Analysis of quantities used in the graphical characterization of the critical inverse temperature in the annealed Potts model on rank-1 random graphs where the vertex weights have the indicator function of the unit interval as pdf

A.J.E.M. Janssen
Eindhoven University of Technology
Department of Mathematics and Computer Science

Abstract.
We consider in this work the quantities t_c, t_b and t_* that are used in the graphical construction in [1], Section 5.1, for the critical inverse temperature β_c in the annealed ferromagnetic q-state Potts model on sparse rank-1 random graphs in which the vertices have as weight density the indicator function $\mathcal{X}_{[0,1)}(w)$, $w \geq 0$, of the unit interval. We work under the assumption that the external field (called B in [1]) is equal to 0. A similar effort has been made for the case of Pareto weight densities $(\tau-1)\, w^{-\tau}\, \mathcal{X}_{[1,\infty)}(w)$, $w \geq 0$, for $\tau \geq 4$ in [2], and we follow the plan of [2] to some extent, although the obtained results and proofs differ considerably. In [1], Section 5.1, a geometric construction of t_c is given by considering the graph of the canonical function $\mathcal{F}_0(t) = \mathbb{E}\,[W(e^{tW}-1)/(\mathbb{E}\,[W]\,(e^{tW}+q-1))]$, $t \geq 0$, where W is the random weight variable. This $\mathcal{F}_0(t)$ increases in $t \geq 0$ from 0 to 1 as t increases from 0 to ∞. Under a rather general condition on the pdf of W, satisfied by the Pareto pdf with $\tau \geq 4$ and by $\mathcal{X}_{[0,1)}(w)$, $w \geq 0$, the function $\mathcal{F}_0(t)$ is strictly convex in $t \in [0, t_*)$ and strictly concave in $t \in (t_*, \infty)$, where $t_* > 0$ is the unique inflection point of $\mathcal{F}_0(t)$,

$t \geq 0$. The critical inverse temperature β_c and t_c are related according to $\beta_c = \ln[1 + \gamma_c]$, where $\gamma_c = t_c/\mathcal{F}_0(t_c)$. As a consequence of the convexity properties of $\mathcal{F}_0(t)$, any straight line $(t, l_\gamma(t))$, $t \geq 0$, through the origin (0,0) with slope γ^{-1} satisfying $\mathcal{F}_0'(0) = \min_{t\geq 0}[\mathcal{F}_0(t)/t] < \gamma^{-1} < \max_{t\geq 0}[\mathcal{F}_0(t)/t]$ intersects the graph of $\mathcal{F}_0$ in exactly three points $(t_0, \mathcal{F}_0(t_0))$, $(t_1, \mathcal{F}_0(t_1))$ and $(t_2, \mathcal{F}_0(t_2))$ with $0 = t_0 < t_1 < t_2$. Furthermore, we have $0 < \mathcal{F}_0(t) < l_\gamma(t)$, $t_0 = 0 < t < t_1$, and $\mathcal{F}_0(t) > l_\gamma(t)$, $t_1 < t < t_2$. Now γ_c is the unique $\gamma > 0$ such that the regions $\{(t, s) \,|\, 0 < t < t_1,\ \mathcal{F}_0(t) < s < l_\gamma(t)\}$ and $\{(t, s) \,|\, t_1 < t < t_2,\ l_\gamma(t) < s < \mathcal{F}_0(t)\}$ have equal area. In [2], Figure 1, we illustrate this "equal area" characterization for the homogeneous case in which $W \equiv 1$. Along with t_* and t_c, a key role in the graphical construction is played by the point t_b which is the unique $t > 0$ such that $\mathcal{F}_0(t)/t$ is maximal; we have $0 < t_* < t_b < t_c$.

More analytially, in [1], Theorem 1.14 (which is about the case $B = 0$), it is shown that t_c can also be obtained as the unique positive zero of a function $\mathcal{K}$ that combines the stationarity condition and the criticality condition imposed on the annealed pressure. From the proof of [1], Theorem 1.14, it is seen that $\mathcal{K}'$ and $\mathcal{K}''$ also have a unique positive zero, which we call t_c' and t_c'', respectively, and that $t_c' = t_b$ and $t_c'' = t_*$. We analyze (in the case of the weight density $\mathcal{X}_{[0,1)}$) t_c, t_c' and t_c'', with general $q > 2$, using, as in [2], an appropriate formulation of their defining equation as unique positive zero of $\mathcal{K}$, $\mathcal{K}'$ and $\mathcal{K}''$, respectively. These defining equations contain in all three cases elementary functions, combined with one and the same integral expression that can be evaluated in terms of the Euler dilogarithm Li_2. Hence, in the case of weight density $\mathcal{X}_{[0,1)}$, the functions $\mathcal{K}(t)$, $\mathcal{K}'(t)$ and $\mathcal{K}''(t)$ can be computed and plotted for $t \geq 0$, using basic software packages such as Mathematica. Using these tools, the bounds $\frac{5}{2}\ln(q-1) < t_c < 3\ln(q-1)$, $\sqrt{3}\ln(q-1) < t_c' < \frac{15}{8}\ln(q-1)$ and $\ln(q-1) < t_c'' < \frac{5}{4}\ln(q-1)$ can be established by numerical inspection for all $q > 2$, and thus suggest what one could prove analytically. We show analytically that $\ln(q-1) < t_c'' < t_c' < 2\ln(q-1) < t_c < 3\ln(q-1)$ for all $q > 2$. Furthermore, we show that $t_c > \frac{5}{2}\ln(q-1)$, $t_c' < \frac{15}{8}\ln(q-1)$ and $t_c'' < \frac{5}{4}\ln(q-1)$ when $q-2$ is small positive and that t_c, t_c' and t_c'' behave as $3\ln(q-1)$, $\sqrt{3}\ln(q-1)$ and $\ln(q-1)$, respectively, as $q \to \infty$. We conclude by presenting a formula for the quantity $\gamma_c = t_c/\mathcal{F}_0(t_c)$, that appears in the expression $\ln(1+\gamma_c)$ for the critical inverse temperature, in which only elementary functions of t_c (and no integrals) occur.

1 Introduction

We repeat, for self-containedness, a large part of [2], Section 1. In [1], a comprehensive study has been made of the annealed ferromagnetic q-state Potts model on sparse rank-1 random graphs, where vertices are equipped with a vertex weight and where the probability of an edge is proportional to the product of the weights of the involved vertices. Under a rather general condition on the weight distribution, phase transition is first order, with a unique discontinuity of the order parameter, see [1], Abstract and Section 1. Let $\beta > 0$ denote the inverse temperature, and let $\gamma = e^{\beta} - 1$ (in [1] one writes β' instead of γ, but in the present work, the prime $'$ has been reserved to indicate differentiation). Assume that the external field B equals 0 and that $\mathbb{E}\,[|W|^2] < \infty$, where W is the non-negative random weight variable. Consider the function

$$\mathcal{F}_0(t) = \mathbb{E}\left[\frac{W}{\mathbb{E}\,[W]}\,\frac{e^{tW}-1}{e^{tW}+q-1}\right], \qquad t \geq 0\ . \tag{1}$$

The function $\mathcal{F}_0(t)$ is non-negative, with $\mathcal{F}(0) = 0$, strictly increasing and $\mathcal{F}_0(t) \to 1$, $t \to \infty$. Assume that $\mathcal{F}_0''(t)$ is first negative and then positive, so that $\mathcal{F}_0(t)$ has a unique inflection point $t_* > 0$ with $\mathcal{F}_0''(t_*) = 0$ and $\mathcal{F}_0''(t) > 0$, $0 < t < t_*$, and $\mathcal{F}_0''(t) < 0$, $t > t_*$. Also consider the annealed pressure

$$p(t,\gamma) = \mathbb{E}\,[\ln(e^{tW}+q-1)] - \mathbb{E}\,[W]\,\frac{\gamma}{2q}\left((q-1)\left(\frac{t}{\gamma}\right)^2 + 2\,\frac{t}{\gamma} - 1\right) \tag{2}$$

for $t \geq 0$ and $\gamma \geq 0$. Under the above condition on $\mathcal{F}_0$, there is a unique pair (t_c, γ_c) with $t_c > 0$, $\gamma_c > 0$ such that simultaneously the stationarity condition

$$\mathcal{F}_0(t) = \frac{t}{\gamma} \tag{3}$$

and the criticality condition

$$p(t,\gamma) = p(0,\gamma) \tag{4}$$

is satisfied by $(t,\gamma) = (t_c,\gamma_c)$. The criticality condition can be written as

$$\frac{1}{\mathbb{E}\,[W]}\,\mathbb{E}\left[\ln\Big(\frac{e^{tW}+q-1}{q}\Big)\right] - \frac{q-1}{2q}\,\frac{t^2}{\gamma} - \frac{t}{q} = 0\ . \tag{5}$$

In Theorem 1.14 of [1] about the critical inverse temperature $\beta_c = \ln(1+\gamma_c)$, there is considered the function

$$\mathcal{K}(t) = \frac{1}{\mathbb{E}\,[W]}\,\mathbb{E}\left[\ln\Big(\frac{e^{tW}+q-1}{q}\Big)\right] - \frac{q-1}{2q}\,t\,\mathcal{F}_0(t) - \frac{t}{q}\ , \qquad t \geq 0\ . \tag{6}$$

This function $\mathcal{K}$ is obtained from the left-hand side of (5) by eliminating γ using (3). By [1], Theorem 1.14, t_c is the unique $t > 0$ such that $\mathcal{K}(t) = 0$, and

$$\beta_c = \ln\Big(1 + \frac{t_c}{\mathcal{F}_0(t_c)}\Big) \ . \tag{7}$$

The proof of [1], Theorem 1.14, furthermore shows that

$$\mathcal{K}'(t) = \frac{q-1}{2q}\,[\mathcal{F}_0(t) - t\,\mathcal{F}_0'(t)] \ , \qquad t \geq 0 \ , \tag{8}$$

$$\mathcal{K}''(t) = -\,\frac{q-1}{2q}\,t\,\mathcal{F}_0''(t) \ , \qquad t \geq 0 \ . \tag{9}$$

According to [1], Section 5.1 for the case $B = 0$, there are unique numbers $t_* > 0$, $t_b > 0$ such that $t_* < t_b < t_c$ and

$$\mathcal{F}_0''(t_*) = 0 \ , \qquad \mathcal{F}_0(t_b) - t_b\,\mathcal{F}_0'(t_b) = 0 \ . \tag{10}$$

Denoting the unique positive zeros of $\mathcal{K}$, $\mathcal{K}'$ and $\mathcal{K}''$ by t_c, t_c' and t_c'', respectively, we thus see that

$$t_c = t_c \ , \qquad t_c' = t_b \ , \qquad t_c'' = t_* \ , \tag{11}$$

where we also refer to [1], Figure 1. Thus, in particular, $0 < t_c'' < t_c' < t_c < \infty$. Hence, $t_c'' = t_*$ and $t_c' = t_b$ have a geometric meaning in terms of the graph of $\mathcal{F}_0$ (inflection point and point determining the non-trivial tangent line that passes through the origin, respectively). We can find for t_c such a geometric meaning as well. Integrating (8) from 0 to $T \geq 0$, using $\mathcal{K}(0) = 0$ and partial integration, we get

$$\mathcal{K}(T) = \frac{q-1}{q}\,\left(\int_0^T \mathcal{F}_0(t)\,dt - \tfrac{1}{2}\,T\,\mathcal{F}_0(T)\right) \ , \qquad T \geq 0 \ . \tag{12}$$

Taking $T = t_c$, the condition $\mathcal{K}(t_c) = 0$ means that

$$\int_0^{t_c} \mathcal{F}_0(t)\,dt = \tfrac{1}{2}\,t_c\,\mathcal{F}_0(t_c) = \int_0^{t_c} t\,\mathcal{F}_0(t_c)/t_c\,dt = \int_0^{t_c} t/\gamma_c\,dt \ , \tag{13}$$

where we recall from (3) that $\gamma_c = t_c/\mathcal{F}_0(t_c)$. The line $(t, t/\gamma_c)$ intersects the graph of $\mathcal{F}_0$ at exactly three points $(t_0, \mathcal{F}_0(t_0))$, $(t_1, \mathcal{F}_0(t_1))$ and $(t_2, \mathcal{F}_0(t_2))$, where $t_0 < t_1 < t_2$ with $t_0 = 0$ and $t_2 = t_c$. Furthermore, $\mathcal{F}_0(t) < t/\gamma_c$, $0 = t_0 < t < t_1$, and $\mathcal{F}_0(t) > t/\gamma_c$, $t_1 < t < t_2 = t_c$. From (13), we have

$\int_0^{t_c} (\mathcal{F}_0(t) - t/\gamma_c)\, dt = 0$, and so the regions $\{(t,s)\,|\,0 < t < t_1,\ \mathcal{F}_0(t) < s < t/\gamma_c\}$ and $\{(t,s)\,|\,t_1 < t < t_c,\ t/\gamma_c < s < \mathcal{F}_0(t)\}$ have equal area. In Figure 1 of [2], this "equal area" condition is illustrated for the case of homogeneous $W \equiv 1$ and $q = 100$ (also compare [1], Proposition 5.6). Figure 1 at the end of Section 3 illustrates the "equal area" condition in the present context.

