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Cross-over phenomena in the asymptotic behaviour of lattice sums

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Abstract. Sums of the form

$$S_\sigma(\boldsymbol{k}, \beta) = \sum_{\boldsymbol{m}}{}' m^{-\sigma} f(\boldsymbol{k} \cdot \boldsymbol{m}) \exp(-\beta m),$$

over a d-dimensional lattice are analysed for small β and $k = |\boldsymbol{k}|$. In particular, for non-integral σ, $S_\sigma(\boldsymbol{k}, \beta)$ is shown to have a singular part which behaves as

$$S_\sigma(\boldsymbol{k}, \beta) \simeq k^{\sigma-d} X_\sigma(\beta/k) \qquad \text{as } \beta \to 0, k \to 0, \beta/k = \mathrm{O}(1),$$

and thus to exhibit cross-over phenomena. Explicit results for the cross-over function $X_\sigma(z)$ are obtained.

1. Introduction

Considerable attention has been devoted recently to the evaluation and analysis of lattice sums of the form

$$S = \sum_{\boldsymbol{m}} \Phi(\boldsymbol{m}) \tag{1.1}$$

where the sum is over all points $\boldsymbol{m}$ of a d-dimensional lattice. An explicit specification of the summand $\Phi(\boldsymbol{m})$, which depends on one or more parameters, will be said to define a *class* of lattice sums.

For certain classes, notably the Madelung class generated by $\Phi(\boldsymbol{m}) = |\boldsymbol{m}|^{-\sigma}$, Glasser (1973a,b, 1974) and Zucker (1974) have shown that for some lattices (1.1) can be evaluated in terms of elementary Dirichlet sums. Other work (see e.g. Hall 1976a, Chaba and Pathria 1975, 1976, Barber and Opie 1977) has investigated the asymptotic properties of S as a function of an additional parameter z in $\Phi(\boldsymbol{m}; z)$ for large and/or small values of z. Hall (1976b) has shown for two particular classes that this asymptotic behaviour can be rather analogous to that found in the theory of critical phenomena. In particular, he found that the leading asymptotic behaviour of $S(z)$ was often independent of the lattice structure and exhibited a kind of *universality*. A similar universality was found for a different class by Barber and Opie (1977).

In this paper, we investigate lattice sums of the form

$$S_\sigma(\boldsymbol{k}, \beta) = \sum_{\boldsymbol{m}}{}' m^{-\sigma} f(\boldsymbol{k} \cdot \boldsymbol{m}) \exp(-\beta m), \tag{1.2}$$

where the prime indicates the omission of the null vector. Here $\boldsymbol{k}$ is a d-dimensional vector of magnitude k, β is a non-negative scalar and $m = |\boldsymbol{m}|$. The restrictions on the parameter σ and the detailed conditions imposed on the function $f(z)$ will be discussed later. Our attention will focus on the asymptotic behaviour of (1.2) in the limits $k \to 0$ *and* $\beta \to 0$. This behaviour is interesting because $S_\sigma(\boldsymbol{k}, \beta)$ is an analytic function of k for fixed positive β but is non-analytic in k if $\beta = 0$. Consequently, the asymptotic properties of $S_\sigma(\boldsymbol{k}, \beta)$ for small k are different in the two regimes $\beta > 0$ and $\beta = 0$, with a 'cross-over' for small β. This behaviour is very analogous to that found in cross-over phenomena in the theory of phase transitions and multi-critical points (see e.g. Fisher 1974).

