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AN INCLUSIVE MINIJET CROSS SECTION AND THE BARE POMERON IN QCD

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An inclusive two-jet cross section is described. The energy dependence of the cross section is calculated within perturbative QCD, and related to a bare pomeron in QCD, in the region where a leading logarithmic expansion is valid.

1. Introduction

As one measures higher and higher energy reactions, the amount of jet production increases rapidly. In their $\sqrt{s} = 900$ GeV data at CERN, UA(1) reported [1,2] an inclusive cross section of about 10 mb for jets having $p_\perp > 5$ GeV and pseudorapidity $|\eta| < 1.5$. This rapid growth of minijet production is expected theoretically [3] and likely accounts for the growth in the average transverse momentum per particle in high multiplicity events as well as the strong violation of KNO scaling in the large-n region of the multiplicity distribution as one goes from ISR to SppS energies [1,4-7].

Although many qualitative aspects of minijet production are understood [8-11] it has been very difficult to obtain precise quantitative predictions of these phenomena. For example, one might attempt to predict the growth, in s, of the inclusive minijet cross section. (In this paper we shall define a minijet as a jet having $p_\perp \geqslant M$ with M^2/s small and M a fixed value.) However, near $\eta = 0$ for example, such cross sections involve quark and gluon distributions having X values of size $M/\sqrt{s}$ and the small X-dependence of such distributions is strongly dependent on the initial distribution used to obtain a solution to the Altarelli-Parisi equation. This is illustrative of a common problem. In general it is very difficult to separate minijet physics from soft hadron physics and at the moment it is still difficult to make precise and reliable predictions of phenomena involving non-perturbative QCD.

Our objective in this paper is to define a measurement involving minijets and to make precise predictions for the energy dependence of that measurement. To that

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end we consider the two-jet inclusive cross section, with each jet having a transverse momentum greater than or equal to M and with the two jets having fixed fractions X_1 and X_2, of the two beam momenta. Variation of s, for X_1, X_2 and M fixed, is then a variation of the rapidity interval, y, between the two jets. It is this s, or y, dependence which we shall describe. As will be discussed in the next section, the y dependence is given by higher order corrections to the hard scattering process. The leading logarithmic corrections in y, terms of the type $[\alpha(M)y]^n$ in perturbation theory, give the y-dependence of the two-jet inclusive cross section in terms of the "bare QCD pomeron" [13–18]. In this approximation the coupling does not run and the resulting pomeron is a fixed branch point in the angular momentum plane. By explicit calculation of the perturbation series through terms of order $(\alpha y)^5$ we show that the y-dependence given by the asymptotic behavior of the bare pomeron is already accurate, to within about 10%, at $y = 1$. This bare pomeron then describes the y-dependence of the inclusive cross section (see eq. (4)) in a region from $y \approx 1$ up to y-values where multiple pomeron exchanges, terms involving $\alpha^q(\alpha y)^p$, become important. (The size of this region is estimated in sect. 2.) This is the y-region where our calculation is systematic and an s-dependence about as strong as $s^{1/2}$ is found in the upper part of this region. In the region where multiple pomeron exchanges are important the s growth should slow to something like $\ln^2 s$ and this regime may well be reached at upper end of the SppS and Tevatron energies. This most interesting region involves short distance, but non-perturbative, QCD which is beyond the scope of the present paper.

In the appendix we describe a general technique used to calculate the perturbation series for the y-dependence through order $(\alpha y)^5$. Unfortunately, we have not been able to find an explicit expression for the general term. The natural variable for this expansion is $\alpha C_A y/\pi$ and it is most remarkable that the asymptotic expansion is already accurate when this variable is about 0.2.

It is likely that there are many other observables involving minijets for which perturbative QCD is the appropriate tool. If such is the case we may have the possibility of describing much of minijet physics in terms of the perturbative QCD pomeron and the associated multi-pomeron exchanges.

2. A two-jet inclusive cross section

In this section we shall define the two-jet inclusive measurement, the energy dependence of whose cross section we shall then describe within perturbative QCD.

Suppose p_1 and p_2 are the momenta of the proton and the antiproton respectively in a high-energy collider reaction. We imagine a coordinate system where p_1 and p_2 are oppositely directed along the z-axis. Further suppose one measures two jets having momenta $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ where $\boldsymbol{k}_1$ is directed into the hemisphere into which $\boldsymbol{p}_1$ points and where $\boldsymbol{k}_2$ is directed into the hemisphere into which $\boldsymbol{p}_2$ points. Then $X_1 X_2 \mathrm{d}\sigma/\mathrm{d}X_1\,\mathrm{d}X_2\,\mathrm{d}^2k_{1\perp}\,\mathrm{d}^2k_{2\perp}$ represents the two-jet inclusive cross section where

X_1 and X_2 are the momentum fractions of the two jets, and $k_{1\perp}$ and $k_{2\perp}$ are the transverse momenta of the two jets with respect to the axis of the collision, the z-axis. If one integrates over phase space regions having $k_{1\perp}^2, k_{2\perp}^2 > M^2$, holding X_1 and X_2 fixed, one obtains the cross section

$$\sigma(M^2, s, X_1, X_2, \varphi) = \int \mathrm{d}k_{1\perp}^2\, \mathrm{d}k_{2\perp}^2\, \Theta(k_{1\perp} - M)\Theta(k_{2\perp} - M)\pi^2 \times \frac{X_1 X_2 \mathrm{d}\sigma}{\mathrm{d}X_1 \mathrm{d}X_2 \mathrm{d}^2k_{1\perp} \mathrm{d}^2k_{2\perp}}, \tag{1}$$

with φ the azimuthal angle, about the z-axis, between the two jets.

