IDENTITIES INVOLVING HARMONIC NUMBERS THAT ARE OF INTEREST FOR PHYSICISTS

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Abstract. We treat a class of combinatorial sums considered by Vermaseren [8] with an elementary approach. The resulting evaluations are in terms of (generalized) harmonic numbers.

1. Introduction

In this paper, we deal with *harmonic sums*, defined by

$$H_n^{(d)} := \sum_{k=1}^{n} \frac{1}{k^d}.$$

Vermaseren [8] presented an algorithm to deal with harmonic numbers, since they are of interest in physics contexts. In his section "Miscellaneous Sums" he writes:

> *In this section some sums are given that can be worked out to any level of complexity, but they are not representing whole classes. Neither is there any proof for the algorithms. The algorithms presented have just been checked up to some rather large values of the parameters.*

In this paper, these (classes!) of identities are treated with different methods, which are very simple and convincing. Basically, partial fraction decomposition is enough! I learned this technique from Wenchang Chu [1]. It avoids complex analysis ("Rice's method") that is often associated with alternating sums involving binomial coefficients, see, e.g., [2].

The next 3 sections treat the classes of identities in question.

Then we consider a related sum in the spirit of Kirschenhofer [4], as well as a sum of Melzik et al., [7, 6].

2. A first set of identities

We perform the following partial fraction decomposition:

$$\frac{(z+1)\dots(z+n)}{z(z-1)\dots(z-n)}\frac{1}{z^d} = \sum_{k=1}^{n} \binom{n}{k}\binom{n+k}{k}(-1)^{n-k}\frac{1}{k^d}\frac{1}{z-k} + \frac{\lambda}{z^{d+1}} + \dots + \frac{\mu}{z}.$$

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Now we multiply this by z, and take the limit $z \to \infty$:

$$0 = \sum_{k=1}^{n} \binom{n}{k} \binom{n+k}{k} (-1)^{n-k} \frac{1}{k^d} + \mu,$$

with

$$\begin{aligned}
(-1)^n \mu &= (-1)^n [z^{-1}] \frac{(z+1)\dots(z+n)}{z(z-1)\dots(z-n)} \frac{1}{z^d} \\
&= (-1)^n [z^d] \frac{(z+1)\dots(z+n)}{(z-1)\dots(z-n)} \\
&= [z^d] \frac{(1+z)\dots(1+\frac{z}{n})}{(1-z)\dots(1-\frac{z}{n})} \\
&= [z^d] \exp\Big(\log(1+z) + \dots + \log\Big(1+\frac{z}{n}\Big) + \log\frac{1}{1-z} + \dots + \log\frac{1}{1-\frac{z}{n}} \Big) \\
&= [z^d] \exp\Big(\sum_{k\ge1} \frac{(-1)^{k-1}}{k} z^k H_n^{(k)} + \sum_{k\ge1} \frac{1}{k} z^k H_n^{(k)} \Big) \\
&= [z^d] \exp\Big(2 \sum_{k \text{ odd}} \frac{1}{k} z^k H_n^{(k)} \Big) \\
&= [z^d] \prod_{k \text{ odd}} \sum_{j\ge0} \frac{1}{j!} \Big(2 \frac{z^k H_n^{(k)}}{k} \Big)^j \\
&= \sum_{1\cdot j_1 + 3\cdot j_3 + \dots = d} \frac{2^{j_1+j_3+\cdots} \big(H_n^{(1)}\big)^{j_1} \big(H_n^{(3)}\big)^{j_3} \dots}{j_1! j_3! \dots 1^{j_1} 3^{j_3} \dots}.
\end{aligned}$$

So we have our first result:

Theorem 1.

$$\sum_{k=1}^{n} \binom{n}{k} \binom{n+k}{k} (-1)^{k-1} \frac{1}{k^d} = \sum_{1\cdot j_1 + 3\cdot j_3 + \dots = d} \frac{2^{j_1+j_3+\cdots} \big(H_n^{(1)}\big)^{j_1} \big(H_n^{(3)}\big)^{j_3} \dots}{j_1! j_3! \dots 1^{j_1} 3^{j_3} \dots}. \qquad \square$$

The polynomials on the right-hand-side can be expressed in the language of *Bell polynomials*; see, e.g., [5].