To illustrate the basic phenomenon in which we are interested and to motivate our subsequent analysis, consider the one-dimensional sum

$$S_{1/2}(k, \beta) = \sum_{m=1}^{\infty} m^{-1/2} \cos(km) \exp(-\beta m). \tag{1.3}$$

For positive β this sum converges for all k, but for $\beta = 0$, it diverges if $k = 0$. For $\beta > 0$, and k small we can expand $\cos(km)$ to obtain

$$S_{1/2}(k, \beta) = F_{1/2}(\beta) - \tfrac{1}{2}k^2 F_{-3/2}(\beta) + \mathrm{O}(k^4) \tag{1.4}$$

where

$$F_\sigma(z) = \sum_{m=1}^{\infty} m^{-\sigma} \exp(-zm) \tag{1.5}$$

is the so called Bose function (Erdélyi 1953, London 1954). For $|z| < 2\pi$ and $\arg|z| < \pi$, these functions possess the convergent expansions (Erdélyi 1953)

$$F_\sigma(z) = \Gamma(1-\sigma) z^{\sigma-1} + \sum_{n=0}^{\infty} (-z)^n \zeta(\sigma - n)/n!, \tag{1.6a}$$

for non-integral σ and

$$F_s(z) = (-z)^{s-1}(\psi(s) - \psi(1) - \ln z)/(s-1)! + \sum_{\substack{n=0 \\ (n \neq s)}}^{\infty} (-z)^n \zeta(s-n)/n!, \tag{1.6b}$$

for σ equal to an integer s. In these formulae $\Gamma(z)$ is the gamma function, $\zeta(z)$ is the Riemann zeta function and $\psi(z) = \mathrm{d}(\ln \Gamma(z))/\mathrm{d}z$.

Equation (1.6a) implies that for small β we can approximate (1.4) by

$$S_{1/2}(k, \beta) \simeq (\pi/\beta)^{1/2}(1 - \tfrac{3}{16}k^2\beta^{-2} + \ldots). \tag{1.7}$$

Thus for β of the order k, the correction term in (1.4) is of the order of the leading term, and (1.4) is a poor representation of $S_{1/2}(k, \beta)$ unless k is extremely small.

On the other hand if $\beta \equiv 0$, we have

$$S_{1/2}(k, \beta) = \mathrm{Re} \sum_{m=1}^{\infty} m^{-1/2} \exp(-\mathrm{i}km) = \mathrm{Re}\, F_{1/2}(\mathrm{i}k) = (\pi/2k)^{1/2} + \mathrm{O}(1), \tag{1.8}$$

where we have used (1.6a). This result explicitly exhibits the non-analyticity of $S_{1/2}(k, \beta)$ as a function of k for $\beta = 0$.

Whilst (1.8) is actually valid only if $\beta \equiv 0$, (1.7) shows that, for any small positive value of β, there exists a range of k for which $S_{1/2}(k, \beta)$ behaves essentially as in (1.8) and only 'crosses-over' to the true asymptotic behaviour of (1.4) for sufficiently small

k. In the following section, we shall establish that in the limit $k \to 0$, $\beta \to 0$ with k/β of order unity, $S_{1/2}(k, \beta)$ has the representation

$$S_{1/2}(k, \beta) \simeq k^{-1/2} X_{1/2}(\beta/k), \tag{1.9}$$

with

$$X_{1/2}(z) = \pi^{1/2}(1+z^2)^{-1/4} \cos(\tfrac{1}{2} \cot^{-1}(z)). \tag{1.10}$$

Two limits of $X_{1/2}(z)$ are now of special interest. In the limit $z \to 0$, corresponding to $\beta \to 0$ at fixed small k, we find

$$X_{1/2}(z) = (\pi/2)^{1/2} + \mathrm{O}(z), \tag{1.11}$$

which yields (1.8). On the other hand, as $z \to \infty$, which corresponds to $k \to 0$ at fixed small β, we obtain

$$X_{1/2}(z) = \pi^{1/2} z^{-1/2}(1 - \tfrac{3}{16} z^{-2} + \mathrm{O}(z^{-3})), \tag{1.12}$$

from which we can recover (1.7). The *cross-over function* $X_{1/2}(z)$ thus affords a complete representation of the non-analytic behaviour of $S_{1/2}(k, \beta)$ over the whole range of small values of both parameters k and β.