Our next task is to factor (1) into a form where a product of structure functions times a hard scattering part occurs. When $y \equiv \ln(X_1 X_2 s/M^2)$ is of order 1, this factorization is the normal factorization where the hard scattering part is given by parton-parton scatterings in the Born approximation. However, when y is large we may classify higher order corrections to the hard scattering part into terms of order $[\alpha(M)y]^p$ and terms of the type $[\alpha(M)]^q[\alpha(M)y]^p$. The former terms, which we shall henceforth call leading logarithmic are the main concern of this paper, although we shall briefly discuss the role of the non-leading logarithmics somewhat later. Then for y large, and in the leading logarithmic approximation

$$\sigma(M^2, s, \varphi) = \left(\frac{\alpha C_A}{\pi}\right)^2 \frac{\pi^3}{2M^2} X_1\left[G(X_1, M^2) + \tfrac{4}{9}Q(X_1, M^2)\right] \times X_2\left[G(X_2, M^2) + \tfrac{4}{9}Q(X_2, M^2)\right] f, \tag{2}$$

where $G + \frac{4}{9}Q$ is the combination of gluon and quark parton densities which naturally appears [19] when y is large. (The jet measurements which have been described above sum over quark and gluon jets indiscriminately.) In (2) the factor

$$\left(\frac{\alpha C_A}{\pi}\right)^2 \frac{\pi^3}{2M^2} f \tag{3}$$

is the two-jet inclusive cross section for gluon-gluon scattering while the remaining factors give the number densities of the gluons and quarks which initiate the collision. Expression (3) may also be viewed as the cross section for gluon-gluon scattering within an impact distance of size about $1/M$. There are a number of points which we would like to make concerning this two-jet inclusive cross section and the resulting eq. (2).

(i) When X_1, X_2 and M^2 are held fixed with s varying, the complete energy dependence is contained in f. This is in contrast to the situation which obtains in the single jet inclusive cross section. In that case all energy dependences are given in terms of the small X dependence of the parton distributions which are strongly dependent on the initial distributions and thus not determinable purely within perturbative QCD. To our knowledge the two-jet inclusive cross section is the simplest measurement which can give energy dependences of quark and gluon cross sections which are then calculable within perturbative QCD.

(ii) Order by order in perturbation theory the coupling dependence of f is given in terms of $\alpha(M)$. This is, of course, what justifies the use of perturbation theory. Nevertheless, as we shall discuss later, there are some subtleties concerning the running of the coupling at extremely high energy. These subtleties do not affect the energy dependence of σ in the energy region in which we shall be concerned, and so we may consider $\alpha(M)$ to be fixed and small.

(iii) We expect soft gluon effects not to modify (2). Though we have not tried to construct a careful proof of soft gluon cancellations we believe that such an argument could be given following the lines of Collins, Soper and Sterman [20].

(iv) We have not investigated the φ dependence of (2) in any detail. Although, as is clear from the work of ref. [14], the φ dependence of f becomes weak for large y we have not carefully studied the rate of approach to the asymptotic expressions for the φ-dependent part of f. Thus we henceforth suppose that a φ-integral has been performed and we define $\sigma(M^2, s) = \int_0^{2\pi} \mathrm{d}\varphi\, \sigma(M^2, s, \varphi)$.

(v) In lowest order perturbation theory $f = 1$. The corrections of order $(\alpha y)^p$ come from both real and virtual gluons. The contributions of the real gluons correspond to the production of additional jets. When αy is of order 1, we expect these leading logarithmic corrections to be large. Thus in general there will be more than two jets produced in the two-jet inclusive events which we are describing. Note that in the leading logarithmic approximation the X_i are strongly ordered so that the longitudinal moments of the two outgoing jets are almost the same as the ones of the two incoming gluons. The additional jets are produced at X near zero but with some transverse momentum.

(vi) Finally, we come to the question of the range of validity, in y, for which we may expect the leading logarithmic terms to dominate the cross section. The formal range of validity of (2) is the region of αy of order 1 and α small. However, we can do a little better in our estimate of where the leading logarithmic approximation will break down in the large y regime. Now αf is proportional to the number of gluon quanta carrying a momentum fraction $X \approx M^2/s$ in an infinite momentum frame of one of the colliding hadrons. These quanta are within a transverse radius $|\Delta X| \lesssim 1/M$. When this number of quanta reaches a value $1/\alpha$ the dilute, one-pomeron, approximation breaks down and multi-pomeron effects become important [3, 21]. Thus the limit in y is reached when $\alpha f = c/\alpha$ with c not yet determined. As we shall soon see the asymptotic behavior of f is

$$f \sim \frac{\exp((\alpha C_{\mathrm{A}} y/\pi) 4 \ln 2)}{\sqrt{\frac{7}{2}\alpha C_{\mathrm{A}} \zeta(3) y}}, \tag{4}$$

so that we may expect two-pomeron and one-pomeron exchanges to be comparable when

$$y = \frac{1}{(\alpha C_A/\pi)4\ln 2}\ln\left[\frac{c}{\alpha^2}\sqrt{\tfrac{7}{2}\alpha C_A\zeta(3)y}\right]. \tag{5}$$

When c varies from 0.1 to 10 the y which satisfies (5) varies from about 4 to about 9 with $(\alpha C_A/\pi)4\ln 2$ taken to be $\frac{1}{2}$. Clearly, it is very important to calculate the constant c, but, in any case, it appears that there should be a region of y for which the two-jet inclusive cross section grows like (4). After growing like (4) the cross section should have a slowed rate of growth as y increases and by the time (5) is achieved the rate of growth should be very slow, perhaps like $\ln^2 s$ [3].

