euler constant (GR). Using (17), the residue of (16) at $p=0$ is

$$\mathrm{res}=\ln(z)-\psi(\alpha)-\psi(1-\alpha)-2\ln 2 \qquad z\neq 0. \tag{18}$$

The integral in the last term of the RHS of (15) is proportional to the inverse Mellin transform of $\Gamma^2(p)$. In fact, one has (Erdélyi 1953b)

$$\frac{1}{4\pi\mathrm{i}}\int_{c''-\mathrm{i}\infty}^{c''+\mathrm{i}\infty}\mathrm{d}p\,\Gamma^2(p)(\pi^2m^2z)^{-p}=K_0(2\pi m\sqrt{z}) \qquad z\neq 0 \tag{19}$$

where $K_\nu(s)$ is the modified Bessel function of the third kind (GR). Using the relation $\psi(\alpha)+1/\alpha=\psi(1+\alpha)$ (GR) and combining (15), (18) and (19), one obtains the final result

$$P^{\alpha}_{1/2,0}(z)=\{\alpha^2+z\}^{-1/2}+\ln(z)-2\ln 2-\psi(1-\alpha)-\psi(1+\alpha)$$
$$-4\sum_{m=1}^{\infty}\cos(2\pi\alpha m)K_0(2\pi m\sqrt{z}). \tag{20}$$

When $\alpha=0$, $P^{\alpha}_{1/2,0}(z)$ reduces to the ordinary remnant function $R^{0}_{1/2,0}(z)=R_{1/2,0}(z)$ (cf (1) and FB). Therefore, the restriction $\alpha\neq 0$ introduced in order to use the Hurwitz formula may be relaxed and equation (20) is thus valid for $0\leqslant\alpha<1$, $z\neq 0$ and $|\arg z|<\pi$. The recursion relation (4), with $P^{\alpha}_{1/2,0}(z)$ given by (20), allows us to obtain $P^{\alpha}_{n+1/2,0}(z)$ for $n>0$. This yields

$$P^{\alpha}_{n+1/2,0}(z)=\frac{\sqrt{\pi}}{\Gamma(n+\frac{1}{2})}[\![\{\alpha^2+z\}^{n-1/2}]\!]_n$$
$$+\frac{z^n}{\Gamma(n+1)}[\ln(z)-C_{\mathrm{E}}-\psi(n+1)-\psi(1-\alpha)-\psi(1+\alpha)-2\ln 2]$$
$$-z^n\sum_{l=1}^{n}\frac{\Gamma(l)}{\Gamma(2l+1)\Gamma(n-l+1)}\left(\frac{z}{4}\right)^{-l}B_{2l}(\alpha)$$
$$-4(-\pi)^{-n}z^{n/2}\sum_{m=1}^{\infty}m^{-n}\cos(2\pi\alpha m)K_n(2\pi m\sqrt{z}) \tag{21}$$

where the function $B_{2l}(\alpha)$ is the Bernoulli polynomial (GR). The restriction $n>0$ can be dropped provided an empty sum in (21) is interpreted as zero (i.e. $\Sigma_{l\in\varnothing}(\ldots)=0$). Therefore (21) holds for all $n\geqslant 0$. It is valid for $0\leqslant\alpha<1$, $z\neq 0$ and $|\arg z|<\pi$.

Using the relation (GR)

$$B_{2l}(0)=-2(-2\pi)^{-2l}\Gamma(2l+1)\zeta(2l) \qquad l>0 \tag{22}$$

where $\zeta(2l)$ is the Riemann zeta function, one can easily show that the equation (21) reduces, in the case $\alpha=0$, to the expression previously obtained by Fisher and Barber (1972) for the ordinary remnant functions. Another interesting case is $\alpha=\frac{1}{2}$. From (2) one has

$$R^{-1/2}_{n+1/2,0}(z)=R^{1/2}_{n+1/2,0}(z)+\frac{2\sqrt{\pi}}{\Gamma(n+\frac{1}{2})}[\![\{\tfrac{1}{4}+z\}^{n-1/2}]\!]_{n+1} \tag{23}$$

and thus (cf (1))

$$P^{1/2}_{n+1/2,0}(z)=R^{1/2}_{n+1/2,0}(z)+\frac{\sqrt{\pi}}{\Gamma(n+\frac{1}{2})}[\![\{\tfrac{1}{4}+z\}^{n-1/2}]\!]_{n+1} \tag{24}$$