In the remainder of this paper, we explicitly calculate the cross-over functions associated with the more general sums (1.3). Section 2 is devoted to an analysis of (1.3) for $d = 1$; the generalisation to arbitrary d is given in § 3. A concluding discussion, in which we mention a few extensions and possible applications of these results, is given in § 4.

2. Analysis of one-dimensional sums

We consider the sum

$$S_\sigma(k, \beta) = \sum_{m=1}^{\infty} m^{-\sigma} f(km) \exp(-\beta m), \qquad \beta \geq 0, k \geq 0. \tag{2.1}$$

The function $f(z)$ is assumed to satisfy both

$$|f(z)| \leq M_1 < \infty \qquad \text{for all } z \tag{2.2a}$$

and

$$\left| \int_0^z f(z')\,\mathrm{d}z' \right| \leq M_2 < \infty \qquad \text{as } z \to \infty. \tag{2.2b}$$

These conditions ensure, by Chartier's test (see e.g. Whittaker and Watson 1965, p 72) that the Mellin transform $\int_0^\infty x^{s-1} f(x)\,\mathrm{d}x$ exists at least for $0 < \mathrm{Re}\, s < 1$. In addition, we shall assume that $f(z)$ possesses a Taylor series

$$f(z) = \sum_{l=0}^{\infty} a_l z^l, \tag{2.3}$$

which converges for all z.

Since for $\beta > 0$, the sum in (2.1) converges uniformly in β, we can differentiate (2.1) term by term to establish,

$$\frac{\partial}{\partial \beta} S_\sigma(k, \beta) = -S_{\sigma-1}(k, \beta). \tag{2.4}$$

Thus we can restrict σ to the interval

$$0<\sigma\leqslant 1. \tag{2.5}$$

Sums corresponding to other values of σ outside this interval can be generated by successive applications of the recurrence relation (2.4) together with

$$\lim_{\beta\to\infty} S_\sigma(k,\beta)=0, \qquad \text{for all } \sigma. \tag{2.6}$$

Hence

$$S_{\sigma-l}(k,\beta)=(-1)^l\frac{\partial^l}{\partial\beta^l}S_\sigma(k,\beta) \tag{2.7}$$

and

$$S_{\sigma+l}(k,\beta)=\int_\beta^\infty \mathrm{d}\beta_1\int_{\beta_1}^\infty \mathrm{d}\beta_2\ldots\int_{\beta_{l-1}}^\infty \mathrm{d}\beta_l\, S_\sigma(k,\beta_l) \tag{2.8}$$

where $l=1,2,\ldots$ and σ satisfies (2.5).

The condition (2.3) implies that $S_\sigma(k,\beta)$ is an analytic function of k for $\beta>0$ with a convergent Taylor series

$$S_\sigma(k,\beta)=\sum_{l=0}^{\infty} a_l k^l F_{\sigma-l}(\beta), \tag{2.9}$$

where $F_\sigma(\beta)$ is the Bose function defined by (1.5). However for sufficiently large l the coefficients of this series (by (1.6)) become very large and ultimately diverge as $\beta\to 0$.

If $\beta\equiv 0$, $S_\sigma(k,0)$ converges by the integral test and (2.2) if $k>0$ but diverges for $k=0$. We shall show† explicitly that

$$S_\sigma(k,0)=k^{\sigma-1}A_\sigma+\mathrm{O}(k^{\sigma-1}) \qquad \text{as } k\to 0. \tag{2.10}$$

To establish this result and to determine the associated cross-over function we introduce the Mellin transform

$$M(p;\beta,k)=\int_0^\infty x^{p-1}f(kx)\exp(-\beta x)\,\mathrm{d}x. \tag{2.11}$$

An obvious change of variable yields

$$M(p;\beta,k)=k^{-p}M(p;z,1)\equiv k^{-p}W(p;z) \tag{2.12}$$

where

$$z=\beta/k. \tag{2.13}$$

Since $f(y)$ satisfies (2.2), $W(p;z)$ is an analytic function of p for all $z\geqslant 0$ in the strip

$$1>\mathrm{Re}\,p>0. \tag{2.14}$$

Thus we can invert (2.11) to obtain

$$f(km)\exp(-\beta m)=\frac{1}{2\pi\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} m^{-p}k^{-p}W(p;z)\,\mathrm{d}p; \tag{2.15}$$