3. The two-jet inclusive cross section as given by the bare pomeron in QCD

In this section we shall relate the two-jet inclusive cross section, defined in the previous section, to the bare pomeron in QCD. To that end it is straightforward, using the arguments given in refs. [17], to write

$$\frac{X_1X_2\,\mathrm{d}\sigma}{\mathrm{d}X_1\,\mathrm{d}X_2\,\mathrm{d}^2k_{1\perp}\,\mathrm{d}^2k_{2\perp}} = \left(\frac{\alpha C_A}{\pi}\right)^2\frac{\pi}{2k_{1\perp}^2k_{2\perp}^2}X_1\left[G(X_1,M^2)+\tfrac{4}{9}Q(X_1,M^2)\right]$$
$$\times X_2\left[G(X_2,M^2)+\tfrac{4}{9}Q(X_2,M^2)\right]f(k_{1\perp},k_{2\perp},y), \tag{6}$$

with f obeying the equation [13,14]

$$\omega f_\omega(k_{1\perp},k_{2\perp}) = \delta(k_{1\perp}^2-k_{2\perp}^2)\delta(\varphi_1-\varphi_2)+\left(\frac{\alpha C_A}{\pi^2}\right)$$
$$\times\int\frac{\mathrm{d}^2k_\perp}{(k_{1\perp}-k_\perp)^2}\left[f_\omega(k_\perp,k_{2\perp})-\frac{k_{1\perp}^2f_\omega(k_{1\perp},k_{2\perp})}{k_\perp^2+(k_{1\perp}-k_\perp)^2}\right]. \tag{7}$$

We have defined

$$f(k_{1\perp},k_{2\perp},y) = \frac{1}{2\pi i}\int_{a-i\infty}^{a+i\infty}\mathrm{d}\omega\,\mathrm{e}^{\omega y}f_\omega(k_{1\perp},k_{2\perp}) \tag{8}$$

and φ_1 and φ_2 are the azimuthal angles of the two-dimensional vectors $k_{1\perp}$ and $k_{2\perp}$.

Now as discussed in ref. [14] one may write

$$f_\omega(k_{1\perp},k_{2\perp}) = \frac{1}{2\pi}\sum_n \mathrm{e}^{in(\varphi_1-\varphi_2)}\times\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\nu\,\frac{(k_{1\perp}^2)^{-1/2-i\nu}(k_{2\perp}^2)^{-1/2+i\nu}}{\omega-\omega_0(\eta,\nu)}, \tag{9}$$

with

$$\omega_0 = 2\frac{\alpha C_A}{\pi}\chi(\eta, \nu), \tag{10}$$

where

$$\chi(\eta, \nu) = \mathrm{Re}\left[\Psi(1) - \Psi\left(\tfrac{1}{2}(|\eta| + 1) + i\nu\right)\right]. \tag{11}$$

Using eqs. (1), (6), (8) and (9) one obtains eq. (2) with

$$f = \frac{1}{2\pi}\sum_{-\infty}^{\infty} e^{in(\varphi_1 - \varphi_2)} \times \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\nu}{\nu^2 + \frac{1}{4}} e^{2z\chi(\eta,\nu)}, \tag{12}$$

with $z = \alpha C_A/\pi$. Eq. (12) gives the y and φ dependence of the two-jet inclusive cross section, at the leading logarithmic level. The fact that χ is a monotically decreasing function of $|\nu|$, for real values of ν, allows one to immediately obtain the asymptotic behavior (4) for large y. A little later in this section we shall discuss the y behavior of f, as given by (12), both in the asymptotic and non asymptotic regimes. Now, we shall discuss some subtleties of the integral equation (7).

As discussed in some detail by Lipatov and his collaborators [13, 14] the large y behavior of $f(k_{1\perp}, k_{2\perp}, y)$ ultimately involves small internal transverse momentum which negate the use of a weak coupling approach to this high energy problem. In our situation we may estimate the y-values at which the coupling variation becomes important by taking $k_{1\perp}^2 \approx k_{2\perp}^2 \approx M^2$. Then the maximum variation in internal transverse momentum can be expected to occur at rapidities about $\frac{1}{2}y$ from either of the observed jets. The internal transverse momenta which are important are then those $k_\perp$ for which $f(M, k_\perp, \frac{1}{2}y)$ is not small. Now

$$f\left(M, k_\perp, \tfrac{1}{2}y\right) = \frac{1}{2\pi}\int d\nu\, e^{z\chi(\nu)}\left(M^2\right)^{-1/2-i\nu}\left(k_\perp^2\right)^{-1/2+i\nu}. \tag{13}$$

At large values of y the ν-values which are important in (11) are determined by $-\frac{3}{2}\chi''(0)\nu^2 \lesssim 1$. Thus the ν-values involved in (11) are (see eq. (22) below)

$$\nu \lesssim \frac{1}{\sqrt{7(\alpha C_A/\pi)\zeta(3) y}}. \tag{14}$$

Thus in order not to have an additional cancellation in (11), due to the factor $(k^2/M^2)^{i\nu}$, one needs to keep

$$\left|\ln\left(M^2/k_\perp^2\right)\right| \lesssim \sqrt{7(\alpha C_A/\pi)\zeta(3) y}. \tag{15}$$

From (14) one sees that at sufficiently large values of y the effective values of $k_\perp$

can be very different from M. It is important to limit the values of y so that $\alpha(M)/\alpha(k)$ is not too far from unity for those values of $k_\perp$ allowed by (13). For M between 5 and 10 GeV there is a significant region in y in which the fixed coupling approach which we have used should be valid. This interval in y will increase as M increases.

Our next task is to evaluate (12). Of course at sufficiently large values of y one may use an asymptotic expansion, however we also must determine the regime, in y, for which the asymptotic expansion is valid. We determine this region of validity by evaluating (12) in a perturbation expansion about $z = 0$. The asymptotic behavior sets in when good agreement is found between the perturbation expansion and the asymptotic expansion. We have found it difficult to evaluate the perturbation expansion including the φ dependence so in what follows we assume that a φ integration of (12) has been performed.