We have $\mathcal{K}(0) = \mathcal{K}'(0) = \mathcal{K}''(0) = 0$ while $\mathcal{K}(t)$ is negative for small positive t and positive for large positive $t > 0$. Hence, $\mathcal{K}$, $\mathcal{K}'$ and $\mathcal{K}''$ are first negative and then positive, and for all $t > 0$, we have

$$t < t_c \Leftrightarrow \mathcal{K}(t) < 0\ ; \qquad t > t_c \Leftrightarrow \mathcal{K}(t) > 0\ , \tag{14}$$

$$t < t_c' \Leftrightarrow \mathcal{K}'(t) < 0\ ; \qquad t > t_c' \Leftrightarrow \mathcal{K}'(t) > 0\ , \tag{15}$$

$$t < t_c'' \Leftrightarrow \mathcal{K}''(t) < 0\ ; \qquad t > t_c'' \Leftrightarrow \mathcal{K}''(t) > 0\ . \tag{16}$$

2 Main results

We are interested in bounds and approximations of t_c, t_c' and t_c'' for $q > 2$ in the particular case that the density of W is given by the indicator function of the unit interval,

$$f_W(w) = \mathcal{X}_{[0,1)}(w)\ , \qquad w \geq 0\ . \tag{17}$$

A similar effort has been done for the case that $f_W(w) = (\tau{-}1)\, w^{-\tau}\, \mathcal{X}_{[0,\infty)}(w)$, $w \geq 0$, with $\tau \geq 4$, in [2], and for the case that $f_W(w) = \exp(-w)\, \mathcal{X}_{[0,\infty)}(w)$, $w \geq 0$, in [3]. In these three cases, $\mathcal{F}_0$ of (1) has a unique positive inflection point $t_* = t_c''$ by Theorem 1.21 in [1].

When the density of W is given by (17), we have $\mathbb{E}[W] = 2$, and, for $q > 2$ and $t > 0$

$$\begin{aligned} \mathcal{F}_0(t) = \mathbb{E}\left[\frac{W}{\mathbb{E}[W]}\ \frac{e^{tW}-1}{e^{tW}+q-1}\right] &= 1 - \frac{q}{\mathbb{E}[W]}\,\mathbb{E}\left[\frac{W}{e^{tW}+q-1}\right] \\ &= 1 - 2q \int_0^1 \frac{w\, dw}{e^{tw}+q-1}\ . \end{aligned} \tag{18}$$

In Section 3, we shall show that for $t \geq 0$, $q > 2$

$$\begin{aligned} \mathcal{K}(t) &= \frac{1}{\mathbb{E}\,[W]}\,\mathbb{E}\,\Big[\ln\Big(\frac{e^{tW}+q-1}{q}\Big)\Big] - \frac{q-1}{q}\,t\,\mathcal{F}_0(t) - \frac{t}{q} \\ &= 2\int\limits_0^1 \ln\Big(\frac{e^{tw}+q-1}{q}\Big)\,dw - \frac{q-1}{2q}\,t\,\mathcal{F}_0(t) - \frac{t}{q}\;, \end{aligned} \tag{19}$$

and from this it follows that

$$\mathcal{K}(t) = 2\ln\Big(\frac{e^t+q-1}{q}\Big) - \frac{3q+1}{2q}\,t + 3(q-1)\,t\int\limits_0^1 \frac{w\,dw}{e^{tw}+q-1}\;, \tag{20}$$

$$\mathcal{K}'(t) = (q-1)\,\Big(\frac{1}{2q} + \frac{1}{e^t+q-1} - 3\int\limits_0^1 \frac{w\,dw}{e^{tw}+q-1}\Big)\;, \tag{21}$$

$$\mathcal{K}''(t) = \frac{q-1}{t}\,\Big(\frac{-t\,e^t}{(e^t+q-1)^2} - \frac{3}{e^t+q-1} + 6\int\limits_0^1 \frac{w\,dw}{e^{tw}+q-1}\Big)\;. \tag{22}$$

Observe that in the last line of (18) and at the right-hand sides of (20), (21) and (22), we have one and the same integral

$$D = D(t) = \int\limits_0^1 \frac{w\,dw}{e^{tw}+q-1}\;, \qquad t \geq 0\,,\quad q > 2\;. \tag{23}$$

Hence, in particular

$$\mathcal{F}_0(t) = 1 - 2q\,D(t)\;, \qquad t \geq 0\,,\quad q > 2\;. \tag{24}$$

In Section 3, we shall also show that for $t \geq 0$, $q > 2$

$$\begin{aligned} (q-1)\,D(t) &= \int\limits_0^1 \frac{w\,dw}{p^{xw-1}+1} \\ &= \frac{-\mathrm{Li}_2(-p) + \mathrm{Li}_2\Big(\dfrac{-1}{p^{x-1}}\Big) - x\ln p\ln\Big(1+\dfrac{1}{p^{x-1}}\Big)}{(x\ln p)^2}\;, \end{aligned} \tag{25}$$

where we have set

$$p = q - 1 \ , \qquad t = x \ln(q-1) = x \ln p \tag{26}$$

with $p > 1$ and $x > 0$. Furthermore, in (25), Li_2 is Euler's dilogarithm which is the analytic continuation to $z \in \mathbb{C}\backslash[1,\infty)$ of the function

$$-\int_0^z \frac{\ln(1-v)}{v}\, dv \ . \tag{27}$$

We refer to [4], [5] for extensive information on Li_2. In particular, we have

$$\mathrm{Li}_2(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^2} \ , \qquad |z| \leq 1 \ . \tag{28}$$

The Li_2-function is available in many software packages, and so the functions $\mathcal{F}_0$, $\mathcal{K}$, $\mathcal{K}'$ and $\mathcal{K}''$ can be computed and plotted. In Section 4, we use this to establish bounds on t_c, t_c' and t_c'' numerically. For instance, for t_c we proceed as follows. Choose an $x > 0$, and check whether $\mathcal{K}(x \ln(q-1)) > 0$ for all $q > 2$, with $\mathcal{K}(x \ln(q-1))$ computed and plotted as a function of $q > 2$ using (20),, (23) and (25). When $\mathcal{K}(x \ln(q-1)) > 0$, $q > 2$, indeed, we have that $t_c < x \ln(q-1)$, $q > 2$, by the criterion (14). When $\mathcal{K}(x \ln(q-1)) < 0$, $q > 2$, we have that $t_c > x \ln(q-1)$, $q > 2$. A similar procedure can be used to find upper and lower bounds for t_c' and t_c'' by using the criterion (15) and (16), respectively. Defining x_c, x_c' and x_c'' by

$$t_c = x_c \ln(q-1) \ , \qquad t_c' = x_c' \ln(q-1) \ , \qquad t_c'' = x_c'' \ln(q-1) \ , \tag{29}$$

it so appears numerically that for $q > 2$

$$\frac{5}{2} < x_c = \frac{t_c}{\ln(q-1)} < 3 \ , \qquad \sqrt{3} < x_c' = \frac{t_c'}{\ln(q-1)} < \frac{15}{8} \ ,$$

$$1 < x_c'' = \frac{t_c''}{\ln(q-1)} < \frac{5}{4} \ . \tag{30}$$

It seems hard to establish the inequalities in (30) by purely analytical means. However, also in Section 4, we shall show analytically for $q > 2$ the weaker result

$$1 < x_c'' < x_c' < 2 < x_c < 3 \ , \tag{31}$$

in which only the proof of the last inequality also requires some numerical help.

In Section 5 we shall show that, as $y = q - 2 \downarrow 0$,

$$t_c = \frac{5}{2}\Big(y - \frac{1}{2}\,y^2 + \Big(\frac{1}{3} + \frac{1}{84}\Big)\,y^3 + O(y^4)\Big)\ , \tag{32}$$

$$t_c' = \frac{15}{8}\Big(y - \frac{1}{2}\,y^2 + \Big(\frac{1}{3} - \frac{1}{336}\Big)\,y^3 + O(y^4)\Big)\ , \tag{33}$$

$$t_c'' = \frac{5}{4}\Big(y - \frac{1}{2}\,y^2 + \Big(\frac{1}{3} - \frac{1}{336}\Big)\,y^3 + O(y^4)\Big)\ . \tag{34}$$

Note that, as $y = q - 2 \downarrow 0$,

$$\ln(q-1) = \ln(1+y) = y - \tfrac{1}{2}\,y^2 + \tfrac{1}{3}\,y^3 + O(y^4)\ , \tag{35}$$

and this shows that in (30) we indeed have $x_c > \frac{5}{2}$, $x_c' < \frac{15}{8}$ and $x_c'' < \frac{5}{4}$ when $y = q - 2$ is small. These results are proved by using properties of the expansion coefficients $a_n(q)$ in

$$\frac{1}{e^z + q - 1} = \sum_{n=0}^{\infty} a_n(q)\,z^n\ , \qquad |z| \le \pi\ , \tag{36}$$

in a similar manner as in [3], Sections 5 and 6, and [2], proof of (193).

In Section 6, we consider the behaviour of t_c, t_c' and t_c'' as $q \to \infty$. With $p = q - 1$, we show that as $p \to \infty$

$$x_c = \frac{t_c}{\ln p} = 2 + \Big(1 - \frac{\pi^2}{\ln^2 p}\Big)^{1/2} + O\Big(\frac{1}{p \ln p}\Big)\ , \tag{37}$$

$$x_c' = \frac{t_c'}{\ln p} = \Big(3 + \frac{\pi^2}{\ln^2 p}\Big)^{1/2} + O\Big(\frac{1}{p^{\sqrt{3}-1}}\Big)\ , \tag{38}$$

$$x_c'' = \frac{t_c''}{\ln p} = 1 + O\Big(\frac{\ln(\ln p)}{\ln p}\Big)\ . \tag{39}$$

The proofs of these results are obtained from (20), (21), (22) and (23), (25), in which we may assume that $x > 1$ (see (31)), and the identity (see [4], [5])

$$-\mathrm{Li}_2(-p) = \tfrac{1}{2}\ln^2 p + \frac{\pi^2}{6} + \mathrm{Li}_2\Big(\frac{-1}{p}\Big)\ , \qquad p > 1\ , \tag{40}$$

so that the right-hand side of (25) can be replaced by an expression in which Li_2 with arguments $-1/p$ and $-1/p^{x-1}$ occurs, these arguments being small negative so that (28) can be used.

