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COMMENT

# On the conjectures of Henkel and Weston

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**Abstract.** Recent conjectures of Henkel and Weston on certain two-dimensional sums are examined, and some significant generalizations of these sums are developed. The results so obtained should be useful in analysing finite-size effects in systems subjected to non-periodic boundary conditions.

In a recent letter Henkel and Weston (1992) have calculated the universal amplitude $A$ of the correlation length $\xi$ of the spherical model of ferromagnetism in geometry $L^2 \times \infty^1$ under *antiperiodic* boundary conditions:

$$A = \frac{\xi}{2L} = \frac{1}{2\sqrt{2}\,\pi}\left(1 + \frac{2y^2}{\pi^2}\right)^{-1/2} \tag{1}$$

where $y$ is the 'thermogeometric parameter' of the system (see Pathria 1983). At the bulk critical temperature, $T = T_c(\infty)$, $y$ is determined by the constraint equation

$$2y = \sum_{q(2)}{}' \, (-1)^{q_x+q_y} q^{-1} \, e^{-2yq} \qquad q = \sqrt{q_x^2 + q_y^2} > 0. \tag{2}$$

In contrast with periodic boundary conditions, equation (2) does not have a real solution. One is then led to the following sums:

$$S(v) = \sum_{q_x=1}^{\infty} \sum_{q_y=0}^{\infty} (-1)^{q_x+q_y} q^{-1} \sin(2vq) \tag{3}$$

and

$$C(v) = \sum_{q_x=1}^{\infty} \sum_{q_y=0}^{\infty} (-1)^{q_x+q_y} q^{-1} \cos(2vq). \tag{4}$$

On the basis of numerical studies, Henkel and Weston conjectured that

$$S(v) = -\tfrac{1}{2}v \qquad \text{if } -\frac{\pi}{\sqrt{2}} < v < \frac{\pi}{\sqrt{2}} \tag{5}$$

and

$$C(v) = 0 \qquad \text{if } v = \pm\tfrac{5}{4} \tag{6}$$

concluding that $y = \pm i\,\frac{5}{4}$ and hence

$$A = \frac{1}{2\sqrt{2}\,\pi}\left(1 - \frac{25}{8\pi^2}\right)^{-1/2} = 0.13614. \tag{7}$$

Our analysis shows that, while (5) is correct, (6) is not. The resulting modification of

$A$ is not that significant but we do acquire a better understanding of the sums involved.

Our initial approach to this problem was to reconsider the exponential sum

$$E_\tau(\alpha)=\sum_{q(2)}{}' \cos(2\pi q_1\tau_1)\cos(2\pi q_2\tau_2)q^{-1}\,e^{-\alpha q}$$
$$0\leqslant\tau_{1,2}\leqslant\tfrac{1}{2}\qquad \tau=|\boldsymbol{\tau}|>0 \tag{8}$$

which had been studied earlier by Chaba and Pathria (1976) with $\alpha$ *real and positive*. The obvious procedure to follow now was to carry out analytic continuation of this sum to *complex* $\alpha$ and then set $\alpha=\pm 2iv$; with $\boldsymbol{\tau}=(\frac{1}{2},\frac{1}{2})$, that would readily provide the desired information about the sums $S(v)$ and $C(v)$. However, keeping in mind the possibility of extending the work of Henkel and Weston to *general* geometry $L^{d^*}\times\infty^{d'}$, we decided to dwell on some of our more recent work on lattice sums (Allen and Pathria 1993) and look at this problem in a somewhat broader context.