Here is a list for $d = 1, 2, 3, 4, 5$ of these polynomials:

$$2H_n, \quad 2H_n^2, \quad \frac{4}{3}H_n^3 + \frac{2}{3}H_n^{(3)}, \quad \frac{2}{3}H_n^4 + \frac{4}{3}H_n H_n^{(3)}, \quad \frac{4}{15}H_n^5 + \frac{4}{3}H_n^2 H_n^{(3)} + \frac{2}{5}H_n^{(5)}.$$

3. A second set of identities

Consider the following partial fraction decomposition

$$\frac{(z+1)\dots(z+n)}{z(z-1)\dots(z-n)} \Big[\frac{1}{j^d} - \frac{1}{(j+z)^d} \Big]$$

$$= \sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{k} (-1)^{n-k} \left[\frac{1}{j^{d+1}} - \frac{1}{(j+k)^{d+1}} \right] \frac{1}{z-k} + \frac{\lambda}{(j+z)^{d+1}} + \cdots + \frac{\mu}{j+z}.$$

Again, we multiply by z, and take the limit $z \to \infty$:

$$\frac{1}{j^{d+1}} = \sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{k} (-1)^{n-k} \left[\frac{1}{j^{d+1}} - \frac{1}{(j+k)^{d+1}} \right] + \mu + \frac{1}{j^{d+1}},$$

with

$$\begin{aligned} \mu &= [(z+j)^{-1}] \frac{(z+1)\dots(z+n)}{z(z-1)\dots(z-n)} \left[\frac{1}{j^{d+1}} - \frac{1}{(j+z)^{d+1}} \right] \\ &= -[(z+j)^{-1}] \frac{(z+1)\dots(z+n)}{z(z-1)\dots(z-n)} \frac{1}{(j+z)^{d+1}} \\ &= -[(z+j)^{d}] \frac{(z+1)\dots(z+n)}{z(z-1)\dots(z-n)} \\ &= -[z^d] \frac{(z+1-j)\dots(z+n-j)}{(z-j)(z-1-j)\dots(z-n-j)}. \end{aligned}$$

So we get

$$\sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{k} (-1)^{n-k} \left[\frac{1}{j^{d+1}} - \frac{1}{(j+k)^{d+1}} \right] = \frac{1}{j^{d+1}} + [z^d] \frac{(z+1-j)\dots(z+n-j)}{(z-j)(z-1-j)\dots(z-n-j)}$$

and by summing over $j \ge 1$:

$$\sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{k} (-1)^{n-k} H_k^{(d+1)} = [z^d] \sum_{j \ge 1} \Big(-\frac{1}{z-j} + \frac{(z+1-j)\dots(z+n-j)}{(z-j)(z-1-j)\dots(z-n-j)} \Big).$$

Now define

$$f(n,j) = \frac{(z+1-j)\dots(z+n-j)}{(z-j)(z-1-j)\dots(z-n-j)}$$

and

$$g(n,j) = f(n,j) \frac{2(-z+j-n-1)}{n+1},$$

then

$$f(n,j) - f(n+1,j) = g(n,j+1) - g(n,j).$$

So, for $d \ge 1$ we can continue

$$\begin{aligned} \sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{k} (-1)^{n-k} H_k^{(d+1)} &= [z^d] \sum_{j \ge 1} \Big(-f(0,j) + f(n,j) \Big) \\ &= [z^d] \sum_{j \ge 1} \sum_{m=0}^{n-1} \Big(g(m,j) - g(m,j+1) \Big) \end{aligned}$$