In Sectìon 7 we express the quantity $\gamma_c = t_c/\mathcal{F}_0(t_c)$, that appears in the formula (7) for the critical inverse temperature β_c, in a form that contains

only elementary functions of $x_c = t_c/\ln p$ (and no integrals). In $p = q-1$, $x = t\ln(q-1)$ notation, this gives the expression

$$\gamma_c = \frac{\frac{3}{4}\,x}{x - \Big(1+\frac{1}{p}\Big)\Big(1-\frac{r(x)}{\ln p}\Big)}\,t_c\ , \qquad x = x_c\ , \tag{41}$$

in which $r(x)$ for $x \geq 2$ is given by

$$r(x) := \ln\Big(\frac{1+p^{1-x}}{1+p^{-1}}\Big) \in \Big(-\ln\Big(1+\frac{1}{p}\Big), 0\Big)\ . \tag{42}$$

This yields for γ_c the inequality

$$\frac{\frac{3}{4}\,x}{x - \dfrac{p+1}{p}}\,t_c < \gamma_c < \frac{\frac{3}{4}\,x}{x - \dfrac{(p+1)\ln(p+1)}{p\ln p}}\,t_c\ , \qquad x = x_c\ , \tag{43}$$

As a consequence of $x_c \to 3$ as $p \to \infty$, we see that $\gamma_c/t_c \to 9/8$ as $p \to \infty$.

3 Proof of the representations (20), (21) and (22) and the identity (25)

We have by (19) for $q > 2$ and $t > 0$

$$\mathcal{K}(t) = 2\int_0^1 \ln\Big(\frac{e^{tw}+q-1}{q}\Big)\,dw - \frac{q-1}{2q}\,t\,\mathcal{F}_0(t) - \frac{t}{q}\ , \tag{44}$$

where $\mathcal{F}_0(t)$ is given by (18) as

$$\mathcal{F}_0(t) = 1 - 2q\int_0^1 \frac{w\,dw}{e^{tw}+q-1}\ . \tag{45}$$

By partial integration, we get

$$\int_0^1 \ln(e^{tw}+q-1)\,dw = w\ln(e^{tw}+q-1)\Big|_0^1 - \int_0^1 w\,\frac{t\,e^{tw}}{e^{tw}+q-1}\,dw$$

$$= \ln(e^t+q-1) - \int_0^1 wt\Big(1-\frac{q-1}{e^{tw}+q-1}\Big)\,dw$$

$$= \ln(e^t+q-1) - \tfrac{1}{2}\,t + (q-1)\,t\int_0^1 \frac{w\,dw}{e^{tw}+q-1}\ . \tag{46}$$

Combining (44), (45) and (46), we arrive at (20).

To show (21), we note that from (20)

$$\mathcal{K}'(t) = \frac{2e^t}{e^t+q-1} - \frac{3q+1}{2q} + 3(q-1)\,\frac{d}{dt}\left(t\int_0^1 \frac{w\,dw}{e^{tw}+q-1}\right)\ . \tag{47}$$

Now

$$\frac{d}{dt}\left(t\int_0^1 \frac{w\,dw}{e^{tw}+q-1}\right) = \frac{d}{dt}\left(\frac{1}{t}\int_0^t \frac{v\,dv}{e^v+q-1}\right)$$

$$= \frac{-1}{t^2}\int_0^t \frac{v\,dv}{e^v+q-1} + \frac{1}{t}\,\frac{t}{e^t+q-1} = -\int_0^1 \frac{w\,dw}{e^{tw}+q-1} + \frac{1}{e^t+q-1}\ , \tag{48}$$

and

$$\frac{2e^t}{e^t+q-1} = 2 - \frac{2(q-1)}{e^t+q-1}\ . \tag{49}$$

From (47), (48), we get (21).

Finally, we get the expression (22) for $\mathcal{K}''(t)$ by differentiation of (21), where we now note that

$$\frac{d}{dt}\left(\int_0^1 \frac{w\,dw}{e^{tw}+q-1}\right) = \frac{d}{dt}\left(\frac{1}{t^2}\int_0^t \frac{v\,dv}{e^v+q-1}\right)$$

$$= \frac{-2}{t}\int_0^1 \frac{w\,dw}{e^{tw}+q-1} + \frac{1}{t}\,\frac{1}{e^t+q-1}\ . \tag{50}$$

We next show the identity (25) with $D = D(t)$ given by (23). With $p = q - 1 > 1$ and $t = x \ln p > 0$, we have

$$(q-1)\, D(t) \;=\; \int\limits_0^1 \frac{(q-1)\, w\, dw}{e^{tw} + q - 1} = \int\limits_0^1 \frac{(q-1)\, w\, dw}{(q-1)^{xw} + q - 1}$$

$$= \int\limits_0^1 \frac{w\, dw}{(q-1)^{xw-1} + 1} = \int\limits_0^1 \frac{w\, dw}{p^{xw-1} + 1}\ . \tag{51}$$

When one uses WolframAlpha for evaluation of the last integral in (51) with integer $p \geq 1$ and integer $x \geq 1$, one gets exactly the expression at the right-hand side of (25). After some try-and-guess work, one is led to propose the required result in (25) for general $p > 1$ and $x > 0$.

We start the proof of (25) by setting $p = e^y$ with $y > 0$. Then we get

$$\int\limits_0^1 \frac{w\, dw}{p^{xw-1} + 1} = \int\limits_0^1 \frac{w\, dw}{p^{-1}\, \exp(xyw) + 1} = \frac{1}{(xy)^2} \int\limits_0^{xy} \frac{t\, dt}{p^{-1}\, e^t + 1}\ . \tag{52}$$

By the substitution $v = p^{-1}\, e^t$, we next get

$$(xy)^2 \int\limits_0^1 \frac{w\, dw}{p^{xw-1} + 1} = \int\limits_{p^{-1}}^{p^{x-1}} \frac{\ln p + \ln v}{v(v+1)}\, dv$$

$$= \int\limits_{p^{-1}}^{p^{x-1}} \ln p \Big(\frac{1}{v} - \frac{1}{v+1}\Big) + \int\limits_{p^{-1}}^{p^{x-1}} \frac{\ln v}{v}\, dv - \int\limits_{p^{-1}}^{p^{x-1}} \frac{\ln v}{v+1}\, dv\ . \tag{53}$$

Now

$$\int\limits_{p^{-1}}^{p^{x-1}} \ln p \Big(\frac{1}{v} - \frac{1}{v+1}\Big) = \ln p \ln(1+p) - \ln p \ln\Big(1 + \frac{1}{p^{x-1}}\Big)\ , \tag{54}$$

$$\int\limits_{p^{-1}}^{p^{x-1}} \frac{\ln v}{v}\, dv = \tfrac{1}{2} \ln^2 p^{x-1} - \tfrac{1}{2} \ln^2 p\ . \tag{55}$$

The last integral on the second line of (53) will produce the Li_2 function. For this we use that for $z > 0$

$$\begin{aligned}\mathrm{Li}_2(-z) &= -\int\limits_0^{-z} \frac{\ln(1-u)}{u}\,du = -\int\limits_0^{z} \frac{\ln(1+v)}{v}\,dv \\ &= -\int\limits_0^{z} \ln(1+v)\,d(\ln v) = -\ln z \ln(1+z) + \int\limits_0^{z} \frac{\ln v}{1+v}\,dv\ ,\end{aligned} \tag{56}$$

and so

$$\int\limits_0^{z} \frac{\ln v}{1+v}\,dv = \mathrm{Li}_2(-z) + \ln z \ln(1+z)\ , \qquad z > 0\ . \tag{57}$$

Thus we get

$$\begin{aligned}\int\limits_{p^{-1}}^{p^{x-1}} \frac{\ln v}{v+1}\,dv &= \mathrm{Li}_2(-p^{x-1}) + \ln(1+p^{x-1}) \ln p^{x-1} \\ &\quad - \Big(\mathrm{Li}_2\Big(-\frac{1}{p}\Big) + \ln\Big(1+\frac{1}{p}\Big) \ln\frac{1}{p}\Big)\ .\end{aligned} \tag{58}$$

Next, we use the formula

$$\mathrm{Li}_2(-z) + \mathrm{Li}_2\Big(-\frac{1}{z}\Big) = -\frac{\pi^2}{6} - \tfrac{1}{2}\ln^2 z\ , \qquad z > 0\ . \tag{59}$$

This gives

$$\begin{aligned}\int\limits_{p^{-1}}^{p^{x-1}} \frac{\ln v}{v+1}\,dv &= -\mathrm{Li}_2\Big(\frac{-1}{p^{x-1}}\Big) + \mathrm{Li}_2(-p) - \tfrac{1}{2}\ln^2 p^{x-1} + \tfrac{1}{2}\ln^2 p \\ &\quad + \ln(1+p^{x-1}) \ln p^{x-1} - \ln\Big(1+\frac{1}{p}\Big) \ln\frac{1}{p}\ .\end{aligned} \tag{60}$$

By combining (53), (54), (55) and (60), we get

$$(xy)^2 \int_0^1 \frac{w\,dw}{p^{xw-1}+1} = \mathrm{Li}_2\Big(\frac{-1}{p^{x-1}}\Big) - \mathrm{Li}_2(-p)$$

$$+ \ln p \ln(1+p) - \ln p \ln\Big(1+\frac{1}{p^{x-1}}\Big) + \tfrac{1}{2}\ln^2 p^{x-1} - \tfrac{1}{2}\ln^2 p$$

$$+ \tfrac{1}{2}\ln^2 p^{x-1} - \tfrac{1}{2}\ln^2 p - \ln(1+p^{x-1})\ln p^{x-1} + \ln\Big(1+\frac{1}{p}\Big)\ln\frac{1}{p}\ . \quad (61)$$

Finally, we use

$$\ln(1+p^{x-1})\ln p^{x-1} = \ln^2 p^{x-1} + (x-1)\ln p \ln\Big(1+\frac{1}{p^{x-1}}\Big)\ , \quad (62)$$

$$\ln\Big(1+\frac{1}{p}\Big)\ln\frac{1}{p} = -\ln p\ln(1+p) + \ln^2 p\ , \quad (63)$$

and we get

$$\begin{aligned}
(xy)^2 &\int_0^1 \frac{w\,dw}{p^{xw-1}+1} \\
&= -\mathrm{Li}_2(-p) + \mathrm{Li}_2\Big(\frac{-1}{p^{x-1}}\Big) + \ln p\ln(1+p) - \ln p\ln\Big(1+\frac{1}{p^{x-1}}\Big) \\
&\quad + \tfrac{1}{2}\ln^2 p^{x-1} - \tfrac{1}{2}\ln^2 p + \tfrac{1}{2}\ln^2 p^{x-1} - \tfrac{1}{2}\ln^2 p \\
&\quad - \Big(\ln^2 p^{x-1} + (x-1)\ln p\ln\Big(1+\frac{1}{p^{x-1}}\Big)\Big) + \ln^2 p - \ln p\ln(1+p) \\
&= -\mathrm{Li}_2(-p) + \mathrm{Li}_2\Big(\frac{-1}{p^{x-1}}\Big) - x\ln p\ln\Big(1+\frac{1}{p^{x-1}}\Big)\ . \quad (64)
\end{aligned}$$

Recalling that $y = \ln p$, we get the required result (25).