In the work cited above, we have studied phase-modulated sums involving modified Bessel functions $K_\nu(z)$ in arbitrary dimensions $m(=1,2,3,\ldots)$; by definition,

$$\mathscr{K}_\tau(\nu\,|\,m;y)=\sum_{q(m)}{}' \cos(2\pi\boldsymbol{q}\cdot\boldsymbol{\tau})(yq)^{-\nu}K_\nu(2yq)$$
$$q=|\boldsymbol{q}(m)|>0\qquad 0\leqslant\tau_j\leqslant\tfrac{1}{2}(j=1,\ldots,m)\qquad \tau=|\boldsymbol{\tau}(m)|>0. \tag{9}$$

In practical applications, $m=d^*$ while $\nu$ is related to $d(=d^*+d')$, the total dimensionality of the system under consideration; the sum appearing in the constraint equation pertains to $\nu=(d-2)/2$. To begin with, the parameter $y$ is *real and positive*; however, making use of the Poisson summation formula, we have rendered these sums into a form that allows analytic continuation into the region $0\geqslant y^2>-\pi^2\tau^2$. Setting $y=\pm iv$, where $v$ is real and $0\leqslant v<\pi\tau$, we obtain some remarkable results for a class of sums involving ordinary Bessel functions, $J_\nu(z)$ and $Y_\nu(z)$, of which $S(v)$ and $C(v)$ are special cases.

First we obtain the following result:

$$\mathscr{J}_\tau(\nu\,|\,m;v)=\sum_{q(m)}{}' \cos(2\pi\boldsymbol{q}\cdot\boldsymbol{\tau})(vq)^{-\nu}J_\nu(2vq)$$
$$=-\frac{1}{\Gamma(\nu+1)}\qquad \nu>-\frac{1}{2}\qquad 0\leqslant v<\pi\tau. \tag{10}$$

We note that, while for $m=1$ the above result is already known (see Morse and Feshbach 1953, Watson 1958), for $m>1$ it seems to be new. From a purely mathematical point of view, the importance of (10) may lie in the fact that, with $\boldsymbol{\tau}=(\frac{1}{2},\ldots,\frac{1}{2})$, it provides a representation of a null-function, over the interval $(0,\pi\sqrt{m})$, by a Schlömilch series in $m$ dimensions with non-vanishing coefficients.

For $\nu=\frac{1}{2}$, (10) gives

$$\sum_{q(m)}{}' \cos(2\pi\boldsymbol{q}\cdot\boldsymbol{\tau})q^{-1}\sin(2vq)=-2v\qquad |v|<\pi\tau. \tag{11}$$

With $m=2$ and $\boldsymbol{\tau}=(\frac{1}{2},\frac{1}{2})$, this yields $4S(v)=-2v$. Conjecture (5) is thereby proved.

Next we obtain

$$\mathscr{Y}_\tau(\nu\,|\,m;v)=\sum_{q(m)}{}' \cos(2\pi\boldsymbol{q}\cdot\boldsymbol{\tau})(vq)^{-\nu}Y_\nu(2vq)$$
$$=A_\tau(\nu\,|\,m;v)+v^{-2\nu}B_\tau(\nu\,|\,m;v^2) \tag{12}$$

where the precise form of the functions $A$ and $B$ depends on whether $\nu$ is, or is not, equal to $k(=0, 1, 2, \ldots)$.

(i) $\nu \neq k$ $(k=0, 1, 2, \ldots)$:

$$A_\tau(\nu \mid m; v) = \pi^{-1} \cos(\pi\nu)\Gamma(-\nu) \tag{13}$$

$$B_\tau(\nu \mid m; v^2) = -\pi^{2\nu-(m/2)-1} \sum_{r=0}^{\infty} D_\tau(\nu - r \mid m) \frac{1}{r!} \left(\frac{v^2}{\pi^2}\right)^r \tag{14}$$

where

$$D_\tau(\nu \mid m) = \begin{cases} \pi^{(m/2)-2\nu}\Gamma(\nu) \sum\limits_{q(m)}' \cos(2\pi \boldsymbol{q}\cdot\boldsymbol{\tau}) q^{-2\nu} & \nu > 0 \quad (15a) \\ \Gamma\left(\frac{1}{2}m - \nu\right) \sum\limits_{l(m)} |\boldsymbol{l} + \boldsymbol{\tau}|^{2\nu-m} & \nu < 0. \quad (15b) \end{cases}$$

