Identities involving harmonic numbers revisited

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Knuth (TAOCP, Vol 3) has an exercise, attributed to S.O.Rice: Show that

$$\begin{aligned} U_n &= \sum_{k \geq 2} \binom{n}{k} (-1)^k \frac{1}{2^{k-1} - 1} \\ &= (-1)^n \frac{n!}{2\pi i} \oint_C \frac{dz}{z(z-1)\ldots(z-n)} \frac{1}{2^{z-1} - 1}, \end{aligned}$$

where C is a skinny closed curve encircling the points $2, 3, \ldots, n$. Changing C to an arbitrarily large circle centered at the origin, derive the convergent series

$$U_n = \frac{(H_{n-1} - 1)n}{\log 2} + \text{further terms}.$$

$$H_n = 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n}$$

(harmonic number)

In Computer Science circles, this method is now called Rice's method, although the integral representation of the alternating sum was known to Nörlund.

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Solving an open problem by Knuth about digital search trees, Flajolet and Sedgewick had to compute

$$n - \sum_{k=2}^{n} \binom{n}{k} (-1)^k R_{k-2},$$

with

$$R_n = Q_n \Big(\frac{1}{Q_0} + \cdots + \frac{1}{Q_n} \Big)$$

and

$$Q_n = \Big(1 - \frac{1}{2}\Big)\Big(1 - \frac{1}{4}\Big) \ldots \Big(1 - \frac{1}{2^n}\Big).$$

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$$\sum_{k=2}^{n} \binom{n}{k} (-1)^k R_{k-2}$$
$$= \frac{1}{2\pi i} \oint \frac{n!(-1)^n}{z(z-1)\dots(z-n)} R(z-2) dz$$

The construction of the meromorphic function $R(z)$ is a bit tricky here.

But the asymptotic evaluation can now be done by computing residues.

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Consider

$$\sum_{k=n_0}^{n} \binom{n}{k} (-1)^k \varphi(k).$$

Rice's method leads to an *identity* in at least the following cases:
$\varphi(z)$ is rational, analytic on $[n_0, \infty)$.
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q-version of Rice's formula (HP):

$$\begin{bmatrix} n \\ k \end{bmatrix}_q := \frac{(q;q)_n}{(q;q)_k (q;q)_{n-k}},$$

with $(z;q)_n := (1-z)(1-zq)\ldots(1-zq^{n-1})$.

$$\sum_{k=1}^{n} (-1)^{k-1} q^{\binom{k}{2}} \begin{bmatrix} n \\ k \end{bmatrix}_q f(q^{-k}) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{(q;q)_n}{(z;q)_{n+1}} f(z)\, dz,$$

where $\mathcal{C}$ encircles the poles $q^{-1}, \ldots, q^{-n}$ and no others.

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For $f(z)$ rational, we get identities:

Van Hamme:

$$S := \sum_{k=1}^{n} \frac{(-1)^{k-1} q^{\binom{k+1}{2}}}{1-q^k} \begin{bmatrix} n \\ k \end{bmatrix}_q = \sum_{k=1}^{n} \frac{q^k}{1-q^k}.$$

For that one, $f(z) = \frac{1}{z-1}$.

Uchimura's generalization for $m \in \mathbb{N}$:

$$S := \sum_{k=1}^{n} \frac{(-1)^{k-1} q^{\binom{k+1}{2}}}{1-q^{k+m}} \begin{bmatrix} n \\ k \end{bmatrix}_q = \sum_{k=1}^{n} \frac{q^k}{1-q^k} \Bigg/ \begin{bmatrix} k+m \\ k \end{bmatrix}_q.$$

Here, $f(z) = \frac{1}{z-q^m}$.

$$\begin{aligned} S &= -\operatorname*{Res}_{z=1} \frac{(q;q)_n}{(z;q)_{n+1}} \frac{1}{z-q^m} - \operatorname*{Res}_{z=q^m} \frac{(q;q)_n}{(z;q)_{n+1}} \frac{1}{z-q^m} \\ &= \frac{1}{1-q^m} - \frac{(q;q)_n (q;q)_{m-1}}{(q;q)_{m+n}}, \end{aligned}$$

which is better (closed form!) than Uchimura's formula.