We illustrate how we can use the result (25) to plot $\mathcal{F}_0(t)$. To that end, we note that $\mathcal{F}_0(t)$ is expressed in terms of $D(t)$ by (24), and this yields

$$\mathcal{F}_0(x\ln p) = 1 + \frac{2q}{q-1}\,\frac{\mathrm{Li}_2(-p) - \mathrm{Li}_2\Big(\frac{-1}{p^{x-1}}\Big) + x\ln p\ln\Big(1+\frac{1}{p^{x-1}}\Big)}{(x\ln p)^2}\ , \quad (65)$$

where $p = q-1$, $t = x\ln p$ as usual. The right-hand side of (65) can be plotted as a function of $x \geq 0$, using the on Mathematica based website Wolfram

Alpha. We have done so in Figure 1 below for $q = p+1 = 100$ and $x \in [0, 4]$. We have also indicated on the x-axis the points x_c'', x_c' and x_c (that lie in $[0, 4]$ by (31)). These points can be computed as $t_c''/\ln p$, $t_c'/\ln p$ and $t_c/\ln p$, where t_c'', t_c' and t_c are the unique positive zeros of $\mathcal{K}''(t)$, $\mathcal{K}'(t)$ and $\mathcal{K}(t)$ given by (20), (21) and (22), respectively. The three functions $\mathcal{K}''$, $\mathcal{K}'$ and $\mathcal{K}$ have a closed-form expression in terms of Li_2 per (25). For the computation of t_c and t_c', we can use Newton's method involving $\mathcal{K}(t)$, $\mathcal{K}'(t)$ and $\mathcal{K}'(t)$, $\mathcal{K}''(t)$ given by (20), (21) and (21), (22), respectively, and where (30) gives a clue as to how to choose appropriate initial values for the Newton iteration. For the computation of t_c'', such a thing can be done as well, in principle, but then we should also have to compute a closed-form expression containing $D(t)$ for $\mathcal{K}'''(t)$. While this can be done, the resulting expressions are somewhat unwieldly. Instead, we have used a quasi-Newton method in which the value of $\mathcal{K}'''(t)$ is estimated from the values of $\mathcal{K}''$ at two successive iterands. The numerical values that we get are $x_c'' = 1.204820$, $x_c' = 1.811137$ and $x_c = 2.799170$. In Figure 1, we have also drawn the two tangent lines to the graph of $\mathcal{F}_0(x \ln p)$, $x \geq 0$, that pass through the origin $(0, 0)$. These tangent lines are given by $\{(x, x \ln p\, \mathcal{F}_0'(0)) \,|\, x \geq 0\}$ and $\{(x, x \ln p\, \mathcal{F}_0(t_c')/t_c') \,|\, x \geq 0\}$, respectively. Finally, we have also drawn the straight line through the origin $(0, 0)$ that passes through the point $(x_c, \mathcal{F}_0(x_c \ln p))$ and that is given by $\{(x, x \ln p/\gamma_c) \,|\, x \geq 0\}$ to illustrate the "equal area" condition.

4 Numerical and analytic bounds on t_c, t_c' and t_c''

The main strategy to find bounds on, for instance, t_c is to fix an $x > 0$ and to consider $\mathcal{K}(x \ln(q-1))$ as a function of $q > 2$. From (14), we have

– when $\mathcal{K}(x \ln(q-1)) > 0$ for all $q > 2$, we have that $t_c < x \ln(q-1))$ for all $q > 2$,

– when $\mathcal{K}(x \ln(q-1)) < 0$ for all $q > 2$, we have that $t_c > x \ln(q-1)$ for all $q > 2$.

With the availability of the formula (25) for $(q-1)\, D(t)$, involving the relatively standard function Li_2, and the formula (20) for $\mathcal{K}(t)$, one can plot $\mathcal{K}(x \ln(q-1))$ as a function of $q > 2$, and tell from the plot whether $\mathcal{K}(x \ln(q-1))$ is positive or negative for all $q > 2$. As to the choice of $x > 0$, we are guided by the results of Sections 5 and 6 that give the limiting behaviour of t_c (and of t_c' and t_c'') as $q - 2 \downarrow 0$ or as $q \to \infty$.

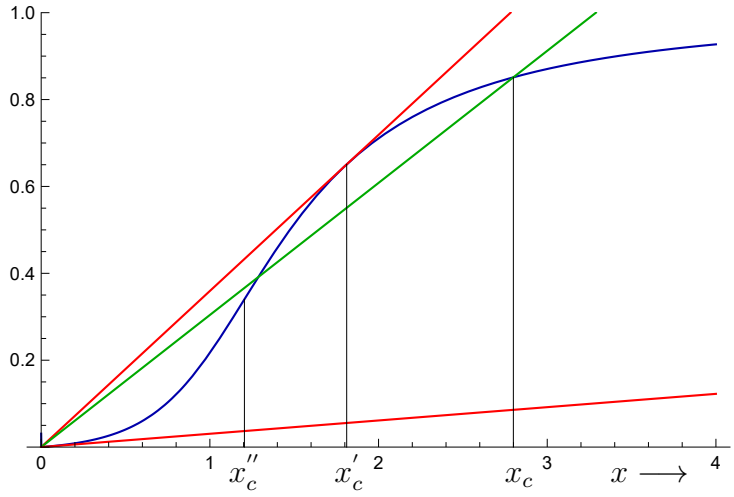

Figure 1: Plot of $\mathcal{F}_0(x \ln p)$, $x \in [0,4]$, where $\mathcal{F}_0$ is given in (24) with $D(t)$ expressed in terms of Li_2 per (25), with $p = q - 1 = 99$ (blue line). On the x-axis there are indicated $x_c'' = t_c''/\ln p$, $x_c' = t_c'/\ln p$ and $x_c = t_c/\ln p$, where t_c'', t_c' and t_c are the unique positive zeros of the functions $\mathcal{K}''(t)$, $\mathcal{K}'(t)$ and $\mathcal{K}(t)$ that are given in terms of $D(t)$ by (22), (21) and (20), respectively. We have $x_c'' = 1.204820$, $x_c' = 1.811137$ and $x_c = 2.799170$. Also drawn are the two tangent lines to the graph of $\mathcal{F}_0(x \ln p)$, $x \geq 0$, that pass through $(0,0)$ with lower slope $\mathcal{F}_0'(0) \ln p$ and higher slope $\mathcal{F}_0(x_c' \ln p)/x_c'$, respectively (red lines). The straight line through $(0,0)$ and $(x_c, \mathcal{F}_0(x_c \ln p))$, exhibiting the "equal area" condition for this case, is displayed as well (green line).

Thus for t_c we consider $\mathcal{K}(\frac{5}{2}\ln(q-1))$ and $\mathcal{K}(3\ln(q-1))$ and ask whether $\mathcal{K}(\frac{5}{2}\ln(q-1)) < 0 < \mathcal{K}(3\ln(q-1))$ for all $q > 2$. Using (25) for $(q-1)\,D$ in the formula (20) for $\mathcal{K}$, we have with $p = q - 1 > 1$

$$\mathcal{K}(\tfrac{5}{2}\ln p) = -\ln((1+p^{3/2})(1+p)^2) \;+\; \Big(\frac{11}{4} - \frac{5}{4\,(1+p)}\Big)\ln p \;-\; \frac{6}{5}\,\frac{\mathrm{Li}_2(-p) - \mathrm{Li}_2\Big(\frac{-1}{p^{3/2}}\Big)}{\ln p}\,, \tag{66}$$

$$\mathcal{K}(3\ln p) = -\ln((1+p^2)(1+p)^2) \;+\; \Big(\frac{7}{2} - \frac{3}{2(1+p)}\Big)\ln p$$

$$- \quad \frac{\mathrm{Li}_2(-p) - \mathrm{Li}_2\Big(\frac{-1}{p^2}\Big)}{\ln p} \ . \qquad (67)$$

In Figure 2 and 3 we display $\mathcal{K}(\frac{5}{2}\ln p)$ and $\mathcal{K}(3\ln p)$, $1 < p \leq 5$, and apparently $\mathcal{K}(\frac{5}{2}\ln p) < 0 < \mathcal{K}(3\ln p)$, $1 < p \leq 5$ (we have done this excercise also with many other ranges of p, always with the same conclusion). At the same time, for instance, $\mathcal{K}(2.8\ln p)$ is first positive (until $p \approx 100$) and then negative. In a similar fashion, we can consider $\mathcal{K}'(\sqrt{3}\ln p)$, $\mathcal{K}'(\frac{15}{8}\ln p)$, $\mathcal{K}''(\ln p)$ and $\mathcal{K}''(\frac{5}{4}\ln p)$, thereby establishing all the inequalities in (30) numerically.

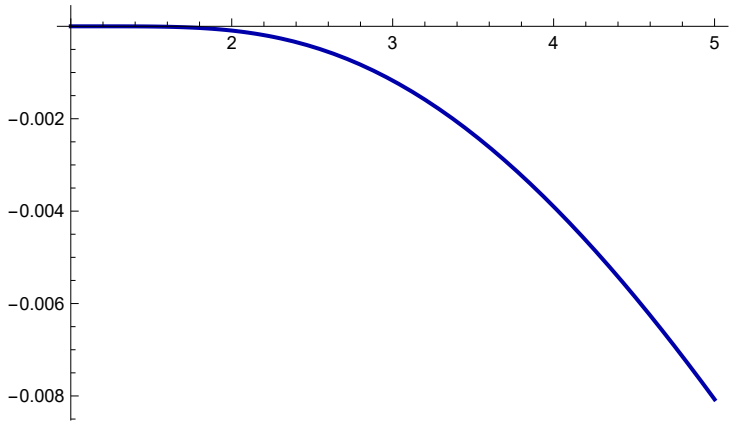

Figure 2: Plot of $\mathcal{K}(\frac{5}{2}\ln p)$, $p = q - 1 \in (1, 5]$ with $\mathcal{K}(\frac{5}{2}\ln p)$ computed according to equation (66).

We proceed now more analytically by proving the chain of (weaker) inequalities in (31). We start with the inequality $t_c'' = x_c'' \ln p > \ln p$ for which we must show that $\mathcal{K}''(\ln p) < 0$, $p > 1$, according to (16). We have from (22) with $t = \ln p$, $e^t = p$,

$$\begin{aligned} \mathcal{K}''(\ln p)\ln p &= \frac{-p^2 \ln p}{(2p)^2} - \frac{3p}{2p} + 6\int_0^1 \frac{pw\,dw}{p^w + p} \\ &= -\tfrac{1}{4}\ln p - \tfrac{3}{2} + 6\int_0^1 \frac{w\,dw}{p^{w-1}+1} \ . \end{aligned} \qquad (68)$$

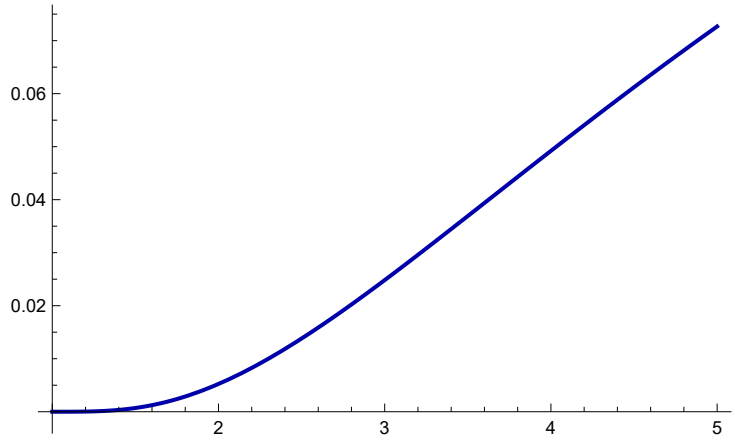

Figure 3: Plot of $\mathcal{K}(3\ln p)$, $p = q - 1 \in (1, 5]$ with $\mathcal{K}(3\ln p)$ computed according to equation (67).