The perturbative expansion of $f(y)$ is readily obtained for small y:

$$f(y) = \sum_{k=0}^{\infty} f_k \left(\frac{\alpha C_A y}{\pi} \right)^k , \tag{16}$$

where

$$f_k = 2(-1)^k \frac{2^k}{k!} \frac{1}{2\pi} \int_0^\infty \frac{d\nu}{\left(\nu^2 + \frac{1}{4}\right)} \left[\operatorname{Re} \Psi\left(\tfrac{1}{2} + i\nu\right) - \Psi(1)\right]^k . \tag{17}$$

We have calculated the first terms of this expansion (see appendix): $f_0 = 1$, $f_1 = 0$, $f_2 = 2\zeta(2)$, $f_3 = 3\zeta(3)$, $f_4 = \frac{53}{6}\zeta(4)$ and $f_5 = \frac{1}{12}[115\zeta(5) + 48\zeta(2)\zeta(3)]$ (see table 1).

It turns out that there exists a good approximation of f_k which works already for k as low as 4 or 5. Indeed, for large ν,

$$\left[\operatorname{Re} \Psi\left(\tfrac{1}{2} + i\nu\right) - \Psi(1)\right] = \ln \frac{\nu}{\nu_0} - \frac{1}{24\nu^2} + O\left(\frac{1}{\nu^4}\right),$$

TABLE 1

k	f_k	h_k	f_k/h_k
0	1	0.3421	2.922
1	0	−0.9836	0
2	3.290	2.167	0.658
3	−3.606	−4.467	1.239
4	9.558	9.021	0.944
5	−17.847	−18.101	1.014

where

$$\nu_0 = \mathrm{e}^{\Psi(1)}. \tag{18}$$

Then if we consider

$$h_k = \frac{(-1)^k 2^k 1}{k!\pi} \int_{\nu_0}^{\infty} \mathrm{d}\nu \left[1 - \frac{1}{4\nu^2}\right] \left\{ \left[\ln \frac{\nu}{\nu_0}\right]^k + \frac{k}{24\nu^2} \left(\ln \frac{\nu}{\nu_0}\right)^{k-1} \right\}, \tag{19}$$

$$h_k = \frac{(-1)^k 2^k}{\nu_0} \frac{1}{\pi} \left\{ 1 - \frac{1}{8\nu_0^2} \frac{1}{3^k} \right\}, \tag{20}$$

$$h(y) = \sum_{k=0}^{\infty} h_k \left(\frac{\alpha C_A y}{\pi} \right)$$

$$= \frac{1}{\pi \nu_0} \left[\frac{1}{(1 + 2\alpha C_A y/\pi)} - \frac{1}{8\nu_0^2} \frac{1}{(1 + \frac{2}{3}\alpha C_A y/\pi)} \right],$$

$$\left(\frac{\alpha C_A y}{\pi} \right) < \frac{1}{2}, \tag{21}$$

so that $f(y) - h(y) = \Sigma_{k=0}^{\infty}(h_k - f_k)(\alpha C_A y/\pi)^k$ is a series the radius of convergence of which is large.

It is interesting to compare our result at small y with the large y regime obtained by Lipatov and collaborators [13]

$$f = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{\mathrm{d}\nu}{\nu^2 + \frac{1}{4}} \exp\left(\frac{2\alpha}{\pi} C_A \chi(\nu) y \right). \tag{22}$$

For large y

$$f^{\mathrm{As}} \simeq \frac{2}{\pi} \int_{-\infty}^{+\infty} \frac{\mathrm{d}\nu}{(1 + 4\nu^2)} \exp\left(\frac{2\alpha C_A}{\pi} \left[\chi(0) + \tfrac{1}{2}\nu^2 \chi''(0) \right] y \right), \tag{23}$$

$$f^{\mathrm{As}} \simeq \frac{2 \exp[(2\alpha C_A/\pi)\chi(0)]\, y}{\sqrt{\pi(-\chi''(0))(\alpha C_A y/\pi)}}, \tag{24}$$

where

$$\chi(0) = \Psi(1) - \Psi\left(\tfrac{1}{2}\right) = 2\ln 2, \tag{25}$$

$$\chi''(0) = \Psi''\left(\tfrac{1}{2}\right) = -14\zeta(3). \tag{26}$$

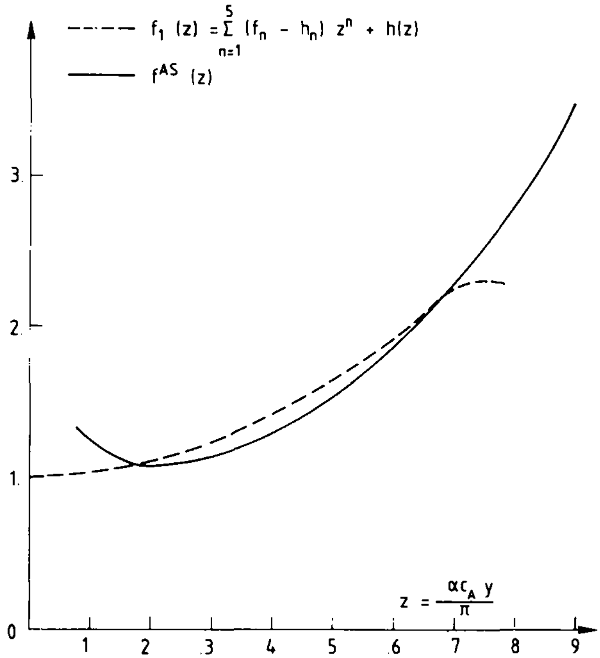

Fig. 1.

Setting $\alpha C_A y/\pi = z$, we have drawn the curve

$$f^{As}(z) = \frac{e^{(4\ln 2)z}}{\sqrt{\pi\zeta(3)\frac{7}{2}z}}, \tag{27}$$

and the curve

$$f_1(z) = \sum_{k=0}^{5}(f_k - h_k)z^k + \frac{1}{\pi\nu_0}\left[\frac{1}{1+2z} - \frac{1}{8\nu_0^2}\frac{1}{1+\frac{2}{3}z}\right] \tag{28}$$

in fig. 1.