Dilcher's sum:

$$\sum_{1\le k\le n} \begin{bmatrix} n \\ k \end{bmatrix}_q (-1)^{k-1} \frac{q^{\binom{k}{2}+mk}}{(1-q^k)^m}$$
$$= \sum_{1\le i_1\le i_2\le\cdots\le i_m\le n} \frac{q^{i_1}}{1-q^{i_1}} \cdots \frac{q^{i_m}}{1-q^{i_m}}.$$

This time,

$$f(z) = \frac{1}{(z-1)^m}.$$

As Dilcher noted, the limit for $q \to 1$ is

$$\sum_{1\le k\le n} \binom{n}{k} (-1)^{k-1} \frac{1}{k^m} = \sum_{1\le i_1\le i_2\le\cdots\le i_m\le n} \frac{1}{i_1 \dots i_m}.$$

If n is replaced by infinity, we are in the realm of *multiple ζ-values*, and there is a big industry about finding identities for them. Hernández proved the following identity:

$$\sum_{1\le k\le n} \binom{n}{k} (-1)^{k-1} \sum_{1\le i_1\le i_2\le\cdots\le i_m=k} \frac{1}{i_1 i_2 \dots i_m} = \sum_{1\le k\le n} \frac{1}{k^m}.$$

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Thus, inverting the q-version of Dilcher's formula, I got a q-Hernández formula:

Assume that $a_0 = b_0 = 0$, then

$$\sum_{1 \le k \le n} b_k = \sum_{1 \le k \le n} \begin{bmatrix} n \\ k \end{bmatrix}_q (-1)^k q^{\binom{k}{2}} a_k,$$

$$\sum_{1 \le k \le n} q^{-k} a_k = \sum_{1 \le k \le n} \begin{bmatrix} n \\ k \end{bmatrix}_q (-1)^k q^{-kn+\binom{k}{2}} b_k.$$

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q-analogue of Hernández' formula

$$\sum_{1\le k\le n} \begin{bmatrix} n \\ k \end{bmatrix}_q (-1)^{k-1} q^{-kn+\binom{k}{2}} \sum_{1\le i_1\le i_2\le\cdots\le i_m=k} \frac{q^{i_1}}{1-q^{i_1}} \cdots \frac{q^{i_m}}{1-q^{i_m}}$$

$$= \sum_{1\le k\le n} \frac{q^{k(m-1)}}{(1-q^k)^m}.$$

Always invert!

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I was able to prove q-identities of Fu and Lascoux using the q-Rice formula:

$$\sum_{i=1}^{n} \begin{bmatrix} n \\ i \end{bmatrix}_q (-1)^{i-1}(x+1)\dots(x+q^{i-1})\frac{q^{mi}}{(1-q^i)^m}$$
$$= \sum_{i=1}^{n} \left(1-(-x)^i\right)\frac{q^i}{1-q^i} \sum_{i\le i_2\le\cdots\le i_m\le n} \frac{q^{i_2}}{1-q^{i_2}}\cdots\frac{q^{i_m}}{1-q^{i_m}}$$

$$\sum_{i=0}^{n} \begin{bmatrix} n \\ i \end{bmatrix}_q (-1)^{i-1}(x+1)\dots(x+q^{i-1})\frac{q^i}{1-tq^i}$$

$$= -\frac{(q;q)_n}{(t;q)_{n+1}} \sum_{i=0}^{n} \frac{(t;q)_i}{(q;q)_i}(-xq)^i.$$

Partial fraction decomposition; Wenchang Chu's method.

Apéry numbers:

$$A(n) = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2.$$

Beukers' conjecture:

$$\sum_{m \geq 1} \alpha(m) q^m = q \prod_{n \geq 1} (1 - q^{2n})^4 (1 - q^{4n})^4$$

$$A\Big(\frac{p-1}{2}\Big) \equiv \alpha(p) \pmod{p^2},$$

for an odd prime p.

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Sufficient (according to Ahlgren and Ono):

$$\sum_{k=1}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2 \left\{1 + 2kH_{n+k} + 2kH_{n-k} - 4kH_k\right\} = 0.$$

$$f(x) = \frac{x(1-x)^2(2-x)^2\dots(n-x)^2}{x^2(x+1)^2\dots(x+n)^2}$$

Partial fraction decomposition

$$f(x) = \frac{1}{x} + \sum_{k=1}^{n} \left\{ \frac{B_k}{(x+k)^2} + \frac{C_k}{x+k} \right\}$$

$$C_k = \binom{n}{k}^2 \binom{n+k}{k}^2 \left\{ 1 + 2kH_{n+k} + 2kH_{n-k} - 4kH_k \right\}$$

Now multiply by x and let $x \to \infty$; this gives the identity.