We have from (25)

$$\int_0^1 \frac{w\,dw}{p^{w-1}+1} = \frac{-\mathrm{Li}_2(-p) + \mathrm{Li}_2(-1) - \ln 2 \ln p}{\ln^2 p} \ . \tag{69}$$

Next, from (40) and $\mathrm{Li}_2(-1) = -\frac{1}{12}\,\pi^2$,

$$-\mathrm{Li}_2(-p) + \mathrm{Li}_2(-1) = \tfrac{1}{2}\ln^2 p + \frac{\pi^2}{6} + \mathrm{Li}_2\Big(\frac{-1}{p}\Big) - \tfrac{1}{12}\,\pi^2$$

$$= \ \tfrac{1}{2}\ln^2 p + \mathrm{Li}_2\Big(-\frac{1}{p}\Big) - \mathrm{Li}_2(-1) = \tfrac{1}{2}\ln^2 p + \int_{1/p}^1 \frac{\ln(1+v)}{v}\,dv \ , \tag{70}$$

where we have used (56). Thus we get

$$\int_0^1 \frac{w\,dw}{p^{w-1}+1} = \frac{1}{2} + \frac{1}{\ln^2 p}\int_{1/p}^1 \frac{\ln(1+v)}{v}\,dv - \frac{\ln 2}{\ln p} \ , \tag{71}$$

and so

$$\mathcal{K}''(\ln p)\ln p = -\tfrac{1}{4}\ln p + \frac{3}{2} - \frac{6\ln 2}{\ln p} + \frac{6}{\ln^2 p}\int_{1/p}^1 \frac{\ln(1+v)}{v}\,dv \ . \tag{72}$$

We shall show that for $p > 1$

$$R(p) := \mathcal{K}''(\ln p)\ln^3 p = -\tfrac{1}{4}\ln^3 p + \tfrac{3}{2}\ln^2 p - 6\ln 2\ln p + 6\int\limits_{1/p}^{1}\frac{\ln(1+v)}{v}\,dv < 0\,. \tag{73}$$

We have $R(1) = 0$, and

$$R'(p) = -\frac{3}{4p}\ln^2 p + \frac{3}{p}\ln p - \frac{6\ln 2}{p} + 6\,\frac{\ln(1+1/p)}{p}\,. \tag{74}$$

We have that

$$p\,R'(p) = -\tfrac{3}{4}\ln^2 p + 3\ln p - 6\ln 2 + 6\ln\Big(1+\frac{1}{p}\Big) \tag{75}$$

vanishes at $p = 1$, while

$$(p\,R'(p))' = -\frac{3}{2}\,\frac{\ln p}{p} + \frac{3}{p} - \frac{6}{p(1+p)}\,. \tag{76}$$

Next

$$p(p\,R'(p))' = -\tfrac{3}{2}\ln p + 3 - \frac{6}{1+p} \tag{77}$$

vanishes at $p = 1$, while

$$(p(p\,R'(p))')' = -\frac{3}{2p} + \frac{6}{(1+p)^2} = -\frac{3}{2p}\Big(\frac{p-1}{p+1}\Big)^2 < 0\,, \qquad p > 1\,. \tag{78}$$

Therefore, we get subsequently that the left-hand sides of (77), (76), (75), (74), (73) and (72) are negative for $p > 1$, showing that $\mathcal{K}''(\ln p) < 0$, $p > 1$, as required.

The second inequality in (31), $x_c'' < x_c'$, follows from general theory (see below (11)), and we shall next show the third inequality in (31), $x_c' < 2$. For this we must show that $\mathcal{K}'(2\ln p) > 0$, $p > 1$, according to (15). We have from (21) with $t = 2\ln p$, $e^t = p^2$

$$\begin{aligned}\mathcal{K}'(2\ln p) &= \frac{p}{2(1+p)} + \frac{p}{p^2+p} - 3\int\limits_0^1 \frac{pw\,dw}{p^{2w}+p} \\ &= \frac{p+2}{2(1+p)} - 3\int\limits_0^1 \frac{w\,dw}{p^{2w-1}+1}\,. \end{aligned}\tag{79}$$

We have from (25)

$$-\int_0^1 \frac{w\,dw}{p^{2w-1}+1} = \frac{\mathrm{Li}_2(-p) - \mathrm{Li}_2\Big(\frac{-1}{p}\Big) + 2\ln p \ln\Big(1+\frac{1}{p}\Big)}{(2\ln p)^2}\ . \tag{80}$$

Next, from (40) and (56) as in (70),

$$\begin{aligned}\mathrm{Li}_2(-p) - \mathrm{Li}_2\Big(\frac{-1}{p}\Big) &= -\tfrac{1}{2}\ln^2 p - \frac{\pi^2}{6} - \mathrm{Li}_2\Big(\frac{-1}{p}\Big) - \mathrm{Li}_2\Big(-\frac{1}{p}\Big) \\ &= -\tfrac{1}{2}\ln^2 p + 2\mathrm{Li}_2(-1) - 2\mathrm{Li}_2\Big(\frac{-1}{p}\Big) = -\tfrac{1}{2}\ln^2 p - 2\int_{1/p}^1 \frac{\ln(1+v)}{v}\,dv\ .\end{aligned} \tag{81}$$

Hence,

$$\begin{aligned}\mathcal{K}'(2\ln p) &= \frac{p+2}{2(1+p)} - \frac{3}{8} + \frac{3}{2}\,\frac{\ln(1+1/p)}{\ln p} - \frac{3}{2\ln^2 p}\int_{1/p}^1 \frac{\ln(1+v)}{v}\,dv \\ &= \frac{1}{8} + \frac{1}{2(1+p)} + \frac{3}{2}\,\frac{\ln(1+1/p)}{\ln p} - \frac{3}{2\ln^2 p}\int_{1/p}^1 \frac{\ln(1+v)}{v}\,dv\ .\end{aligned} \tag{82}$$

We shall show that for $p > 1$

$$\begin{aligned}S(p) := \mathcal{K}'(2\ln p)\ln^2 p = \tfrac{1}{8}\ln^2 p + \frac{\ln^2 p}{2(1+p)} &+ \tfrac{3}{2}\ln p \ln(1+1/p) \\ &- \frac{3}{2}\int_{1/p}^1 \frac{\ln(1+v)}{v}\,dv > 0\ .\end{aligned} \tag{83}$$

We have $S(1) = 0$, and

$$\begin{aligned} S'(p) &= \frac{\ln p}{4p} + \frac{\frac{1}{p}\,(1+p)\ln p - \frac{1}{2}\ln^2 p}{(1+p)^2} + \frac{3\ln(1+1/p)}{2p} \\ &\quad - \frac{3\ln p}{2p(1+p)} - \frac{3\ln(1+1/p)}{2p} \\ &= \frac{\ln p}{4p} + \frac{\frac{1}{p}\,(1+p)\ln p - \frac{1}{2}\ln^2 p}{(1+p)^2} - \frac{3\ln p}{2p(1+p)}\ . \end{aligned} \tag{84}$$

We have $S'(1) = 0$. Furthermore,

$$\frac{p(1+p)^2}{\ln p}\,S'(p) = \tfrac{1}{4}\,(1+p)^2 - \tfrac{1}{2}\,(1+p) - \tfrac{1}{2}\,p\ln p \tag{85}$$

vanishes at $p = 1$, while

$$\Big(\frac{p(1+p)^2}{\ln p}\,S'(p)\Big)' = \tfrac{1}{2}\,(p - 1 - \ln p) > 0\ , \qquad p > 1\ . \tag{86}$$

Therefore, we get subsequently that the left-hand sides of (85), (84), (83) and (82) are positive for $p > 1$, showing that $\mathcal{K}'(2\ln p) > 0$, $p > 1$, as required.

We next show the fourth inequality in (31), $x_c > 2$. For this we must show that $\mathcal{K}(2\ln p) < 0$, $p > 1$, according to (14). We have from (20) with $t = 2\ln p$, $e^t = p^2$

$$\begin{aligned} \mathcal{K}(2\ln p) &= 2\ln\Big(\frac{p^2+p}{1+p}\Big) - \frac{3p+4}{p+1}\ln p + 6\ln p \int\limits_0^1 \frac{pw\,dw}{p^{2w}+p} \\ &= \left(2 - \frac{3p+4}{p+1} + 6\int\limits_0^1 \frac{w\,dw}{p^{2w-1}+1}\right)\ln p \\ &= \left(-\frac{p+2}{p+1} + 6\int\limits_0^1 \frac{w\,dw}{p^{2w-1}+1}\right)\ln p = -2\mathcal{K}'(2\ln p)\ln p < 0\ , \end{aligned} \tag{87}$$

see (79), for $p > 1$, as required.

We finally consider the last inequality in (31), $x_c < 3$. For this, we should show that $\mathcal{K}(3\ln p) > 0$, $p > 1$, according to (14). It will appear that a sufficient condition for this is given by $F(p) > 0$, $p > 1$, with $F(p)$ defined in (99). We have from (20) with $t = 3\ln p$, $e^t = p^3$

$$\begin{aligned}\mathcal{K}(3\ln p) &= 2\ln\Big(\frac{p^3+p}{1+p}\Big) - \frac{3p+4}{2p+2}\,3\ln p + 9\ln p \int\limits_0^1 \frac{pw\,dw}{p^{3w}+p} \\ &= 2\ln\Big(\frac{1+p^2}{1+p}\Big) - \Big(\frac{5}{2}+\frac{3}{2p+2}\Big)\ln p + 9\ln p \int\limits_0^1 \frac{w\,dw}{p^{3w}+1}\ .\end{aligned} \tag{88}$$

We have from (25), (40) and (56) as before

$$\begin{aligned}\int\limits_0^1 \frac{w\,dw}{p^{3w-1}+1} &= \frac{-\mathrm{Li}_2(-p)+\mathrm{Li}_2(-1/p^2)-3\ln p\ln(1+1/p^2)}{9\ln^2 p} \\ &= \frac{\frac{1}{2}\ln^2 p + \frac{\pi^2}{6} + \mathrm{Li}_2(-1/p) + \mathrm{Li}_2(-1/p^2) - 3\ln p\ln(1+1/p^2)}{9\ln^2 p} \\ &= \frac{1}{18} - \frac{\ln(1+1/p^2)}{3\ln p} + \frac{\frac{\pi^2}{6} + \mathrm{Li}_2(-1/p) + \mathrm{Li}_2(-1/p^2)}{9\ln^2 p} \\ &= \frac{1}{18} - \frac{\ln(1+1/p^2)}{3\ln p} + \frac{1}{9\ln^2 p}\left(\int\limits_{1/p}^1 \frac{\ln(1+v)}{v}\,dv + \int\limits_{1/p^2}^1 \frac{\ln(1+v)}{v}\,dv\right)\ .\end{aligned} \tag{89}$$

With

$$\ln\Big(\frac{1+p^2}{1+p}\Big) = \ln(1+p^2) - \ln(1+p)\,, \quad \ln(1+1/p^2) = \ln(1+p^2) - 2\ln p\,, \tag{90}$$

we then arrive at

$$\begin{aligned}\mathcal{K}(3\ln p) &= \Big(4 - \frac{3}{2p+2}\Big)\ln p - \ln(1+p^2) - 2\ln(1+p) \\ &\quad + \frac{1}{\ln p}\left(\int\limits_{1/p}^1 \frac{\ln(1+v)}{v}\,dv + \int\limits_{1/p^2}^1 \frac{\ln(1+v)}{v}\,dv\right)\ .\end{aligned} \tag{91}$$