We observe that the large y regime obtained by Lipatov and collaborators is already valid for z as small as 0.2 and up. For very small z ($0 \leqslant y \leqslant 1$ if $\alpha C_A/\pi \sim \frac{1}{5}$) we are in the perturbative regime. Then there is a large region of overlap between the perturbative and the asymptotic behaviour for $0.2 \leqslant z \leqslant 0.6$ ($1 \leqslant y \leqslant 6$) where either the perturbative expansion or the asymptotic expression coincides within a few percent.

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Appendix

CALCULATION OF $f_k = (1/2\pi)\int_{-\infty}^{\infty} d\nu\,[2\Psi(1) - \Psi(\frac{1}{2}+i\nu) - \Psi(\frac{1}{2}-i\nu)]^k/(\nu^2+\frac{1}{4})$

We use a contour integral (c) in the upper half plane and the symmetry $\nu \to -\nu$ of the integrand ($\Psi(\frac{1}{2}-i\nu)$ has poles in the lower half plane) to get at once.

$$f_0 = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\nu}{\nu^2+\frac{1}{4}} = 1, \tag{A.1}$$

$$f_1 = 2\times\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\nu\,\frac{\left[\Psi(1)-\Psi(\frac{1}{2}-i\nu)\right]}{\nu^2+\frac{1}{4}} = 2[\Psi(1)-\Psi(1)] = 0. \tag{A.2}$$

CALCULATION OF $f_2 = 1/2\pi\times 2\int_{-\infty}^{+\infty} d\nu[\Psi(1)-\Psi(\frac{1}{2}-i\nu)]^2/(\nu^2+\frac{1}{4}) + (2/2\pi)\int_{-\infty}^{+\infty} d\nu\,[\Psi(1)-\Psi(\frac{1}{2}-i\nu)][\Psi(1)-\Psi(\frac{1}{2}+i\nu)]/(\nu^2+\frac{1}{4})$

Thus

$$f_2 = \frac{1}{\pi}\int_{-\infty}^{+\infty} d\nu\,\frac{\left[\Psi(1)-\Psi(\frac{1}{2}-i\nu)\right]\left[\Psi(1)-\Psi(\frac{1}{2}+i\nu)\right]}{\nu^2+\frac{1}{4}}.$$

The simple poles contribution at $\nu = \frac{1}{2}i(2k+1)$ for $k = 1,2,\ldots$ yields

$$(f_2)_s = 2\sum_{k=1}^{\infty}\frac{S_1(k)}{k(k+1)},$$

where

$$S_p(k) = \sum_{j=1}^{k}(1/j^p), \quad p = 1,\ldots, \tag{A.3}$$

with the convention $S_p(0) = 0$

$$(f_2)_s = 2\left\{\sum_{k=1}^{\infty}\frac{\left[S_1(k-1)+\frac{1}{k}\right]}{k} - \sum_{k=1}^{\infty}\frac{S_1(k)}{k+1}\right\}$$

$$= 2\sum_{k=1}^{\infty}\frac{1}{k^2} = 2\zeta(2),$$

where $\zeta(x)$ is the Riemann function ($\zeta(n) = \sum_{k=1}^{\infty} 1/k^n$, $n > 1$). The double-pole contribution at $\nu=\frac{1}{2}i$ yields

$$(f_2)_{\mathrm{d}}=2\psi'(1)=2\zeta(2),$$

so that

$$f_2=4\zeta(2). \tag{A.4}$$

CALCULATION OF $f_3=(3\times 2/2\pi)\int_{-\infty}^{+\infty}\mathrm{d}\nu\,[\psi(1)-\psi(\frac{1}{2}-i\nu)]^2[\psi(1)-\psi(\frac{1}{2}+i\nu)]/(\nu^2+\frac{1}{4})$

There is no contribution from the double pole at $\nu=\frac{1}{2}i$. As far as the single poles are concerned, we get

$$f_3=-6\sum_{k=1}^{\infty}\frac{S_1^2(k)}{k(k+1)}=-6\left\{\sum_{k=1}^{\infty}\frac{\left(S_1(k-1)+1/k\right)^2}{k}-\sum_{k=1}^{\infty}\frac{S_1^2(k)}{k+1}\right\},$$

$$f_3=-6\left\{2\sum_{k=1}^{\infty}\left(S_1(k)-\frac{1}{k}\right)\frac{1}{k^2}+\sum_{k=1}^{\infty}\frac{1}{k^3}\right\}$$

$$=-6\left\{2\sum_{k=1}^{\infty}\frac{S_1(k)}{k^2}-\zeta(3)\right\}.$$

It can be shown (see below) that $\sum_{k=1}^{\infty}S_1(k)/k^2=2\zeta(3)$, so that

$$f_3=-18\zeta(3). \tag{A.5}$$

CALCULATION OF $f_4=(2\times 4/2\pi)\int_{-\infty}^{+\infty}\mathrm{d}\nu\,[\psi(1)-\psi(\frac{1}{2}-i\nu)]^3\,[\psi(1)-\psi(\frac{1}{2}+i\nu)]/(\nu^2+\frac{1}{4})+(6/2\pi)\int_{-\infty}^{+\infty}\mathrm{d}\nu\,[\psi(1)-\psi(\frac{1}{2}-i\nu)]^2[\psi(1)-\psi(\frac{1}{2}-i\nu)]^2/(\nu^2+\frac{1}{4})$

Here again no contribution at $\nu=\frac{1}{2}i$ for the first term but $6\zeta^2(2)$ for the second one. The single-pole contribution yields

$$(f_4)=8\left\{\sum_{k=1}^{\infty}\frac{\left(S_1(k-1)+1/k\right)^3}{k}-\sum_{k=1}^{\infty}\frac{S_1^3(k)}{k+1}\right\}$$

$$=8\left\{3\sum_{k=1}^{\infty}\frac{S_1^2(k)}{k^2}-3\sum_{k=1}^{\infty}\frac{S_1(k)}{k^3}+\zeta(4)\right\}.$$