† This result is true for $0<\sigma<1$. The corresponding behaviour for $\sigma=1$ will be given later (see (2.25)).

where the contour is such that $c = \mathrm{Re}\, p$ satisfies (2.14). If the contour is further restricted to the strip

$$1 > \mathrm{Re}\, p > 1 - \sigma \geq 0, \tag{2.16}$$

we can substitute (2.15) in (2.1) and interchange the order of summation and integration to yield the integral representation

$$S_\sigma(k, \beta) = \frac{1}{2\pi \mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} k^{-p} \zeta(p+\sigma) W(p; z)\, \mathrm{d}p, \tag{2.17}$$

where, as before, $\zeta(z)$ is the Riemann zeta function and $c = \mathrm{Re}\, p$ satisfies (2.16).

Since $W(p; z)$ is analytic in the strip (2.16) the leading behaviour of $S_\sigma(k, \beta)$ as $k \to 0$ with $z = \beta/k = \mathrm{O}(1)$ comes from the pole of the zeta function in (2.17) at $p = 1 - \sigma$. For $1 > \sigma > 0$, we thus obtain

$$S_\sigma(k, \beta) \approx k^{\sigma-1} X_\sigma(\beta/k) \tag{2.18}$$

with

$$X_\sigma(z) = W(1-\sigma; z) = \int_0^\infty x^{-\sigma} f(x) \exp(-zx)\, \mathrm{d}x. \tag{2.19}$$

For $z = 0$, i.e. $\beta \equiv 0$, these results confirm (2.10) with

$$A_\sigma = X_\sigma(0) = W(1-\sigma; 0). \tag{2.20}$$

To estimate the order of the correction term in (2.18) and to include the case $\sigma = 1$, we require some knowledge of the analytic properties of $W(p; z)$ for $\mathrm{Re}\, p \leq 0$. A suitable analytic continuation follows by writing

$$W(p; z) = \int_0^\infty y^{p-1}(f(y) - f(0))\, \mathrm{e}^{-zy}\, \mathrm{d}y + f(0) z^{-p} \Gamma(p). \tag{2.21}$$

Since $f(y)$ satisfies (2.3), the integral in this expression converges for $\mathrm{Re}\, p > -1$, while the second term shows that $W(p; z)$ has a simple pole at $p = 0$ with residue $f(0) = a_0$. Thus the correction term in (2.18) and (2.10) is $\mathrm{O}(1)$ for small k.

The case $\sigma = 1$ is complicated by the fact that the integrand of (2.17) has a double pole at $p = 0$ arising from the coincidence of the poles of $W(p; z)$ and $\zeta(p+1)$. From (2.21) we find that

$$W(p; z) = \frac{a_0}{p} - a_0(\ln z - \psi(1)) + \int_0^\infty y^{-1}(f(y) - a_0)\, \mathrm{e}^{-zy}\, \mathrm{d}y + \mathrm{O}(p) \qquad \text{as } p \to 0, \tag{2.22}$$

where

$$\psi(1) = \Gamma'(1)/\Gamma(1) = -C_\mathrm{E} = -0{\cdot}577216\ldots \tag{2.23}$$

with C_E denoting Euler's constant. The corresponding expansion of $\zeta(1+p)$ is (see Whittaker and Watson 1965, p 271)

$$\zeta(1+p) = \frac{1}{p} + C_\mathrm{E} + \mathrm{O}(p). \tag{2.24}$$

Combining (2.23) and (2.24) yields, after some elementary analysis,

$$S_1(k, \beta) = -a_0 \ln k + X_1(\beta/k) + \mathrm{O}(k) \qquad \text{as } k \to 0,\ \beta/k = \mathrm{O}(1), \tag{2.25}$$

where

$$X_1(z) = -a_0 \ln z + \int_0^\infty y^{-1}(f(y) - a_0)\,e^{-zy}\,dy. \tag{2.26}$$

The correction term in (2.25) comes from the pole in $W(p, z)$ at $p = -1$.

