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Evaluation of certain lattice sums in arbitrary dimensions†

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Abstract. For the two mutually reciprocal, unit, Bravais lattices $\{\tau\}$ and $\{\gamma\}$ in an m-dimensional Euclidean space, we present exact results for (i) a class of lattice sums $J_\tau(a, k, m) = \Sigma'_\tau \exp(-a\tau^2)/\tau^{2k}$ for $a > 0$ and k any real number and (ii) the class of complementary lattice sums $S_\gamma(q, l, j, m) = \Sigma'_\gamma \gamma^{-2l}(\gamma^2 + q^2)^{-j}$ for $j > 0$, l any real number and $(2l+2j) > m$. These results may be useful in dealing with finite as well as infinite physical systems—in particular, the ones undergoing phase transitions. The asymptotic results following from our expressions are in qualitative agreement with those of Hall, though quantitatively a slight discrepancy is noted in the case $k < m/2$ for $J_\tau(a, k, m)$ and in the case $l < m/2$ for $S_\gamma(q, l, j, m)$.

1. Introduction

Recently, Hall (1976a) has considered the class of lattice sums defined by

$$J_\tau(a, k, m) \equiv \sum_\tau{}' \exp(-a\tau^2)/\tau^{2k} \qquad (a > 0, k > 0) \tag{1}$$

and a class of complementary sums (Hall 1976b) defined by

$$S_\gamma(q, l, j, m) \equiv \sum_\gamma{}' \gamma^{-2l}(\gamma^2 + q^2)^{-j} \qquad l, j > 0, 2l + 2j > m, \tag{2}$$

where $\{\tau\}$ and $\{\gamma\}$ are mutually reciprocal, unit, Bravais lattices in an m-dimensional Euclidean space. Earlier, Chaba and Pathria (1975a; hereafter this will be referred to as I) had found exact expressions for $J_\tau(a, k, m)$, as applied to an isotropic lattice in m dimensions, for $k = 1$ and asymptotic expressions for $k = 2, 3, 4 \ldots$. Although Hall (1976a) has extended these sums to general lattices and to all positive values of k, he has derived asymptotic results which hold only in the limit $a \to 0$. For the various applications of the sums $J_\tau(a, k, m)$ for positive integer k, the reader may refer to I. The motivation for the extension to all positive k has been given by Hall (1976a) and we shall not repeat it here. For the sums $S_\gamma(q, l, j, m)$, also, Hall (1976b) has given asymptotic results which are valid for the limit $q \to \infty$. Further, Hall (1976b) has mentioned that, for $m = 3$ and $j = 2$, the sums $S_\gamma(q, l, j, m)$ arose in the calculations, concerning a physical problem, by Plasket and Hall and so these sums are also of interest in physics.

The purpose of this paper is to derive exact expressions for the sums $J_\tau(a, k, m)$ where k, now, is any real number and also for the sums $S_\gamma(q, l, j, m)$ for any real value of

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l, with $j>0$ and $(2l+2j)>m$. The results obtained here may be of interest for three main reasons. (i) In the study of an infinite system, that is, in the thermodynamic limit, the physical parameters a and q may be extremely small and large respectively and the asymptotic results of Hall (1976a, b) may be sufficient for analysis; for a finite system, however, this may not be true and one may require subsequent terms of the sums as well. (ii) For certain studies a in $J_\tau(a, k, m)$ may not be small or q in $S_\gamma(q, l, j, m)$ may not be too large, irrespective of the fact that the system is finite or infinite. Such a situation arises, for instance, in the rigorous study of Bose–Einstein condensation (Chaba and Pathria 1975b, Zasada and Pathria 1976), where one encounters the sum $\Sigma'_\tau \exp(-a\tau)/\tau$, with the simple cubic lattice, τ, related to the sum $J_\tau(a, k, m)$, and there a varies drastically in the temperature range of interest. (iii) As pointed out by Hall (1976b), such sums may also be useful in the study of other phase transitions. For instance, if one of such sums occupies a dominant position in some of the basic expressions pertaining to a given physical system, then useful conclusions regarding the onset of a phase transition in the system may be drawn from the behaviour of the sum as a function of the parameters.

The asymptotic results following from our expressions for $J_\tau(a, k, m)$ and $S_\gamma(q, l, j, m)$ are in agreement with those of Hall (1976a, b), except for the case $k<m/2$ in the former and $l<m/2$ in the latter, where slight discrepancies are noted.