To get the double-pole contribution, we use the relation $\psi'(k+1) = -S_2(k) + \zeta(2)$

$$(f_4)_{\mathrm{d}} = -6\left\{ \sum_{k=1}^{\infty} S_1^2(k)\left[\frac{1}{k^2} - \frac{1}{(k+1)^2}\right] \right.$$

$$\left. -2S_1(k)(\zeta(2) - S_2(k))\left[\frac{1}{k} - \frac{1}{k+1}\right] - 2S_1^3(k)\left\{\frac{1}{k} - \frac{1}{k+1}\right\}\right\}$$

$$= -6\left\{ -5\zeta(4) - 2\zeta^2(2) + 10\sum_{k=1}^{\infty}\frac{S_1(k)}{k^3} - 6\sum_{k=1}^{\infty}\frac{S_1^2(k)}{k^2} + 2\sum_{k=1}^{\infty}\frac{S_2(k)}{k^2}\right\}.$$

Thus

$$f_4 = 38\zeta(4) + 18\zeta^2(2) + 60\sum_{k=1}^{\infty}\frac{\left(S_1^2(k) + S_2(k)\right)}{k^2} - 72\sum_{k=1}^{\infty}\frac{S_2(k)}{k^2} - 84\sum_{k=1}^{\infty}\frac{S_1(k)}{k^3},$$

with (see below),

$$\sum_{k=1}^{\infty}\frac{S_1(k)}{k^3} = \tfrac{5}{4}\zeta(4) = \tfrac{1}{2}\zeta^2(2),$$

$$\sum_{k=1}^{\infty}\frac{S_2(k)}{k^2} = \tfrac{1}{2}\left\{\zeta^2(2) + \zeta(4)\right\},$$

$$\sum_{k=1}^{\infty}\frac{\left(S_1^2(k) + S_2(k)\right)}{k^2} = 6\zeta(4),$$

and we get

$$f_4 = 8\left[4!\zeta(4) + \zeta^2(2)\right]. \tag{A.6}$$

Similar formulas can be obtained for g_5. Indeed

$$g_5 = \frac{2\times 5}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}\nu\,\frac{\left[\psi(1) - \psi\left(\tfrac{1}{2} - i\nu\right)\right]^4\left[\psi(1) - \psi\left(\tfrac{1}{2} + i\nu\right)\right]}{\nu^2 + \tfrac{1}{4}}$$

$$+ \frac{2\times 10}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}\nu\,\frac{\left[\psi(1) - \psi\left(\tfrac{1}{2} - i\nu\right)\right]^3\left[\psi(1) - \psi\left(\tfrac{1}{2} + i\nu\right)\right]^2}{\nu^2 + \tfrac{1}{4}}.$$

We get

$$f_5 = -10\left[-13\zeta(5) + 18\zeta(2)\zeta(3) + 20\sum_{k=1}^{\infty}\frac{[S_1^3(k) + 3S_1(k)S_2(k) + 2S_3(k)]}{k^2}\right.$$

$$-42\sum_{k=1}^{\infty}\frac{[S_1^2(k) + S_2(k)]}{k^3} + 38\sum_{k=1}^{\infty}\frac{S_1(k)}{k^4} + 48\sum_{k=1}\frac{S_2(k)}{k^3}$$

$$\left.-72\sum_{k=1}^{\infty}\frac{S_1(k)S_2(k) + S_3(k)}{k^2} + 32\sum_{k=1}^{\infty}\frac{S_3(k)}{k^2}\right].$$

With (see below)

$$\sum_{k=1}^{\infty}\left\{\frac{S_1^3(k) + 3S_1(k)S_2(k) + 2S_3(k)}{k^2}\right\} = 4!\zeta(5),$$

$$\sum_{k=1}^{\infty}\frac{\{S_1^2(k) + S_2(k)\}}{k^3} = 2\zeta(2)\zeta(3) - \zeta(5),$$

$$\sum_{k=1}^{\infty}\frac{S_1(k)}{k^4} = 3\zeta(5) - \zeta(2)\zeta(3),$$

$$\sum_{k=1}^{\infty}\frac{S_2(k)}{k^3} = \frac{1}{2}[6\zeta(2)\zeta(3) - 9\zeta(5)]$$

$$= \zeta(2)\zeta(3) + \zeta(5) - \sum_{k=1}^{\infty}\frac{S_3(k)}{k^2},$$

$$\sum_{k=1}^{\infty}\frac{S_1(k)S_2(k) + S_3(k)}{k^2} = \zeta(5) + \zeta(2)\zeta(3),$$

we get

$$f_5 = -10[115\zeta(5) + 48\zeta(2)\zeta(3)]. \tag{A.7}$$

The higher orders contributions can be calculated the same way. It involves more and more resummations. But since we have already obtained a very good approximation for f_k, we do not compute the 6th order contribution although it can be done exactly.*

To conclude this appendix, we show how to get the different terms. This can be done using the following technique which implies the properties of the Mellin moments.

* After the submission of this paper, we have computed the 6th order term. As expected, the ratio f_6/h_6 is very close to 1, $f_6/h_6 = 1.0026$.