Equations (2.18), (2.19), (2.25) and (2.26) are the main results of this section and establish the asymptotic properties of (2.1) for $0 < \sigma \leq 1$ and all (small) values of β and k. The results reported in § 1 follow by specialising (2.18) and (2.19). For $f(x) = \cos x$, (2.19) gives

$$X_\sigma(z) = \int_0^\infty x^{-\sigma} \cos x \exp(-zx)\,dx, \tag{2.27}$$

which may be evaluated by reference to Erdélyi (1954). Explicitly we find

$$X_\sigma(z) = \Gamma(1-\sigma)(1+z^2)^{-(1-\sigma)/2} \cos[(1-\sigma)\cot^{-1} z], \qquad 0 < \sigma < 1. \tag{2.28}$$

Equation (1.10) is a special case of this for $\sigma = \frac{1}{2}$.

The cross-over functions for other choices of $f(x)$ in (2.1) are given in table 1. These results all follow from the tables of Laplace and Mellin transforms given by Erdélyi (1954). Additional examples can be found in this reference.

Table 1. Cross-over functions for various one-dimensional sums.

$f(x)$	$X_\sigma(z)$
$\sin x$	$\Gamma(1-\sigma)(1+z^2)^{(\sigma-1)/2} \sin[(1-\sigma)\cot^{-1} z]$
$J_0(x)$ $(\sigma \neq 1)$	$\Gamma(1-\sigma) z^{\sigma-1}\, {}_2F_1(\frac{1}{2}(1-\sigma), 1-\frac{1}{2}\sigma; 1; -z^{-2})$
$J_\nu(x)$ $(\nu > \sigma - 1)$	$\dfrac{\Gamma(1-\sigma+\nu)}{\Gamma(1+\nu)} z^{\sigma-1-\nu}\, {}_2F_1(\frac{1}{2}(1-\sigma+\nu), 1-\frac{1}{2}(\sigma-\nu); \nu+1; -z^{-2})$
$I_\nu(x)$ $(\nu > \sigma - 1)$	$\dfrac{2^{-\sigma}\Gamma(\frac{1}{2}(1-\sigma+\nu))\Gamma(1-\frac{1}{2}(\sigma-\nu))}{\pi^{1/2} z^{1-\sigma+\nu}\Gamma(\nu+1)}\, {}_2F_1(1-\frac{1}{2}(\sigma-\nu), \frac{1}{2}(1-\sigma+\nu); \nu+1; z^2)$

Notation: $J_\nu(x)$ is the Bessel function of the first kind, $I_\nu(x)$ is the Bessel function of purely imaginary argument and ${}_2F_1(a, b; c; z)$ denotes the hypergeometric function.

Two points remain for discussion. Firstly, we should check that in the limit $z \to \infty$, corresponding to $k \to 0$ at fixed positive β, $X_\sigma(z)$ behaves in such a way as to cancel the apparent non-analyticity in (2.18) for small k. Secondly we shall briefly comment on the extension of these results to arbitrary real σ.

The behaviour of $X_\sigma(z)$ for large z follows almost immediately from (2.19). We find that

$$X_\sigma(z) \approx z^{\sigma-1} a_0 \Gamma(\sigma-1) + O(z^{\sigma-2}), \tag{2.29}$$

which precisely cancels the $k^{\sigma-1}$ behaviour apparent in (2.18), in accord with (2.9).