(ii) $\nu = k$ $(k=0, 1, 2, \ldots)$:

$$A_\tau(k \mid m; v) = -\frac{v^{2k}}{\pi k!} \left[\ln\left(\frac{v^2}{\pi^2}\right) - \psi(k+1) + \pi^{-(m/2)} \bar{D}_\tau(m)\right] \tag{16}$$

$$B_\tau(k \mid m; v^2) = -\pi^{2k-(m/2)-1} \sum_{\substack{r=0 \\ (r \neq k)}}^{\infty} D_\tau(k - r \mid m) \frac{1}{r!} \left(\frac{v^2}{\pi^2}\right)^r \tag{17}$$

where $\psi(k+1)$ is the digamma function while

$$\bar{D}_\tau(m) = \lim_{\nu \to 0} \left[D_\tau(\nu \mid m) + \frac{\pi^{(m/2)}}{\nu}\right]. \tag{18}$$

Explicit expressions for the functions $D_\tau(\nu \mid m)$ and $\bar{D}_\tau(m)$ for some special values of $\boldsymbol{\tau}$ and $m$ are given in Allen and Pathria (1993); clearly, for cases like those, the $m$-dimensional sum in (12) is effectively reduced to a one-dimensional sum, as in (14) or (17).

For $\nu = \frac{1}{2}$, we obtain

$$\sum_{q(m)}' \cos(2\pi \boldsymbol{q}\cdot\boldsymbol{\tau}) q^{-1} \cos(2vq)$$

$$= \pi^{(1-m)/2} \sum_{r=0}^{\infty} D_\tau\left(\frac{1}{2} - r \mid m\right) \frac{1}{r!} \left(\frac{v^2}{\pi^2}\right)^r \qquad |v| < \pi\tau. \tag{19}$$

For $m=1$, the sum on the left can be evaluated by elementary means, giving $-\ln\{4[\sin^2(\pi\tau) - \sin^2 v]\}$ which, for $\tau = \frac{1}{2}$, vanishes at $v = \pm\pi/3$. It was the existence of this exact result (see Singh and Pathria 1985, Singh *et al* 1986) that triggered Henkel and Weston (1992) to explore the corresponding problem with $m=2$, leading to the sum $C(v)$, and (erroneously) hope that once again an exact zero would result. We now find that, for $|v| < \pi/\sqrt{2}$,

$$C(v) = \frac{1}{\sqrt{\pi}} \sum_{r=0}^{\infty} \frac{1}{r!} (2^{r+1/2} - 1) \Gamma\left(r + \frac{1}{2}\right) \zeta\left(r + \frac{1}{2}\right) \beta\left(r + \frac{1}{2}\right) \left(\frac{v^2}{\pi^2}\right)^r$$

$$= \sqrt{2}\left(1 - \frac{2v^2}{\pi^2}\right)^{-1/2} + \sqrt{\frac{2}{\pi}}$$

$$\times \sum_{r=0}^{\infty} \frac{1}{r!} \Gamma\left(r + \frac{1}{2}\right) \left\{(1 - 2^{-r-1/2}) \zeta\left(r + \frac{1}{2}\right) \beta\left(r + \frac{1}{2}\right) - 1\right\} \left(\frac{2v^2}{\pi^2}\right)^r \tag{20}$$

where $\zeta(\nu)$ is the Riemann zeta function while

$$\beta(\nu) = \sum_{l=0}^{\infty} (-1)^l (2l+1)^{-\nu} \qquad \nu > 0. \tag{21}$$

In the above form, the sum $C(v)$ converges much faster than in the original form (4). Working with (4) and employing $1600 \times 1600$ terms in $q_x$ and $q_y$, we found that the zero of this sum was approximately 1.252; working with (20) and employing only 10 terms in $r$, we concluded that this number was more like 1.25213. Conjecture (6) is thereby disproved, though the resulting value of $A$, viz. 0.13624 . . . , is not very different from the one given in (7).

## References

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