Let $a_n(b_n)$ be the nth Mellin moment of a function $a(x)$ $(b(x))$, namely $an = \int_0^1 x^{n-1} a(x)\,\mathrm{d}x$. Then

$$\sum_{n=1}^{\infty} a_n = \int_0^1 \frac{a(x)\,\mathrm{d}x}{1-x} = \int_0^1 a'(x) \ln(1-x)\,\mathrm{d}x \qquad \text{if } a(1)=0,$$

and

$$\sum_{n=1}^{\infty} a_n b_n = \int_0^1 \frac{c(x)\,\mathrm{d}x}{1-x} = +\int_0^1 c'(x)\ln(1-x)\,\mathrm{d}x,$$

where $c(x) = \int_x^1 a(x')b(x/x')\,\mathrm{d}x'/x'$ is the convolution of $a(x)$ and $b(x)$; $c(1)=0$. The last trick [23] is to calculate $d_n = \Sigma_{k=1}^{n} a_k$. d_n is the Mellin moment of $d(x) = -[xa(x)/(1-x)]_+ + \delta(1-x)$, where $[xa(x)/(1-x)]_+$ is the usual distribution. Indeed,

$$\begin{aligned} d_n &= -\int_0^1 (x^{n-1} - 1)\frac{xa(x)}{1-x}\,\mathrm{d}x + 1 \\ &= \sum_{k=1}^{n} \int_0^1 x^{k-1} a(x)\,\mathrm{d}x = \sum_{k=1}^{n} a(k). \end{aligned}$$

In the following, we will use extensively the notations and results of Kölbig [24], Duke and Devoto [25] and Lewin [26].

Let us define the Nielsen functions [27]

$$L_{n,p}(z) = \frac{(-1)^{n-p+1}}{(n-1)!p!}\int_0^z \ln^{n-1}t \ln^p(1-t)\frac{\mathrm{d}t}{t}, \qquad L_{0,p}(z) \equiv 0,$$

$$S_{n,p}(z) = \frac{(-1)^{n-p+1}}{(n-1)!p!}\int_0^z \ln^{n-1}t \ln^p(1-zt)\frac{\mathrm{d}t}{t}, \qquad \frac{\mathrm{d}}{\mathrm{d}z}S_{n,p}(z) = \frac{1}{z}S_{n-1,p}(z),$$

$$L_{n,p}(z) = \sum_{j=0}^{n-1} \frac{(-1)^j z}{j!} S_{n-j,p}(z),$$

and $S_{n,1}(z) \equiv \mathrm{Li}_{n+1}(z)$ [26] where $\mathrm{Li}_p(z)$ is the polylogarithm function of order p, $\mathrm{Li}_2(z) = -\int_0^z \ln(1-t)\,\mathrm{d}t/t$. Then for $q \geqslant 1$, $S_q(n)/n$ is the nth moment of

$$G_q(x) = L_{q-1,1}(x) + \frac{(-1)^q}{(q-1)!}\ln^{q-1}x \ln(1-x);$$

for instance

$$G_1(x) = -\ln(1-x),$$

$$G_2(x) = \mathrm{Li}_2(x) + \ln x \ln(1-x),$$

$$G_3(x) = \mathrm{Li}_3(x) - \ln x\,\mathrm{Li}_2(x) - \tfrac{1}{2}\ln^2 x \ln(1-x).$$

As an illustration, for $q=1$, $S_1(n)/n$ is the nth moment of $G_1(x) = -\ln(1-x)$. Thus $S_1(n)/n^2$ is the moment of $1 \otimes G_1 = -\int_\rho^1 \ln(1-x)\,\mathrm{d}x/x = \zeta(2) - \mathrm{Li}_2(x)$ and

$$\sum_{n=1}^{\infty} \frac{S_1(n)}{n^2} = \int_0^1 [\zeta(2) - \mathrm{Li}_2(x)] \frac{\mathrm{d}x}{1-x}$$

$$= -\int_0^1 \ln(1-x) G_1(x) \frac{\mathrm{d}x}{x} = 2\zeta(3).$$

Noticing that $\mathrm{Li}_p(x) = \sum_{n=1}^{\infty} x^n/n^p$, then

$$\int_0^1 G_q(x) \mathrm{Li}_{p-1}(x) \frac{\mathrm{d}x}{x} = \sum_{n=1}^{\infty} \frac{1}{n^{p-1}} \int_0^1 x^{n-1} G_q(x)\,\mathrm{d}x = \sum_{n=1}^{\infty} \frac{S_q(n)}{n^p}$$

and

$$\sum_{n=1}^{\infty} \frac{S_1(n)}{n^2} = \int_0^1 \ln^2(1-\rho) \frac{\mathrm{d}\rho}{\rho} = 2\zeta(3),$$

$$\sum_{n=1}^{\infty} \frac{S_1(n)}{n^3} = -\int_0^1 \ln(1-\rho) \mathrm{Li}_2(\rho) \frac{\mathrm{d}\rho}{\rho} = \tfrac{1}{2}\zeta^2(2),$$

$$\sum_{n=1}^{\infty} \frac{S_1(n)}{n^4} = -\int_0^1 \ln(1-\rho) \mathrm{Li}_3(\rho) \frac{\mathrm{d}\rho}{\rho} = 3\zeta(5) - \zeta(2)\zeta(3),$$

$$\sum_{n=1}^{\infty} \frac{S_2(n)}{n^2} = -\int_0^1 [\mathrm{Li}_2(\rho) + \ln\rho \ln(1-\rho)] \ln(1-\rho) \frac{\mathrm{d}\rho}{\rho} = \tfrac{1}{2}[\zeta^2(2) + \zeta(4)],$$

$$\sum_{n=1}^{\infty} \frac{S_2(n)}{n^3} = -\int_0^1 [\mathrm{Li}_2(\rho) + \ln\rho \ln(1-\rho)] \mathrm{Li}_2(\rho) \frac{\mathrm{d}\rho}{\rho} = 3\zeta(2)\zeta(3) - \tfrac{9}{2}\zeta(5).$$

Note that

$$\sum_{n=1}^{\infty} \left(\frac{S_p(n)}{n^q} + \frac{S_q(n)}{n^p} \right) = \zeta(p)\zeta(q) + \zeta(p+q),$$

provided p and $q > 1$, so that

$$\sum_{n=1}^{\infty} \frac{S_3(n)}{n^2} = \zeta(2)\zeta(3) + \zeta(5) - \sum_{n=1}^{\infty} \frac{S_2(n)}{n^3} = -\zeta(2)\zeta(3) + \tfrac{11}{2}\zeta(5).$$