The extension of the preceding results to values of σ outside the half-open interval (0, 1] is also fairly straightforward. For $\sigma \leq 0$, (2.7), together with (2.19) and (2.26), immediately gives

$$S_\sigma(k, \beta) \approx k^{-|1-\sigma|} X_\sigma(\beta/k) \tag{2.30}$$

with

$$X_\sigma(z)=(-1)^l\,\mathrm{d}^l X_{\sigma+l}(z)/\mathrm{d}z^l, \tag{2.31}$$

where l is such that

$$0<\sigma+l\leqslant 1. \tag{2.32}$$

For $\sigma>1$, the situation is somewhat more difficult since we observe that in this case $S_\sigma(0, 0)$ exists being given by

$$S_\sigma(0,0)=\zeta(\sigma)f(0). \tag{2.33}$$

This limit obviously cannot be recovered by a direct application of (2.8) to (2.19) or (2.26). Nevertheless, for $\sigma>1$, $S_\sigma(\beta, k)$ does possess a *singular part*, which varies as

$$S_{\sigma,\mathrm{sing}}(k,\beta)\approx k^{\sigma-1}X_\sigma(\beta/k) \qquad k\to 0,\ \beta/k=\mathrm{O}(1) \tag{2.34}$$

for non-integral σ with $X_\sigma(z)$ given by

$$X_\sigma(z)=\int_z^\infty \mathrm{d}z_1\int_{z_1}^\infty \mathrm{d}z_2\ldots\int_{z_{l-1}}^\infty \mathrm{d}z_l\,X_{\sigma-l}(z_l) \tag{2.35}$$

and l such that

$$0<\sigma-l<1. \tag{2.36}$$

One can show that (2.34) gives the lowest *non-analytic* term in the expansion of $S_\sigma(k, \beta)$ for small k; all terms of lower order being integral powers of k. If σ is a positive integer, say s, a similar analysis shows that

$$S_{s,\mathrm{sing}}(k,\beta)=\mathrm{O}(k^{s-1}\ln k). \tag{2.36}$$

We shall not, however, discuss the details of this case, except to note that if the Taylor coefficient of x^s in (2.3) vanishes, then the singular part of $S_s(k, \beta)$ is of order k^s.

3. Higher-dimensional sums

We turn now to the analysis of d-dimensional sums of the type (1.2) with $d>1$. Since $S_\sigma(\boldsymbol{k}, \beta)$ again satisfies the recurrence relations (2.7) and (2.5) we can restrict the parameter σ to a unit interval, which we take to be

$$d-1<\sigma\leqslant d. \tag{3.1}$$

Furthermore, since the sum in (1.2) is over all lattice points, we can, without loss of generality, assume that $f(x)$ is even. Defining

$$\gamma=\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{m}} \tag{3.2}$$

where $\hat{\boldsymbol{k}}$ and $\hat{\boldsymbol{m}}$ denote unit vectors in the direction of $\boldsymbol{k}$ and $\boldsymbol{m}$ respectively, we can then write (1.2) as

$$S_\sigma(\boldsymbol{k},\beta)=2\sum_{\boldsymbol{m},\gamma>0} m^{-\sigma}f(\gamma k m)\exp(-\beta m)+f(0)\sum_{\boldsymbol{m},\gamma=0} m^{-\sigma}\exp(-\beta m). \tag{3.3}$$

The second sum in this expression is over a $(d-1)$-dimensional sub-lattice of the whole lattice and thus converges for all $\beta\geqslant 0$ if σ satisfies (3.1). Consequently, to investigate the asymptotic behaviour of $S_\sigma(\boldsymbol{k}, \beta)$ for small $k=|\boldsymbol{k}|$ and small β it suffices to consider

$$\hat{S}_\sigma(k, \beta)=2 \sum_{\boldsymbol{m}, \gamma>0} m^{-\sigma} f(\gamma k m) \exp(-\beta m). \tag{3.4}$$

Proceeding, as earlier, we introduce the Mellin transform

$$M(p; \beta, k, \gamma)=\int_0^{\infty} x^{p-1} f(\gamma k x) \mathrm{e}^{-\beta x} \mathrm{d}x=k^{-p} W(p; \beta/k, \gamma), \tag{3.5}$$

where

$$W(p; z, \gamma)=\int_0^{\infty} y^{p-1} f(\gamma y) \mathrm{e}^{-zy} \mathrm{d}y. \tag{3.6}$$