We should show that for $p > 1$

$$T(p) := \mathcal{K}(3\ln p)\ln p$$

$$= \Big(4 - \frac{3}{2p+2}\Big)\ln^2 p - \ln p \ln(1+p^2) - 2\ln p \ln(1+p) + \int\limits_{1/p}^{1} \frac{\ln(1+v)}{v}\,dv$$

$$+ \int\limits_{1/p^2}^{1} \frac{\ln(1+v)}{v}\,dv > 0\ . \qquad (92)$$

We have $T(1) = 0$, and, using

$$\Big(\frac{3}{2p+2}\ln^2 p\Big)' = \frac{3}{2}\ \frac{2(p+1)\ln p - p\ln^2 p}{p(p+1)^2}\ , \qquad (93)$$

we have

$$T'(p) = \frac{8\ln p}{p} - \frac{3}{2}\ \frac{2(p+1)\ln p - p\ln^2 p}{p(p+1)^2} - \frac{\ln(1+p)^2}{p} - \frac{2p\ln p}{1+p^2}$$

$$- \frac{2\ln(1+p)}{p} - \frac{2\ln p}{1+p} + \frac{\ln(1+1/p)}{p} + \frac{2\ln(1+1/p^2)}{p}\ . \qquad (94)$$

Hence,

$$p\,T'(p) = 8\ln p - \frac{3}{2}\ \frac{2(p+1)\ln p - p\ln^2 p}{(p+1)^2} - \frac{2p^2\ln p}{1+p^2} - \frac{2p\ln p}{1+p}$$

$$+ \left[-\ln(1+p^2) - 2\ln(1+p) + \ln(1+1/p) + 2\ln(1+1/p^2)\right]\ . \qquad (95)$$

The quantity in [ ] on the right-hand side of (95) equals $\ln(1+p^2) - \ln(1+p) - 5\ln p$, and so

$$p\,T'(p) = 3\ln p - \frac{2p^2\ln p}{1+p^2} - \frac{2p\ln p}{1+p} - \frac{3}{2}\ \frac{2(p+1)\ln p - p\ln^2 p}{(p+1)^2} + \ln\Big(\frac{1+p^2}{1+p}\Big)\ . \qquad (96)$$

Using

$$\ln\Big(\frac{1+p^2}{1+p}\Big) = \ln p + \ln\Big(\frac{1+p^2}{p(1+p)}\Big)\ , \qquad (97)$$

we get

$$
\begin{aligned}
& p\,T'(p) \\
&= \frac{2\ln p}{1+p^2} + \frac{2\ln p}{1+p} - \frac{3}{2}\,\frac{2(p+1)\ln p - p\ln^2 p}{(p+1)^2} + \ln\Big(\frac{1+p^2}{p(1+p)}\Big) \\
&= \frac{2\ln p}{1+p^2} - \frac{(p+1)\ln p}{(p+1)^2} + \frac{3}{2}\,\frac{p\ln^2 p}{(p+1)^2} + \ln\Big(\frac{1+p^2}{p(1+p)}\Big) \\
&= \frac{1}{(p+1)^2}\,\Big(\Big(2\,\frac{(p+1)^2}{(1+p)^2} - p - 1 + \tfrac{3}{2}\,p\ln p\Big)\ln p + (p+1)^2\ln\Big(\frac{1+p^2}{p(1+p)}\Big)\Big) \\
&= \frac{1}{(p+1)^2}\,\Big(\Big(\frac{4p}{(1+p)^2} + \tfrac{3}{2}\,p\ln p - p + 1\Big)\ln p + (p+1)^2\ln\Big(\frac{1+p^2}{p(1+p)}\Big)\Big)\,.
\end{aligned}
\tag{98}
$$

Therefore, positivity of $T(p)$ for all $p > 1$ would follow from

$$
F(p) := \Big(\frac{4p}{1+p^2} + \tfrac{3}{2}\,p\ln p - p + 1\Big)\ln p + (p+1)^2\ln\Big(\frac{1+p^2}{p(1+p)}\Big) > 0\,, \quad p > 1\,. \tag{99}
$$

While $F(p)$ is built from elementary functions (unlike the right-hand side of (67)), it is still a bit too complicated to show $F(p) > 0$, $p > 1$, analytically. In Figure 4, we display $F(p)$, $1 < p \leq 5$, and it is seen that $F(p) > 0$, $1 < p \leq 5$, indeed (we have checked this also for many other ranges of p, always with the same conclusion).

5 Behaviour of t_c, t_c' and t_c'' as $q \downarrow 2$

We shall determine the behaviour of t_c, t_c' and t_c'' as $q \downarrow 2$, where we follow the approach of [3], Section 5, in which the behaviour of t_c as $q \downarrow 2$ is found for the case of the exponential weight density. We begin with t_c. We have $\mathcal{K}(t_c) = 0$, where

$$
\mathcal{K}(t) = 2\ln\Big(\frac{e^t + q - 1}{q}\Big) - \frac{3q+1}{2q}\,t + 3(q-1)\,t\int\limits_0^1 \frac{w\,dw}{e^{tw} + q - 1}\,, \tag{100}
$$

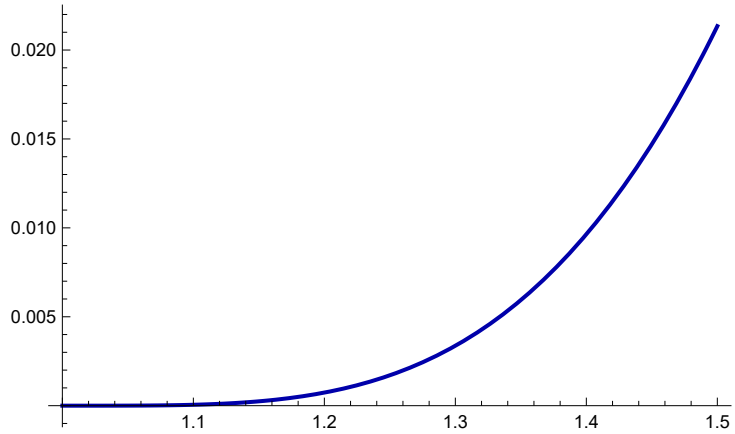

Figure 4: Plot of $F(p)$, given in (99), for $p = q - 1 \in (1, 5]$.

see (20). We have by [3], (75) for $q > 2$

$$\frac{1}{e^t + q - 1} = \sum_{n=0}^{\infty} a_n(q)\, t^n \ , \qquad |t| < \pi \ , \tag{101}$$

where $a_n(q)$ are given and studied in detail in [3], Section 5. Now

$$\frac{d}{dt}\left[\ln\Big(\frac{e^t + q - 1}{q}\Big)\right] = \frac{e^t}{e^t + q - 1} = 1 - \frac{q-1}{e^t + q - 1} \ . \tag{102}$$

Hence, when

$$\ln\Big(\frac{e^t + q - 1}{q}\Big) = \sum_{n=0}^{\infty} b_n(q)\, t^n \ , \tag{103}$$

we have $b_0(q) = 0$, and

$$\sum_{n=1}^{\infty} n\, b_n(q)\, t^{n-1} = 1 - (q-1) \sum_{m=0}^{\infty} a_m(q)\, t^m \ . \tag{104}$$

We have $a_0(q) = 1/q$, and so

$$b_1(q) = 1 - (q-1)\,\frac{1}{q} = \frac{1}{q} \ , \tag{105}$$

and

$$b_n(q) = -\,\frac{q-1}{n}\, a_{n-1}(q) \ , \qquad n = 2, 3, \ldots \ . \tag{106}$$

It follows that

$$\ln\Big(\frac{e^t+q-1}{q}\Big) = \frac{t}{q} - \sum_{n=2}^{\infty} \frac{q-1}{n}\, a_{n-1}(q)\, t^n \ , \qquad |t| < \pi \ . \tag{107}$$

Next,

$$t \int_0^1 \frac{w\, dw}{e^{tw}+q-1} = \frac{1}{t} \int_0^t \frac{v\, dv}{e^v+q-1}$$

$$= \sum_{m=0}^{\infty} a_m(q)\, \frac{1}{t} \int_0^t v^{m+1}\, dv = \sum_{m=0}^{\infty} \frac{a_m(q)}{m+2}\, t^{m+1} \ , \qquad |t| < \pi \ . \tag{108}$$

Thus, we obtain from (100), (107) and (108)

$$\begin{aligned}
\mathcal{K}(t) &= \frac{2t}{q} - 2\sum_{n=2}^{\infty} \frac{q-1}{n}\, a_{n-1}(q)\, t^n - \frac{3q+1}{2q}\, t + 3(q-1) \sum_{n=1}^{\infty} \frac{a_{n-1}(q)}{n+1}\, t^n \\
&= \frac{2t}{q} - \frac{3q+1}{2q}\, t + \frac{3(q-1)}{2q}\, t \\
&\quad - 2\sum_{n=2}^{\infty} \frac{q-1}{n}\, a_{n-1}(q)\, t^n + 3(q-1) \sum_{n=2}^{\infty} \frac{a_{n-1}(q)}{n+1}\, t^n \\
&= 0 + \sum_{n=2}^{\infty} a_{n-1}(q) \Big(\frac{3(q-1)}{n+1} - \frac{2(q-1)}{n} \Big)\, t^n \\
&= (q-1) \sum_{n=3}^{\infty} \frac{(n-2)\, a_{n-1}(q)}{n(n+1)}\, t^n \ , \qquad |t| < \pi \ .
\end{aligned} \tag{109}$$

Using (109), the condition $\mathcal{K}(t) = 0$ for $t = t_c$ can be written as

$$\tfrac{1}{12}\, a_2(q) + \tfrac{1}{10}\, a_3(q)\, t + \tfrac{1}{10}\, a_4(q)\, t^2 + \tfrac{2}{21}\, a_5(q)\, t^3 + ... = 0 \ . \tag{110}$$

Therefore, we have for $t = t_c$

$$t = -\frac{5}{6}\, \frac{a_2(q)}{a_3(q)} - \frac{a_4(q)}{a_3(q)}\, t^2 - \frac{20}{21}\, \frac{a_5(q)}{a_3(q)}\, t^3 + O(t^4) \ . \tag{111}$$

We shall show below analytically that it follows from (109) that

$$t_c < 3(q-2) \ , \qquad q-2 \text{ sufficiently small} \ , \tag{112}$$

where we avoid to rely on the bound $t_c < 3\ln(q-1)$, $q > 2$, that was obtained at the end of Section 4 by numerical means. We proceed with (111) for which we note, see [2], (188)–(191),

$$-\frac{a_2(q)}{a_3(q)} = 3y - \tfrac{3}{2}\,y^2 + 3y^3 - \tfrac{15}{4}\,y^4 + O(y^5)\ , \qquad y = q-2\ , \tag{113}$$

$$a_2(2) = a_4(2) = ... = 0\ , \tag{114}$$

$$a_4(q) = -5a_5(2)\,y + O(y^2)\ , \qquad y = q-2\ , \tag{115}$$

$$a_3(2) = \frac{1}{48}\ , \qquad a_5(2) = \frac{-1}{480}\ , \tag{116}$$

also see [3], (94), (95) and (166). Then combining (113)–(116) and using that $t = t_c = O(y)$, see (112), we get

$$t = \tfrac{5}{6}\,(3y - \tfrac{3}{2}\,y^2 + 3y^3 + O(y^4)) - \tfrac{1}{2}\,y\,t^2 + \tfrac{2}{21}\,t^3 + O(y^4)\ . \tag{117}$$

Using that $t = O(y)$, we first get from (117) that $t = \frac{5}{2}\,y + O(y^2)$. Inserting this into the right-hand side of (117), we get for $t = t_c$

$$\begin{aligned} t &= \tfrac{5}{2}\,y - \tfrac{5}{4}\,y^2 + \tfrac{5}{2}\,y^3 - \left(\tfrac{25}{8} - \tfrac{250}{168}\right)\,y^3 + O(y^4) \\ &= \tfrac{5}{2}\left(y - \tfrac{1}{2}\,y^2 + \left(\tfrac{1}{3} + \tfrac{1}{84}\right)\,y^3 + O(y^4)\right)\ , \qquad y = q-2 \downarrow 0\,, \end{aligned} \tag{118}$$

and this is (32).