which yields, using (21) and the fact that $\psi(\frac{1}{2}) = -C_E - 2\ln 2$ and $\psi(\frac{3}{2}) = \psi(\frac{1}{2}) + 2$ (GR),

$$R^{1/2}_{n+1/2,0}(z) = \frac{z^n}{\Gamma(n+1)}[\ln(z) + C_E + 2\ln 2 - \psi(n+1)]$$
$$- z^n \sum_{l=1}^{n} \frac{\Gamma(l)}{\Gamma(2l+1)\Gamma(n-l+1)}\left(\frac{z}{4}\right)^{-l} B_{2l}(\tfrac{1}{2})$$
$$- 4(-\pi)^{-n} z^{n/2} \sum_{m=1}^{\infty} m^{-n}(-1)^m K_n(2\pi m\sqrt{z}). \tag{25}$$

Using the relation (22) and the relation between $B_{2l}(\frac{1}{2})$ and $\zeta(2l)$ (Erdélyi 1953a), one obtains

$$B_{2l}(\tfrac{1}{2}) = -(1 - 2^{1-2l})B_{2l}(0). \tag{26}$$

Combining (26), (25) and (21) (with $\alpha = 0$) yields

$$R^{1/2}_{n+1/2,0}(z) = 4^{1/2-n} R_{n+1/2,0}(4z) - R_{n+1/2,0}(z) \tag{27}$$

a result that can be derived directly from (2) (FB).

Since $K_\nu(s) = (\pi/2s)^{1/2} e^{-s}[1 + O(s^{-1})]$ as $|s| \to \infty$ and $|\arg s| < 3\pi/2$ (GR), one concludes that the RHS of equations (21) and (25) decrease to zero exponentially fast as $|z| \to \infty$. No dependence upon α survives in this limit and the behaviour of $P^\alpha_{n+1/2,0}(z)$, $R^{1/2}_{n+1/2,0}(z)$, as well as the behaviour of the ordinary remnant function $R_{n+1/2,0}(z)$ (FB), become asymptotically identical. These fuunctions are $O(z^n \ln z)$.

We conclude this letter with the derivation of a convergent power expansion of $P^\alpha_{n+1/2,0}(z)$ for arbitrary z (except possibly, as for the ordinary remnant functions, at branch points of (2) (FB)). Let us introduce the integer k_μ defined by

$$k_\mu = [\mu\alpha + |z|^{1/2}] \tag{28}$$

where $\mu = \pm 1$ and where $[a]$ stands for the largest integer less than or equal to the real number a. Removing the first k_μ terms in (2) and expanding the remainder, one obtains, for the function $P^\alpha_{n+1/2,0}(z)$ defined by (1) ($n \geq 0$),

$$P^\alpha_{n+1/2,0}(z) = \frac{-\sqrt{\pi}}{\Gamma(n+\frac{1}{2})} \sum_\mu \sum_{k=1}^{k_\mu} [\![\{(k-\mu\alpha)^2 + z\}^{n-1/2}]\!]_{n+1}$$
$$- \pi^{-1/2} z^n \sum_{l=1}^{\infty} \frac{\Gamma(l+\frac{1}{2})}{\Gamma(n+1+l)}\left(\sum_\mu \zeta(2l+1, 1-\mu\alpha+k_\mu)\right)(-z)^l. \tag{29}$$

Note that $\Sigma_{k\in\varnothing}(\ldots) = 0$ in (29). As $z \to 0$, equation (29) yields

$$P^\alpha_{n+1/2,0}(z) = \frac{z^{n+1}}{2(n+1)!}[\zeta(3, 1+\alpha) + \zeta(3, 1-\alpha)](1 + O(z)) \tag{30}$$

which shows explicitly the dependence of $P^\alpha_{n+1/2,0}(z)$ on α in this limit. Again, when $\alpha = 0$, the expansion (29) coincides with the expansion of the ordinary remnant function previously obtained by Fisher and Barber (1972).

Note finally that (21), with $n \neq 0$, constitutes, to our knowledge, a new series involving modified Bessel functions of the third kind and Bernoulli polynomials. For the special case $n = 0$, it reduces to the analytical continuation of a known series of Bessel functions (see, for instance, GR, equation (8.526.1)).

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