Inverting (3.5) and substituting in (3.1) yields the integral representation

$$\hat{S}_\sigma(k, \beta)=\frac{1}{2\pi\mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} k^{-p} \Psi(p; \beta/k) \mathrm{d}p \tag{3.7}$$

with

$$\Psi(p; z)=2 \sum_{\boldsymbol{m}, \gamma>0} m^{-p-\sigma} W(p; z, \gamma). \tag{3.8}$$

The contour in (3.7) is to be chosen such that

$$1>c=\operatorname{Re} p>d-\sigma \geqslant 0, \tag{3.9}$$

for which (3.5) and (3.8) converge.

As before, the leading asymptotic behaviour of $\hat{S}_\sigma(\boldsymbol{k}, \beta)$ for small k with $\beta/k=$ O(1) comes from the pole of the integrand of (3.7) closest to the strip (3.9). We shall show that $\Psi(p; z)$ has a pole at $d-\sigma$. To do so we consider

$$X_\sigma(z)=\lim_{p \to d-\sigma+} (p-d+\sigma) \Psi(p; z), \tag{3.10}$$

where our notation anticipates the identification of the limit with the required crossover function. Applying the Euler–Maclaurin expansion to the sum in (3.4) allows us to write

$$X_\sigma(z)=\lim_{p \to d-\sigma+} 2(p-d+\sigma) \int_{|\boldsymbol{m}|>m_0, \gamma>0} \mathrm{d}^d m\, m^{-p-\sigma} W(p; \gamma, z), \tag{3.11}$$

where m_0 is a fixed positive number. The difference between this integral and the original sum can be shown to vanish in the indicated limit. Introducing polar coordinates in the d-dimensional space about the direction $\hat{\boldsymbol{k}}$, yields

$$\begin{aligned} X_\sigma(z) &=\lim_{p \to d-\sigma+} K_d(p-d+\sigma) \int_{m_0}^{\infty} m^{d-1-p-\sigma} \mathrm{d}m \int_0^1 \mathrm{d}\gamma (1-\gamma^2)^{(d-3)/2} W(p; \gamma, z) \\ &=-K_d \int_0^1 \mathrm{d}\gamma (1-\gamma^2)^{(d-3)/2} W(d-\sigma; \gamma, z), \end{aligned} \tag{3.12}$$

where

$$K_d=2^{1-d} \pi^{(2-d)/2} / \Gamma((d-1)/2). \tag{3.13}$$

Thus for p near $d-\sigma$,

$$\Psi(p,z)=\frac{X_\sigma(z)}{p-d+\sigma}+\mathrm{o}[(p-d+\sigma)^{-1}]. \tag{3.14}$$

Equation (3.7) now immediately implies that $\hat{S}_\sigma$ varies for small k as

$$\hat{S}_\sigma(\boldsymbol{k},\beta)=k^{\sigma-d}X_\sigma(\beta/k)+\mathrm{o}(k^{\sigma-d}) \tag{3.15}$$

with the cross-over function $X_\sigma(z)$ given by (3.12). This result is again only valid for $d-1<\sigma<d$. If $\sigma=d$, $\Psi(p;z)$ possesses a double pole at $p=d-\sigma=0$, which implies that

$$\hat{S}_d(k,\beta)=\mathrm{O}(\ln k). \tag{3.16}$$

This case is, however, rather more difficult to analyse but it can be done along the lines used by Barber and Opie (1977) in their discussion of a special case of (1.2).

The extension of these results to σ outside the interval (3.1) is completely analogous to that given in the preceding section. The conclusion is very similar; namely that for arbitrary σ, $S_\sigma(\boldsymbol{k},\beta)$ has a singular piece which for non-integral σ varies as

$$k^{\sigma-d}X_\sigma(\beta/k) \tag{3.17}$$

as $k\to 0$ with $\beta/k=\mathrm{O}(1)$.