Before we proceed to t_c' and t_c'', we shall establish (112). We have from (109)

$$\begin{aligned} \mathcal{K}(t) &= (q-1)\left(\tfrac{1}{12}\,a_2(q)\,t^3 + \tfrac{1}{10}\,a_3(q)\,t^4 + \tfrac{1}{10}\,a_4(q)\,t^5 + ...\right) \\ &= \tfrac{1}{12}\,(q-1)\,a_2(q)\,t^3\Big(1 + \frac{6}{5}\,\frac{a_3(q)}{a_2(q)}\,t + \frac{6}{5}\,\frac{a_4(q)}{a_2(q)}\,t^2 + ...\Big)\ . \end{aligned} \tag{119}$$

We use the explicit forms of $a_n(q)$ as given in [3], p. 18. Thus

$$0 > a_2(q) = \frac{-1}{2q} + \frac{1}{q^3} = -\,\frac{q-2}{2q^3} = -\,\tfrac{1}{16}\,(q-2)(1 + O(q-2))\ , \tag{120}$$

$$a_3(q) = \frac{1}{q^4}\,(q - 1 - \tfrac{1}{6}\,q^2) = \tfrac{1}{48}\,(1 + O(q-2))\ , \tag{121}$$

when $q - 2 \downarrow 0$. We aim at showing that $\mathcal{K}(3(q-2)) > 0$ when $q-2$ is sufficiently small, so that, by (14), $t_c < 3(q-2)$ when $q-2$ is sufficiently small. Using (120) and (121), we have

$$\frac{6}{5}\,\frac{a_3(q)}{a_2(q)}\,3(q-2) = -\,\tfrac{6}{5}\,(1 + O(q-2))\ , \qquad q-2 \downarrow 0\ . \tag{122}$$

Furthermore, we have from (109) being valid for $|t| < \pi$,

$$\frac{6}{5}\,\frac{a_4(q)}{a_2(q)}\,(3(q-2))^2 + ... = O(q-2)\ , \qquad q-2 \downarrow 0\ . \tag{123}$$

Hence,

$$1 + \frac{6}{5}\,\frac{a_3(q)}{a_2(q)}\,3(q-2) + \frac{6}{5}\,\frac{a_4(q)}{a_2(q)}\,(3(q-2))^2 + ... \to -\tfrac{1}{5}\,, \qquad q-2 \downarrow 0\,. \tag{124}$$

Therefore, we have from $a_2(q) < 0$ that $\mathcal{K}(3(q-2)) > 0$, see (119), when $q-2$ is sufficiently small.

We now consider t_c' and t_c''. From (109), we have

$$\mathcal{K}'(t) = (q-1)\sum_{n=2}^{\infty}\frac{n-1}{n+2}\,a_n(q)\,t^n\ , \qquad |t| < \pi\ . \tag{125}$$

The condition $\mathcal{K}'(t) = 0$ for $t = t_c'$ can be written as

$$\tfrac{1}{4}\,a_2(q)\,t^2 + \tfrac{2}{5}\,a_3(q)\,t^3 + \tfrac{1}{2}\,a_4(q)\,t^4 + \tfrac{4}{7}\,a_5(q)\,t^5 + ... = 0\ , \tag{126}$$

so that

$$t = -\frac{5}{8}\,\frac{a_2(q)}{a_3(q)} - \frac{5}{4}\,\frac{a_4(q)}{a_3(q)}\,t^2 - \frac{10}{7}\,\frac{a_5(q)}{a_3(q)}\,t^3 - ...\ . \tag{127}$$

Then proceeding as in (117) and (118) (with $t_c' < 2\ln(q-1) < 2(q-2)$), we find for $t = t_c'$

$$t = \tfrac{15}{8}\,(y - \tfrac{1}{2}\,y^2 + (\tfrac{1}{3} - \tfrac{1}{336})\,y^3 + O(y^4))\ , \qquad y = q-2 \downarrow 0\ . \tag{128}$$

Similarly, we have from (125)

$$\mathcal{K}''(t) = (q-1)\sum_{n=1}^{\infty}\frac{n(n+1)}{n+3}\,a_{n+1}(q)\,t^n\ , \qquad |t| < \pi\ , \tag{129}$$

and the condition $\mathcal{K}''(t) = 0$ for $t = t_c''$ can be written as

$$\tfrac{1}{2}\,a_2(q)\,t + \tfrac{6}{5}\,a_3(q)\,t^2 + 2a_4(q)\,t^3 + \tfrac{20}{7}\,a_5(q)\,t^4 + ... = 0\ . \tag{130}$$

This leads for $t = t_c''$ to

$$t = \tfrac{5}{4}\,(y - \tfrac{1}{2}\,y^2 + (\tfrac{1}{3} - \tfrac{1}{336})\,y^3 + O(y^4))\ , \qquad y = q-2 \downarrow 0\ . \tag{131}$$

6 Asymptotics of t_c, t_c' and t_c'' as $q \to \infty$

The asymptotics of t_c, t_c' and t_c'' as $q \to \infty$ is obtained by solving the equations $\mathcal{K}(t) = 0$, $\mathcal{K}'(t) = 0$ and $\mathcal{K}''(t) = 0$ approximately, using (20), (21) and (22), respectively, in which an appropriate form of the result (25) is used for the common integral $(q-1)\,D(t)$. This form of (25) is derived from (40), so that, with $t = x \ln p$, $p = q - 1 > 1$ as usual

$$
\begin{aligned}
(q-1)\,D(t) &= \int_0^1 \frac{(q-1)\,w\,dw}{e^{tw} + q - 1} = \int_0^1 \frac{w\,dw}{p^{xw-1} + 1} \\
&= \frac{-\mathrm{Li}_2(-p) + \mathrm{Li}_2(-1/p^{x-1}) - x \ln p \ln(1 + 1/p^{x-1})}{(x \ln p)^2} \\
&= \frac{\frac{1}{2}\ln^2 p + \frac{1}{6}\,\pi^2 + \mathrm{Li}_2(-1/p) + \mathrm{Li}_2(-1/p^{x-1}) - x \ln p \ln(1 + 1/p^{x-1})}{(x \ln p)^2} \\
&= \frac{1}{2x^2} + \frac{\pi^2}{6(x \ln p)^2} - \frac{\ln(1 + 1/p^{x-1})}{x \ln p} + \frac{\mathrm{Li}_2(-1/p) + \mathrm{Li}_2(-1/p^{x-1})}{(x \ln p)^2}\ .
\end{aligned}
\tag{132}
$$

According to (31), we may assume $x > 1$, so that (28) applies to the expressions involving Li_2 on the last line of (132).

We start by showing the asymptotic result (37) for $t_c = x_c \ln p$ as $p \to \infty$. We take in (20) $t = x \ln p$ with $x > 2$, see (31), so that

$$
\mathcal{K}(x \ln p) = 2 \ln\Big(\frac{p^x + p}{1 + p}\Big) - \frac{3p + 4}{2p + 2}\, x \ln p + 3x \ln p \int_0^1 \frac{w\,dw}{p^{xw-1} + 1}\ . \tag{133}
$$

We write

$$
\ln\Big(\frac{p^x + p}{1 + p}\Big) = (x - 1) \ln p + r(x)\ , \tag{134}
$$

where, since $x > 2$,

$$
r(x) = \ln(1 + 1/p^{x-1}) - \ln(1 + 1/p) \in (-1/p, 0)\ . \tag{135}
$$

Therefore,

$$
\mathcal{K}(x \ln p) = \left(2(x-1) - \tfrac{3}{2}\,x - \frac{x}{2p+2} + 3x \int_0^1 \frac{w\,dw}{p^{xw-1} + 1} + \frac{2r(x)}{\ln p} \right) \ln p\ . \tag{136}
$$

Furthermore, from (132),

$$3x \int_0^1 \frac{w\,dw}{p^{xw-1}+1} = \frac{3}{2x} + \frac{\pi^2}{2x\ln^2 p} - \frac{3\ln(1+1/p^{x-1})}{\ln p} + \frac{3\delta(x)}{x}\ , \qquad (137)$$

where

$$\delta(x) = \frac{\mathrm{Li}_2(-1/p) + \mathrm{Li}_2(-1/p^{x-1})}{\ln^2 p} \in \Big(\frac{-2}{p\ln^2 p}, 0\Big) \qquad (138)$$

on account of $x > 2$ and (28). Thus

$$\begin{aligned}
&\mathcal{K}(x\ln p) \\
&= \Big(\frac{1}{2}\,\frac{p}{p+1}\,x - 2 + \frac{3}{2x} + \frac{\pi^2}{2x\ln^2 p} - \frac{3\ln(1+1/p^{x-1})}{\ln p} + \frac{3\delta(x)}{x} + \frac{2r(x)}{\ln p}\Big)\ln p \\
&= \Big(\frac{p}{p+1}\,x^2 - 2\Big(2 + \frac{3\ln(1+1/p^{x-1})}{\ln p} - \frac{2r(x)}{\ln p}\Big)x + 3 + \frac{\pi^2}{\ln^2 p} + 6\delta(x)\Big)\,\frac{\ln p}{2x}\,.
\end{aligned} \qquad (139)$$

Therefore, $x = x_c$ satisfies

$$0 = \frac{2x\,\mathcal{K}(x\ln p)}{\ln p} = \Big(1 - \frac{1}{p+1}\Big)\,x^2 - (4 + 2\varepsilon(x))\,x + 3 + \frac{\pi^2}{\ln^2 p} + 6\delta(x)\ , \qquad (140)$$

where, since $x > 2$ and (135),

$$\varepsilon(x) = \frac{3\ln(1+1/p^{x-1}) - 2r(x)}{\ln p} \in \Big(0, \frac{5}{p\ln p}\Big)\ . \qquad (141)$$

Ignoring at the right-hand side of (140) all expressions that are exponentially small in $\ln p$ (such as $1/p$, $1/p^{x-1}$), we get for $x = x_c$ in leading order the equation

$$x^2 - 4x + 3 + \frac{\pi^2}{\ln^2 p} = 0\ , \qquad (142)$$

which has the solution, when $\ln p > \pi$,

$$\hat{x} = 2 + \sqrt{1 - \frac{\pi^2}{\ln^2 p}}\ . \qquad (143)$$

Since

$$\frac{d}{dx}\,\Big(x^2 - 4x + 3 + \frac{\pi^2}{\ln^2 p}\Big)\Big|_{x=\hat{x}} = 2\sqrt{1 - \frac{\pi^2}{\ln^2 p}} > 1 \qquad (144)$$

when $\ln p > \frac{2}{3}\pi\sqrt{3}$, the actual solution x_c of (140) deviates from $\hat{x}$ by an amount that is of the order $1/p$. This gives (37).