2. Evaluation of sums $J_\tau(a, k, m)$

2.1. When k is a positive number, $k>0$

2.1.1. $m=2$. We start with the integral representation (Gradshteyn and Ryzhik 1965)

$$J_\tau(a, k, 2) = a^k \Gamma^{-1}(k) \sum_\tau{}' \int_0^1 x^{-k-1}(1-x)^{k-1} \exp(-a\tau^2/x)\, \mathrm{d}x \qquad (k>0) \tag{3}$$

where the primed summation Σ' excludes the term with $\tau=0$. In order to proceed further, it is convenient to study two separate cases, namely when k is an integer and when it is not an integer.

Firstly, we take up the case when k is an integer, $k=n\geqslant 1$. Then we have

$$\begin{aligned}
&\Gamma(n)a^{-n}J_\tau(a, n, 2)\\
&\quad= \sum_{l=0}^{n-1} (-1)^l \binom{n-1}{l} \sum_\tau{}' \int_0^1 x^{l-n-1} \exp(-a\tau^2/x)\, \mathrm{d}x\\
&\quad= (-1)^{n-1} \sum_\tau{}' \int_1^\infty \exp(-a\tau^2 y)\, \mathrm{d}y + \sum_{l=0}^{n-2} (-1)^l \binom{n-1}{l}\\
&\qquad\times \sum_\tau{}' \int_0^\infty y^{n-l-1} \exp(-a\tau^2 y)\, \mathrm{d}y - \sum_{l=0}^{n-2} (-1)^l \binom{n-1}{l}\\
&\qquad\times \int_1^\infty x^{l-n-1}\Big((\pi x/a) \sum_\gamma \exp(-\pi^2\gamma^2 x/a) - 1\Big)\, \mathrm{d}x\\
&\quad= (-1)^{n-1} a^{-1} \sum_\tau{}' \exp(-a\tau^2)/\tau^2 + \sum_{l=0}^{n-2} (-1)^l \binom{n-1}{l} \Gamma(n-l) J_\tau(0, n-l, 2) a^{l-n}
\end{aligned}$$

$$-\P a^{-1}\sum_{l=0}^{n-2}(-1)^l\binom{n-1}{l}(n-l-1)^{-1}+\sum_{l=0}^{n-2}(-1)^l\binom{n-1}{l}(n-l)^{-1}$$

$$-\sum_{l=0}^{n-2}(-1)^l\binom{n-1}{l}\P^{2n-2l-1}a^{-n+l}\sum_{\gamma}{}'\gamma^{2n-2l-2}\Gamma(1+l-n,\P^2\gamma^2/a), \qquad (4)$$

where $\binom{k-1}{l}=(k-1)(k-2)\dots(k-l)/l!$, $\Gamma(a,x)$ is the incomplete gamma function, and

$$J_\tau(0,k,m)=\lim_{a\to 0}\,[J_\tau(a,k,m)\ \textit{minus}\ \text{its divergent part (if any)}]; \qquad (5)$$

for $k>m/2$, $J_\tau(0,k,m)$ is simply $\Sigma'_\tau\,\tau^{-2k}$. In the second line of (4) we have separated out the term corresponding to $l=n-1$ and split the integral in the remaining sum into two parts, and in the second part we have made use of the Poisson summation formula (PSF) (Stein and Weiss 1971) which, in two dimensions, reads as follows:

$$\sum_\tau \exp(-a\tau^2)=(\P/a)\sum_\gamma \exp(-\P^2\gamma^2/a). \qquad (6)$$

Now using equation (A2) of the appendix and noting that

$$\sum_{l=0}^{n-1}(-1)^l\binom{n-1}{l}(n-l)^{-1}=(-1)^{n-1}n^{-1},$$

we can finally write

$$J_\tau(a,n,2)=\sum_{l=0}^{n}(-1)^l(l!)^{-1}J_\tau(0,n-l,2)a^l+\P A(n,2)[(n-1)!]^{-1}a^{n-1}$$

$$+(-1)^{n-1}\P a^{n-1}[(n-1)!]^{-1}\ln(1/a)-\P a^{n-1}\sum_{l=0}^{n-1}(-1)^l$$

$$\times[l!(n-l-1)!]^{-1}\sum_\gamma{}'(\P^2\gamma^2/a)^{n-l-1}\Gamma(1+l-n,\P^2\gamma^2/a), \qquad (7)$$

where

$$A(n,2)=\sum_{l=0}^{n-2}(-1)^{l-1}\binom{n-1}{l}(n-l-1)^{-1}=(-1)^{n-1}(\psi(n)+C), \qquad (8)$$

ψ being the digamma function and C Euler's constant.