4. Discussion

In the preceding two sections, we analysed sums of the form

$$S_\sigma(\boldsymbol{k},\beta)=\sum_{\boldsymbol{m}}{}' m^{-\sigma}f(\boldsymbol{k}\,.\,\boldsymbol{m})\exp(-\beta m) \tag{4.1}$$

in the limit $\beta\to 0$, $k\to 0$ with β/k of order unity. These sums, for non-integral σ, were found to possess a singular part, which varies in the limit of interest as

$$S_{\sigma,\mathrm{sing}}(\boldsymbol{k},\beta)\simeq k^{\sigma-d}X_\sigma(\beta/k). \tag{4.2}$$

Several aspects of these results are worth comment.

Firstly, for $\beta=0$, we note that the leading asymptotic behaviour as $k^{\sigma-d}$ is independent of both the lattice structure and the specific choice of the function $f(z)$. The cross-over function $X_\sigma(z)$ is also lattice independent, but does depend upon $f(z)$ (recall (2.19) and (3.12)). This universality is wider than that discussed by Hall (1976b) and appears to be rather common to lattice sums. Of course, if $\sigma>d$, (4.2) does not give the *leading* behaviour of $S_\sigma(\boldsymbol{k},\beta)$ for small k. In general, this will be analytic and not universal.

It is possible to extend the analysis presented in this paper in several directions. One extension, which can be treated by the methods developed here, is to sums of the form

$$T_{\sigma,\kappa}(\boldsymbol{k},\beta)=\sum_{\boldsymbol{m}} m^{-\sigma}f(\boldsymbol{k}\,.\,\boldsymbol{m})\exp(-\beta m^{\kappa}). \tag{4.3}$$

The analogue of (4.2) now becomes

$$T_{\sigma,\kappa;\mathrm{sing}}=k^{\sigma-d}Y(\beta/k^{\kappa}) \tag{4.4}$$

with $Y(z)$ given in terms of the Mellin transform of $f(y)\exp(-zy^{\kappa})$ evaluated at $d-\sigma$. It would also be possible to handle functions $f(z)$ which were non-analytic for small z.

Finally, we briefly mention a possible application of these results. Sums of the form (4.1) with $f(x)=\cos x$ and $d=3$ arise in the calculation of dispersion relations in inert gas solids (Opie, private communication). In this example, β arises from many-body effects which screen the simple pairwise additive forces. Since β is probably small, the results of this paper should be relevant to the calculation of dispersion relations for small k. The relevant cross-over function follows from (3.13) and (3.6). Reference to Erdélyi (1954, p 320) gives

$$W(d-\sigma;\gamma,z)=\Gamma(d-\sigma)(z^2+\gamma^2)^{(\sigma-d)/2}\cos[(d-\sigma)\tan^{-1}(\gamma/z)]. \quad (4.5)$$

Hence the cross-over function is given by

$$X_\sigma(z)=-K_d\Gamma(d-\sigma)\int_0^1 \mathrm{d}\gamma(1-\gamma^2)^{(d-3)/2}(z^2+\gamma^2)^{(\sigma-d)/2}\cos[(d-\sigma)\tan^{-1}(\gamma/z)], \quad (4.6)$$

where K_d is given in (3.13).

While this integral cannot be evaluated in closed form for arbitrary σ and d, it is possible to confirm the essential features of the cross-over. In particular, in the limit $z\to 0$, corresponding to $\beta\to 0$ at fixed small k, we obtain

$$X_\sigma(0)=\frac{-2^{1-d}\pi^{(3-d)/2}\Gamma(d-\sigma)}{\Gamma(\frac{1}{2}\sigma)\Gamma(\frac{1}{2}(d-\sigma+1))}. \quad (4.7)$$

This result, together with (3.15), generalises the results of Barber and Opie (1977) to arbitrary d. Similarly, one can easily check that for $z\to\infty$, the non-analytic k dependence in (3.15) is removed.

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