A short assessment of the result (37) is as follows With $q = p + 1$ and $t_c = x_c \ln(q-1)$, we can write (37) as

$$t_c = 2\ln(q-1) + (\ln^2(q-1) - \pi^2)^{1/2} + O\Big(\frac{\ln q}{q}\Big) \ . \tag{145}$$

There is the table

q	t_c	$2\ln(q-1) + (\ln^2(q-1) - \pi^2)^{1/2}$
10	5.7466	—
100	12.8625	12.5437
1000	20.0038	19.9644
10000	27.0833	27.0784

We next show the asymptotic result (38) for $t'_x = x'_c \ln p$ as $p \to \infty$. We take in (21) $t = x \ln p$, $p = q - 1$, where we now assume, see (31), that $1 \le x \le 2$. The condition $\mathcal{K}'(x \ln p) = 0$ for $x = x'_c$ can be written as

$$0 = \frac{p}{2(1+p)} + \frac{p}{p^x + p} - 3 \int_0^1 \frac{pw\,dw}{p^{xw} + 1} \ , \tag{146}$$

i.e., as

$$0 = \frac{1}{2(1+1/p)} + \frac{1}{1+p^{x-1}} - 3 \int_0^1 \frac{w\,dw}{p^{xw-1} + 1} \ . \tag{147}$$

By (132), we have for $x = x'_c$

$$\begin{aligned} &\frac{1}{2} + \frac{1}{1+p^{x-1}} - \frac{3}{2x^2} - \frac{\pi^2}{2(x\ln p)^2} \\ &= \ \frac{1}{2(p+1)} - \frac{3\ln(1+1/p^{x-1})}{x\ln p} + 3\,\frac{\mathrm{Li}_2(-1/p) + \mathrm{Li}_2(-1/p^{x-1})}{(x\ln p)^2} \ . \end{aligned} \tag{148}$$

The right-hand side of (148) tends to 0 as $p \to \infty$, and does so uniformly in $x \in [1,2]$. Since $p > 1$ and $x \ge 1$, the left-hand side of (148) is less than $1 - 3/2x^2$, and this is negative when $x^2 < 3/2$. Hence, for fixed $\varepsilon \in (0, \sqrt{3/2} - 1)$, we have $x = x_c \ge \sqrt{3/2} - \varepsilon > 1$ for large p. Therefore, both $(1 + p^{x-1})^{-1}$ and the right-hand side of (148) are $O(p^{-\alpha})$, $p \to \infty$, where $\alpha = \sqrt{3/2} - \varepsilon > 0$. This implies that for large p

$$\frac{1}{2} - \frac{3}{2x^2} - \frac{\pi^2}{2x^2 \ln^2 p} = O(p^{-\alpha}) \ . \tag{149}$$

Since x is bounded by 2, this gives for $x = x_c'$

$$x = \Big(3 + \frac{\pi^2}{\ln^2 p}\Big)^{1/2} + O(p^{-\alpha}) \ . \tag{150}$$

The right-hand side of (150) exceeds $\sqrt{3}$ when p is large, and then returning to (148), we see that $x = x_c'$ satisfies

$$\frac{1}{2} - \frac{3}{2x^2} - \frac{\pi^2}{2x^2 \ln^2 p} = O(p^{-(\sqrt{3}-1)}) \ . \tag{151}$$

This gives

$$x = \Big(3 + \frac{\pi^2}{\ln^2 p}\Big)^{1/2} + O(p^{-(\sqrt{3}-1)}) \ , \tag{152}$$

and this is (38).

For the case that $q = p + 1 = 1000$, we have $t_c' = x_c' \ln(q-1) = 12.3045$ while $(3\ln^2(q-1) + \pi^2)^{1/2} = 12.3685$.

We finally show the asymptotic result for $t_c'' = x_c'' \ln p$ as $p \to \infty$. We take in (22) $t = x \ln p$, $p = q - 1$, and we assume , see (31), that $1 \le x \le 2$. The condition $\mathcal{K}''(x \ln p) = 0$ for $x = x_c''$ can be written as

$$0 = \frac{-x\, p^{x-1} \ln p}{(p^{x-1}+1)^2} - \frac{3}{p^{x-1}+1} + 6 \int\limits_0^1 \frac{w\, dw}{p^{xw-1}+1} \ . \tag{153}$$

By (132), we have for $x = x_c''$

$$\begin{aligned} 0 \ &= \ \frac{3}{x^2} + \frac{\pi^2}{x^2 \ln^2 p} - \frac{x \ln p}{p^{x-1}+1} \Big(1 - \frac{1}{p^{x-1}+1} + \frac{3}{x \ln p}\Big) \\ &\quad - 6\, \frac{\ln(1 + 1/p^{x-1})}{x \ln p} + 6\, \frac{\mathrm{Li}_2(-1/p) + \mathrm{Li}_2(-1/p^{x-1})}{x^2 \ln^2 p} \ . \end{aligned} \tag{154}$$

Suppose that $x = x_c$ does not converge to 1 as $p \to \infty$. Then there are arbitrarily large p such that all terms at the right-hand side of (154) after $3/x^2$ are arbitrarily small. Hence, for such p (154) would not hold. Therefore, $x = x_c \to 1$ as $p \to \infty$. In leading order, we have for $x = x_c$ from (154) the equation

$$\frac{3}{x^2} - \frac{x \ln p}{p^{x-1}+1} = 0 \ , \tag{155}$$

so that, in leading order,

$$x = 1 + \frac{\ln(\frac{1}{3}\, x^3 \ln p)}{\ln p} = 1 + O\Big(\frac{\ln(\ln p)}{\ln p}\Big) \tag{156}$$

since $x \in [1,2]$.

With $p = 999$, $q = 1000$, we have $t_c'' = 8.14441$, and for $x \in [1,2]$ satisfying the first equation in (156), we find $x = 1.199887$, i.e., $x \ln(q-1) = 8.28732$.

7 Expressing γ_c as an elementary function of $x_c = t_c/\ln(q-1)$

We have

$$\gamma_c = \frac{t_c}{\mathcal{F}_0(t_c)} \ , \tag{157}$$

where

$$\mathcal{F}_0(t) = 1 - 2q \int_0^1 \frac{w\,dw}{e^{tw} + q - 1} \ , \qquad t \geq 0 \ , \tag{158}$$

and t_c is the unique positive zero t of $\mathcal{K}(t)$, where

$$\mathcal{K}(t) = 2\ln\Big(\frac{e^t + q - 1}{q}\Big) - \frac{3q+1}{2q}\,t + 3(q-1)\,t \int_0^1 \frac{w\,dw}{e^{tw} + q - 1} \ . \tag{159}$$

When we take $t = t_c$ in (159), the right-hand side vanishes, and we can express the integral for $t = t_c$ as an elementary function of t_c. This same integral also occurs in $\mathcal{F}_0(t_0)$, and we obtain γ_c as an elementary function of t_c.

Set $p = q - 1$, $t = x \ln p$, $t_c = x_c \ln p$ with $x > 2$, $x_c > 2$, see (31). We shall show that

$$\gamma_c = \frac{\frac{3}{4}\,x_c}{x_c - \Big(1 + \frac{1}{p}\Big)\Big(1 - \frac{r(x_c)}{\ln p}\Big)}\,t_c \ , \tag{160}$$

where

$$r(x) = \ln\Big(\frac{1 + 1/p^{x-1}}{1 + 1/p}\Big) \in (-\ln(1 + 1/p), 0) \ , \qquad x > 2 \ , \tag{161}$$

as in (134), (135). In this notation, we have

$$\mathcal{F}_0(x \ln p) = 1 - 2\,\frac{p+1}{p}\,I(x) \ , \tag{162}$$

$$\mathcal{K}(x \ln p) = 2(x-1)\ln p + 2r(x) - \frac{3p+4}{2p+2}\,x \ln p + 3x \ln p\, I(x) \ , \tag{163}$$

where

$$I(x) = \int_0^1 \frac{w\,dw}{p^{xw-1}+1}\ . \tag{164}$$

For $x = x_c$, we have $\mathcal{K}(x\ln p) = 0$, and we find for $I(x)$ the result

$$I(x) = \frac{1}{3}\,\frac{3p+4}{2p+2} - \frac{2}{3}\,\frac{(x-1)\ln p + r(x)}{x\ln p} = \frac{-p}{6(p+1)} + \frac{2}{3x}\left(1 - \frac{r(x)}{\ln p}\right)\ . \tag{165}$$

Thus, for $x = x_c$,

$$\begin{aligned}\mathcal{F}_0(x\ln p) &= 1 - 2\,\frac{p+1}{p}\left(\frac{-p}{6(p+1)} + \frac{2}{3x}\left(1 - \frac{r(x)}{\ln p}\right)\right)\\ &= \frac{4}{3} - \frac{4}{3x}\,\frac{p+1}{p}\left(1 - \frac{r(x)}{\ln p}\right)\ .\end{aligned} \tag{166}$$

This gives (160) via (157).

To show the inequalities in (43), we use (161) that bounds $r(x)$ between $-\ln(1+1/p)$ and 0. Thus,

$$\gamma_c < \frac{\frac{3}{4}\,x_c}{x_c - \left(1+\frac{1}{p}\right)\left(1 + \frac{\ln(1+1/p)}{\ln p}\right)}\,t_c = \frac{\frac{3}{4}\,x_c}{x_c - \frac{p+1}{p}\,\frac{\ln(p+1)}{\ln p}}\,t_c\ , \tag{167}$$

and

$$\gamma_c > \frac{\frac{3}{4}\,x_c}{x_c - \left(1+\frac{1}{p}\right)}\,t_c = \frac{\frac{3}{4}\,x_c}{x_c - \frac{p+1}{p}}\,t_c\ . \tag{168}$$

We illustrate this for the case that $q = p+1 = 100$. Then we have $t_c = 12.86252$, $x_c = 2.799170$ and $\mathcal{F}_0(t_c) = 0.8511647$. This yields, with γ_c computed either from (157) and (158) or from (160),

$$15.09348 < \gamma_c = 15.11167 < 15.11214\ , \tag{169}$$

where the two inequalities come from (168) and (167), respectively.

NB. In [2], p. 17, on the Pareto case, there is given an inequality for γ_c (and resulting large-q behaviour). There are some errors on this p. 17. Going from [2], (90) to [2], (91), a "q" has been forgotten. The correct version of [2], (93) therefore reads

$$\gamma_c = t_c\Big(1 + O\Big(\frac{q}{(q-1)^\alpha}\Big)\Big)\ , \qquad q\to\infty\ . \tag{170}$$

Also, in the sentence containing [2], (91), a factor "2" in front of $(\tau{-}2)/(\tau{-}1)$ has been forgotten twice.

The approach presented in this section for γ_c in the case of density $\mathcal{X}_{[0,1)}(w)$ can also be used for γ_c in the case of Pareto density $(\tau{-}1)\, w^{-\tau}\, \mathcal{X}_{[1,\infty)}$. Indeed, then we have again $\gamma_c = t_c/\mathcal{F}_0(t_c)$, but now with

$$\mathcal{F}_0(t) = 1 - q(\tau-2)\, E(t)\ , \qquad t \geq 0\ , \tag{171}$$

and with t_c the unique positive zero t of

$$\mathcal{K}(t) = \frac{\tau{-}2}{\tau{-}1} \ln\Big(\frac{e^t + q - 1}{q}\Big) + \Big(\frac{1}{\tau{-}2} - \frac{q+1}{2q}\Big)\, t + \frac{(\tau{-}2)(\tau{-}3)}{2(\tau{-}1)}\, (q-1)\, t\, E(t)\,, \tag{172}$$

where

$$E(t) = \int_1^\infty \frac{w^{-\tau+1}\, dw}{e^{tw} + q - 1}\ . \tag{173}$$

Hence, from $\mathcal{K}(t_c) = 0$, we can express $E(t_c)$ in an elementary way in terms of t_c, and this can be inserted into the expression (171) for $\mathcal{F}_0(t)$ with $t = t_c$. Omitting further details, this then leads to the result

$$\gamma_c = \frac{1}{2}\, \frac{\tau-2}{\tau-3}\, \frac{x}{x - \dfrac{p+1}{p}\Big(1 - \dfrac{r(x)}{\ln p}\Big)}\, t_c\ , \tag{174}$$

where we have set $p = q - 1$, $t = x \ln p$, $t_c = x_c \ln p$, and $r(x)$ is as in (134), (135) and (161) for $x \geq 1$.

References

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