$$
\begin{aligned}
&= [z^d]\sum_{m=0}^{n-1}\sum_{j\ge1}\Big(g(m,j)-g(m,j+1)\Big)\\
&= [z^d]\sum_{m=0}^{n-1} g(m,1)\\
&= -2[z^d]\sum_{m=1}^{n}\frac{1}{m}\frac{z\dots(z+m-1)}{(z-1)(z-2)\dots(z-m)}\\
&= 2[z^{d-1}]\sum_{m=1}^{n}\frac{(-1)^{m-1}}{m^2}\frac{(1+z)\dots(1+\frac{z}{m-1})}{(1-z)(1-\frac{z}{2})\dots(1-\frac{z}{m})}\\
&= 2\sum_{m=1}^{n}\frac{(-1)^{m-1}}{m^2}\sum_{l_1+2l_2+\dots=d-1}\frac{(s_{m,1})^{l_1}(s_{m,2})^{l_2}\dots}{l_1!l_2!\dots1^{l_1}2^{l_2}\dots}
\end{aligned}
$$

with

$$s_{m,j}=(-1)^{j-1}H_{m-1}^{(j)}+H_m^{(j)}.$$

For $d=0$, the modified computation goes like this:

$$
\begin{aligned}
\sum_{k=0}^{n}\binom{n}{k}\binom{n+k}{k}(-1)^{n-k}H_k &= [z^0]\sum_{j\ge1}\Big(-f(0,j)+f(n,j)\Big)\\
&= [z^0]\sum_{j\ge1}\sum_{m=0}^{n-1}\Big(g(m,j)-g(m,j+1)\Big)\\
&= \lim_{J\to\infty}[z^0]\sum_{m=0}^{n-1}\sum_{j=1}^{J}\Big(g(m,j)-g(m,j+1)\Big)\\
&= \lim_{J\to\infty}[z^0]\sum_{m=0}^{n-1}\Big[g(m,1)-g(m,J+1)\Big]\\
&= \sum_{m=0}^{n-1}\frac{2}{m+1}=2H_n.
\end{aligned}
$$

Theorem 2. *For $d\ge1$,*

$$\sum_{k=0}^{n}\binom{n}{k}\binom{n+k}{k}(-1)^{n-k}H_k^{(d+1)}=2\sum_{m=1}^{n}\frac{(-1)^{m-1}}{m^2}\sum_{l_1+2l_2+\dots=d-1}\frac{(s_{m,1})^{l_1}(s_{m,2})^{l_2}\dots}{l_1!l_2!\dots1^{l_1}2^{l_2}\dots}$$

with

$$s_{m,j}=(-1)^{j-1}H_{m-1}^{(j)}+H_m^{(j)}.$$

For $d=0$,

$$\sum_{k=0}^{n}\binom{n}{k}\binom{n+k}{k}(-1)^{n-k}H_k=\sum_{m=0}^{n-1}\frac{2}{m+1}=2H_n. \quad\square$$

For instance we get for $d = 3$

$$\sum_{m=1}^{n} \frac{(-1)^{m-1}}{m^2} \left(\frac{s_{m,1}^3}{3} + s_{m,1} s_{m,2} + \frac{2 s_{m,3}}{3} \right).$$

All the appearing quantities could be rewritten in terms of some standardized sums:

$$\sum_{1 \le j_1 \le \cdots \le j_h \le n} \frac{\varepsilon_1^{j_1}}{j_1^{a_1}} \cdots \frac{\varepsilon_h^{j_h}}{j_h^{a_h}},$$

with $\varepsilon_i \in \{\pm 1\}$ and some natural numbers a_i.