For the other sums, we use the trick that $\frac{1}{2}(S_1^2(n) + S_2(n)$ is the nth moment of $(\rho(\ln(1-\rho))/(1-\rho))_+ + \delta(1-\rho)$, $\frac{1}{6}\{S_1^3(n) + 3S_1(n)S_2(n) + 2S_3(n)\}$ is the nth moment of $-\frac{1}{2}(\rho(\ln^2(1-\rho)/(1-\rho))_+ + \delta(1-\rho)$ and $S_1(n)S_2(n) + S_3(n)$ is the nth moment of $-(\rho(\zeta(2) + \ln\rho\ln(1-\rho))/(1-\rho))_+ + 2\delta(1-\rho)$. Indeed

$$\sum_{i \leqslant j=1}^{n} \frac{1}{ij} = \tfrac{1}{2}\left(S_1^2(n) + S_2(n)\right),$$

$$\sum_{i \leqslant j \leqslant k=1}^{n} \frac{1}{ijk} = \tfrac{1}{6}S_1^3(n) + \tfrac{1}{2}S_1(n)S_2(n) + \tfrac{1}{3}S_3(n),$$

and

$$S_1(n)S_2(n) + S_3(n) = \sum_{k=1}^{n} \frac{S_1(k)}{k^2} + \sum_{k=1}^{n} \frac{S_2(k)}{k},$$

$$1 \otimes \left[\left(\frac{\rho\ln(1-\rho)}{1-\rho}\right)_+ + \delta(1-\rho)\right] = \tfrac{1}{2}\ln^2(1-\rho),$$

$$-1 \otimes \left[\left(\frac{\rho\ln^2(1-\rho)}{1-\rho}\right)_+\right] + \delta(1-\rho) = -\tfrac{1}{3}\ln^3(1-\rho),$$

$$1 \otimes \left[-\frac{(\rho(\zeta(2) + \ln\rho\ln(1-\rho)))}{1-\rho}\right]_+ + 2\delta(1-\rho)$$

$$= S_{1,2}(\rho) - \tfrac{1}{2}\ln\rho\ln^2(1-\rho) - \zeta(2)\ln(1-\rho),$$

so that

$$\sum_{n=1}^{\infty} \frac{S_1^2(n) + S_2(n)}{n^2} = -\int_0^1 \ln^2(1-\rho)\ln(1-\rho)\frac{\mathrm{d}\rho}{\rho} = 3!\zeta(4),$$

$$\sum_{n=1}^{\infty} \frac{S_1^3(n) + 3S_1(n)S_2(n) + 2S_3(n)}{n^2} = \int_0^1 \ln^3(1-\rho)\ln(1-\rho)\frac{\mathrm{d}\rho}{\rho} = 4!\zeta(5).$$

Similarly

$$1 \otimes 1 \otimes \left[\left(\frac{\rho\ln(1-\rho)}{1-\rho}\right)_+ + \delta(1-\rho)\right] = \tfrac{1}{2}\int_0^1 \ln^2(1-\rho')\frac{\mathrm{d}\rho'}{\rho'} = -S_{1,2}(\rho) + \zeta(3).$$

Thus

$$\frac{1}{2}\sum_{n=1}^{\infty}\left(\frac{S_1^2(n)+S_2(n)}{n^3}\right)=-\int_0^1[\zeta(3)-S_{1,2}(\rho)]\frac{\ln(1-\rho)}{\rho}\,\mathrm{d}\rho$$

$$=\zeta(2)\zeta(3)-\tfrac{1}{2}\zeta(5).$$

More generally,

$$\sigma_q(n)=\sum_{1\leqslant i_1\leqslant i_2\leqslant\cdots\leqslant i_q\leqslant n}\frac{1}{i_1\ldots i_q}$$

is the nth moment of

$$\frac{(-1)^q}{(q-1)!}\left(\frac{\rho\ln^{q-1}(1-\rho)}{1-\rho}\right)_+ +\delta(1-\rho),$$

where $\sigma_q(n)$ is the permanent of the $q\times q$ matrix M [28]

$$M=\frac{1}{1!}\begin{vmatrix} S_1(n) & S_2(n) & S_3(n) & S_q(n)\\ 1 & S_1(n) & S_2(n) & S_{q-1}(n)\\ & 2 & S_1(n) & S_{q-2}(n)\\ 0 & & \cdots & \cdots\\ & & (q-1) & S_1(n)\end{vmatrix}.$$

For instance,

$$\sum_{1\leqslant i_1\leqslant n}\frac{1}{i_1}=S_1(n),$$

$$\sum_{1\leqslant i_1\leqslant i_2\leqslant n}\frac{1}{i_1 i_2}=\left[S_1^2(n)+S_2(n)\right]\frac{1}{2!},$$

$$\sum_{i\leqslant i_1\leqslant i_2\leqslant i_3\leqslant n}\frac{1}{i_1 i_2 i_3}=\left[S_1^3(n)+3S_1(n)S_2(n)+2S_3(n)\right]\frac{1}{3!}.$$

Thus $(1/n)\sigma_q(n)$ is the nth moment of

$$\frac{(-1)^q}{(q-1)!}1\otimes\left[\left(\frac{\rho\ln^{q-1}(1-\rho)}{1-\rho}\right)_+ +\delta(1-\rho)\right]=\frac{(-1)^q}{q!}\ln^q(1-\rho)$$

and

$$\sum_{n=1}^{\infty} \frac{\sigma_q(n)}{n^2} = -\frac{(-1)^q}{q!} \int_0^1 \ln^q(1-\rho)\ln(1-\rho)\frac{\mathrm{d}\rho}{\rho} = (q+1)\zeta(q).$$

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