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Human proofs of Identities by Osburn and Schneider
(as opposed to Carsten Schneider's computer proofs)
Consider

$$\frac{(z+1)\ldots(z+n)}{z(z-1)\ldots(z-n)} = \sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{k} (-1)^{n-k} \frac{1}{z-k}.$$

Multiplying this by z, and letting $z \to \infty$, by obtain

$$\sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{k} (-1)^{n-k} = 1.$$

Consider

$$\frac{(z+1)\dots(z+n-1)}{z(z-1)\dots(z-n)}\frac{1}{z+n}$$
$$=\sum_{k=0}^{n}\binom{n}{k}\binom{n+k}{k}(-1)^{n-k}\frac{1}{(n+k)^2}\frac{1}{z-k}+\frac{(n-1)!^2}{(2n)!}\frac{1}{z+n}.$$

The limit form is

$$\sum_{k=0}^{n}\binom{n}{k}\binom{n+k}{k}(-1)^{n-k}\frac{1}{(n+k)^2}=-\frac{(n-1)!^2}{(2n)!}.$$

$$\frac{(z+1)\dots(z+n)}{(z-1)\dots(z-n)}\frac{1}{j(j+z)} = \sum_{k=1}^{n}\binom{n}{k}\binom{n+k}{k}(-1)^{n-k}\frac{k}{j(j+k)}\frac{1}{z-k} + \frac{(j-1)!^2}{(j-n-1)!(n+j)!}\frac{1}{j+z}.$$

The limit form is

$$\sum_{k=1}^{n}\binom{n}{k}\binom{n+k}{k}(-1)^{n-k}\frac{k}{j+k} = -\frac{(j-1)!^2}{(j-n-1)!(n+j)!} + \frac{1}{j}.$$

Summing on $j \geq 1$ (and shifting the index), we get

$$\sum_{k=1}^{n} \binom{n}{k} \binom{n+k}{k} (-1)^{n-k} H_k = \sum_{j \geq 0} \left[\frac{1}{j+1} - \frac{j!^2}{(j-n)!(n+1+j)!} \right].$$

This can be summed (creative telescoping):

$$\sum_{k=1}^{n} \binom{n}{k} \binom{n+k}{k} (-1)^{n-k} H_k = 2H_n.$$

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A few more, for example

$$\sum_{k=1}^{n} \binom{n}{k} \binom{n+k}{k} (-1)^{n-k} H_k^{(2)} = 2 \sum_{k=1}^{n} \frac{(-1)^{k-1}}{k^2}.$$

Vermaseren (a physisist) 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.*

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Wenchang Chu's method works here as well!

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

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

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

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

Theorem

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

$$= \sum_{1 \cdot j_1 + 3 \cdot j_3 + \cdots = d} \frac{2^{j_1 + j_3 + \cdots} \left(H_n^{(1)}\right)^{j_1} \left(H_n^{(3)}\right)^{j_3} \ldots}{j_1! j_3! \ldots 1^{j_1} 3^{j_3} \ldots}. \quad \square$$

Theorem

For $d \geq 1$,

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

with

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

For $d = 0$,

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

Theorem

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

$$= \frac{n!(m-1)!}{(n+m)!} \sum_{l_1+2l_2+\cdots=d} \frac{\left(U_1\right)^{l_1} \left(U_2\right)^{l_1} \ldots}{l_1 l_2! \ldots 1^{l_1} 2^{l_2} \ldots},$$

with

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

An old exercise vom AMM (Melzak):

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

with a polynomial $f(x)$ of degree $\leq n$.

Díaz-Barrero, Gibergans-Báguena and Popescu:

$$\sum_{k=1}^{n} \binom{n}{k} (-1)^{k-1} \frac{1}{\binom{x+k}{k}} \sum_{1 \le i \le j \le k} \frac{1}{x^2 + (i+j)x + ij} = \frac{n}{(x+n)^3},$$

$$\sum_{k=1}^{n} \binom{n}{k} (-1)^{k-1} \text{complicated}(k) = \frac{n}{(x+n)^4}.$$

INVERT!

Compute

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

Of course, Wenchang Chu's rational fraction decomposition works here again.

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Theorem

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

$$= \frac{1}{\binom{x+n}{n}} \sum_{l_1+2l_2+3l_3+\cdots=d} \frac{s_{n,1}^{l_1} s_{n,2}^{l_2} \ldots}{l_1! l_2! \ldots 1^{l_1} 2^{l_2} \ldots}$$

with

$$s_{n,j} = \sum_{k=1}^{n} \frac{1}{(k+x)^j}.$$

Recently, I ran into this:

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

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$$S(n,m) = \sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{1}{2^k(m+k)}.$$

Using Pfaff's reflection law (or simply induction!)

$$S(n,m) = \frac{n!(m-1)!}{2^n(n+m)!} \sum_{k=0}^{n} \binom{m+n}{k}.$$

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$$S(n, n+d) = \frac{n!(n+d-1)!}{2^n(2n+d)!}\left[2^{2n+d-1} - \sum_{k=n+1}^{n+d-1}\binom{2n+d}{k}\right]$$