4. A third set of identities

Consider for $0 < m \le n$ the following partial fraction decomposition:

$$\begin{aligned} T &:= \frac{(m+1+z)\dots(n+z)}{z(z-1)\dots(z-n)} \frac{n!}{(n-m)!} \frac{1}{(m+z)^{d+1}} \\ &= \sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{m+k} (-1)^{n-k} \frac{1}{(m+k)^{d+1}} \frac{1}{z-k} + \frac{\lambda}{(m+z)^{d+1}} + \cdots + \frac{\mu}{m+z} \end{aligned}$$

and the limit of $z \cdot T$ for $z \to \infty$:

$$0 = \sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{m+k} (-1)^{n-k} \frac{1}{(m+k)^{d+1}} + \mu,$$

with

$$\begin{aligned} \mu &= [(m+z)^{-1}] \frac{(m+1+z)\dots(n+z)}{z(z-1)\dots(z-n)} \frac{n!}{(n-m)!} \frac{1}{(m+z)^{d+1}} \\ &= \frac{n!}{(n-m)!} [(m+z)^d] \frac{(m+1+z)\dots(n+z)}{z(z-1)\dots(z-n)} \\ &= \frac{n!}{(n-m)!} [z^d] \frac{(1+z)\dots(n-m+z)}{(z-m)(z-1-m)\dots(z-n-m)} \\ &= \frac{n!(m-1)!(-1)^{n-1}}{(n+m)!} [z^d] \frac{(1+z)\dots(1+\frac{z}{n-m})}{(1-\frac{z}{m})(1-\frac{z}{m+1})\dots(1-\frac{z}{m+n})} \\ &= \frac{n!(m-1)!(-1)^{n-1}}{(n+m)!} [z^d] \exp\left(\sum_{i=1}^{n-m} \log(1+\frac{z}{i}) + \sum_{i=m}^{m+n} \log \frac{1}{1-\frac{z}{i}} \right) \\ &= \frac{n!(m-1)!(-1)^{n-1}}{(n+m)!} [z^d] \exp\left(\sum_{j \ge 1} \frac{z^j U_j}{j} \right) \end{aligned}$$

with

$$U_j = (-1)^{j-1} \sum_{i=1}^{n-m} \frac{1}{i^j} + \sum_{i=m}^{m+n} \frac{1}{i^j} = (-1)^{j-1} H_{n-m}^{(j)} + H_{n+m}^{(j)} - H_{m-1}^{(j)}.$$

This leads to

$$\mu = \frac{n!(m-1)!(-1)^{n-1}}{(n+m)!} \sum_{l_1+2l_2+\cdots=d} \frac{\big(U_1\big)^{l_1}\big(U_2\big)^{l_1}\dots}{l_1 l_2!\dots 1^{l_1}2^{l_2}\dots}.$$

Theorem 3.

$$\sum_{k=0}^{n} \binom{n}{k}\binom{n+k}{m+k}(-1)^k \frac{1}{(m+k)^{d+1}} = \frac{n!(m-1)!}{(n+m)!} \sum_{l_1+2l_2+\cdots=d} \frac{\big(U_1\big)^{l_1}\big(U_2\big)^{l_1}\dots}{l_1 l_2!\dots 1^{l_1}2^{l_2}\dots},$$

with

$$U_j = (-1)^{j-1}H^{(j)}_{n-m} + H^{(j)}_{n+m} - H^{(j)}_{m-1}.$$

Remark 1. *An almost identical computation gives for integers $0 < p \le m \le n$ the following formula: ($p = m$ is the previous result.)*

$$\sum_{k=0}^{n} \binom{n}{k}\binom{n+k}{m+k}(-1)^k \frac{1}{(p+k)^{d+1}} = \frac{n!(n-p)!(p-1)!(-1)^{n-1}}{(m-p)!(n-m)!(p+n)!} \sum_{l_1+2l_2+\cdots=d} \frac{\big(U_1\big)^{l_1}\big(U_2\big)^{l_1}\dots}{l_1 l_2!\dots 1^{l_1}2^{l_2}\dots},$$

with

$$U_j = (-1)^{j-1}H^{(j)}_{n-p} - (-1)^{j-1}H^{(j)}_{m-p} + H^{(j)}_{n+p} - H^{(j)}_{p-1}.$$

5. Identities in the spirit of Kirschenhofer

Kirschenhofer [4] has found identities for sums

$$\sum_{0\le k\le n,\ k\ne M} \binom{n}{k}(-1)^k \frac{1}{(k-M)^d},$$

where M is an integer with $0 \le M \le n$. We are now investigating the analogous sum

$$\sum_{0\le k\le n,\ k\ne M} \binom{n}{k}\binom{n+k}{k}(-1)^k \frac{1}{(k-M)^d}.$$

Of course, we start from

$$T := \frac{(z+1)\dots(z+n)}{z(z-1)\dots(z-n)}\frac{1}{(z-M)^d},$$

write it in partial fraction decomposition, multiply by z, and consider the limit $z \to \infty$, with the result

$$0 = \sum_{0\le k\le n,\ k\ne M} \binom{n}{k}\binom{n+k}{k}(-1)^{n-k} \frac{1}{(k-M)^d} + \mu,$$

with

$$\begin{aligned}(-1)^n\mu &= (-1)^n[(z-M)^{-1}]\frac{(z+1)\dots(z+n)}{z(z-1)\dots(z-n)}\frac{1}{(z-M)^d}\\ &= (-1)^n[(z-M)^d]\frac{(z+1)\dots(z+n)}{z(z-1)\dots(z-M+1)\cdot(z-M-1)\dots(z-n)}\end{aligned}$$

$$= (-1)^n [z^d] \frac{(z+M+1)\dots(z+M+n)}{(z+M)\dots(z+1)\cdot(z-1)\dots(z+M-n)}$$
$$= (-1)^M \frac{(M+n)!}{M!M!(n-M)!} [z^d] \frac{(1+\frac{z}{M+1})\dots(1+\frac{z}{M+n})}{(1+\frac{z}{M})\dots(1+z)\cdot(1-z)\dots(1-\frac{z}{n-M})}$$
$$= (-1)^M \frac{(M+n)!}{M!M!(n-M)!} [z^d] \exp\biggl(\sum_{k\ge1} \frac{s_k}{k} z^k\biggr),$$

with

$$s_k = (-1)^{k-1}\Bigl(H_{M+n}^{(k)} - 2H_M^{(k)}\Bigr) + H_{n-M}^{(k)}.$$

Hence

$$\sum_{0\le k\le n,\ k\ne M} \binom{n}{k}\binom{n+k}{k}(-1)^{k-1}\frac{1}{(k-M)^d}$$
$$= (-1)^M \frac{(M+n)!}{M!M!(n-M)!} \sum_{j_1+2j_2+\dots=d} \frac{\bigl(s_1\bigr)^{j_1}\bigl(s_2\bigr)^{j_2}\dots}{j_1!j_2!\dots 1^{j_1}2^{j_2}\dots}.$$

Once again here is the comment that one could write the result in the terminology of Bell polynomials.

6. A sum by Melzak et al.

The sum in question appears in [7, 6], viz.

$$f(x+y) = y\binom{y+n}{n}\sum_{k=0}^{n}\binom{n}{k}(-1)^k\frac{f(x-k)}{y+k},$$

with a polynomial $f(x)$ of degree $\le n$. (Compare also [3].)

This formula, too, can easily be derived by partial fraction decomposition:

$$\frac{n!}{z(z-1)\dots(z-n)}\frac{f(x-z)}{y+z}$$
$$= \sum_{k=0}^{n}\binom{n}{k}(-1)^{n-k}\frac{f(x-k)}{(y+k)(z-k)} + \frac{n!(-1)^{n+1}}{y(y+1)\dots(y+n)}\frac{f(x+y)}{y+z}.$$

(The degree restriction is essential here, otherwise there would be extra polynomial terms.)

Now we multiply, as usual, by z, and perform the limit $z\to\infty$:

$$0 = \sum_{k=0}^{n}\binom{n}{k}(-1)^{n-k}\frac{f(x-k)}{y+k} + \frac{n!(-1)^{n+1}f(x+y)}{y(y+1)\dots(y+n)}.$$

This is already the desired formula, after rewriting it.

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