We may point out here that equation (7) can also be obtained by integrations of equation (6) with respect to a. However, the method developed here is such that it can be applied even when k is not an integer. We further observe that, for $n=1$, equation (7) goes back to (A2), and the cases $n=1$, 2 and 3 provide identities which are generalisations of equations I(11), I(16) and I(17), respectively, to arbitrary lattices. It may also be noted that for any lattice $J_\tau(0,0,m)\equiv -1$ and for a square lattice (I)

$$J(0,1,2)=C_2=\P(C-\ln[\Gamma^4(1/4)/4\P^3])=0{\cdot}771\,605$$

and

$$J(0,k,2)=4\zeta(k)\beta(k) \qquad (k>1)$$

where

$$\zeta(k)=\sum_{l=0}^{\infty}(l+1)^{-k} \qquad \text{and} \qquad \beta(k)=\sum_{l=0}^{\infty}(-1)^l(2l+1)^{-k}.$$

Next we consider the case when k is not an integer. Let $n=[k]$ be the integral part of k. We then have

$$\begin{aligned}
&\Gamma(k)a^{-k}J_\tau(a,k,2)\\
&\quad=\sum_{l=0}^{\infty}(-1)^l\binom{k-1}{l}\sum_\tau{}'\int_0^1 \mathrm{d}x\,x^{-k+l-1}\exp(-a\tau^2/x)\\
&\quad=\sum_{l=0}^{n-1}(-1)^l\binom{k-1}{l}\sum_\tau{}'\int_0^\infty y^{k-l-1}\exp(-a\tau^2y)\,\mathrm{d}y-\sum_{l=0}^{n-1}(-1)^l\binom{k-1}{l}\\
&\qquad\times\int_1^\infty \mathrm{d}x\,x^{-k+l-1}\Big((\P x/a)\sum_\gamma\exp(-\P^2\gamma^2x/a)-1\Big)+(-1)^n\binom{k-1}{n}\\
&\qquad\times\int_0^1 \mathrm{d}x\,x^{-k+n-1}\Big((\P x/a)\sum_\gamma\exp(-\P^2\gamma^2x/a)-1\Big)+\sum_{l=n+1}^{\infty}(-1)^l\binom{k-1}{l}\\
&\qquad\times\int_0^1 \mathrm{d}x\,x^{-k+l-1}\Big((\P x/a)\sum_\gamma\exp(-\P^2\gamma^2x/a)-1\Big)\\
&\quad=\sum_{l=0}^{n-1}(-1)^l\binom{k-1}{l}\Gamma(k-l)J_\tau(0,k-l,2)a^{-k+l}\\
&\qquad+\sum_{l=n+1}^{\infty}(-1)^l\binom{k-1}{l}\P^{2k-2l-1}\Gamma(l-k+1)\\
&\qquad\times J_\gamma(0,l-k+1,2)a^{-k+l}-(\P/a)\\
&\qquad\times\sum_{l=0}^{\infty}(-1)^l\binom{k-1}{l}(k-l-1)^{-1}+\sum_{l=0}^{\infty}(-1)^l\binom{k-1}{l}(k-l)^{-1}\\
&\qquad-\sum_{l=0}^{\infty}(-1)^l\binom{k-1}{l}\P^{2k-2l-1}a^{-k+l}\sum_\gamma{}'\gamma^{2k-2l-2}\Gamma(1+l-k,\P^2\gamma^2/a)\\
&\qquad+(-1)^n\binom{k-1}{n}\lim_{\epsilon\to0}\Big(\P^{2k-2n-1}a^{-k+n}\sum_\gamma{}'\gamma^{2k-2n-2}\\
&\qquad\times\Gamma(1+n-k,\P^2\gamma^2\epsilon/a)-(k-n)^{-1}\epsilon^{n-k}\Big),
\end{aligned}\tag{9}$$

where we have separated out the terms corresponding to $l\leqslant(n-1)$, $l=n$ and $l\geqslant(n+1)$, split the integral in the first partial sum into two parts and made use of the PSF. Using (A3), to calculate the limit of the expression in large round brackets, and (A6), and noting that

$$\sum_{l=0}^{\infty}(-1)^l\binom{k-1}{l}(k-l)^{-1}=0,$$

we can finally write

$$\begin{aligned}
J_\tau(a,k,2)=&\sum_{l=0}^{\infty}(-1)^l(l!)^{-1}J_\tau(0,k-l,2)a^l+\P A(k,2)\Gamma^{-1}(k)a^{k-l}-\P a^{k-1}\\
&\times\sum_{l=0}^{\infty}(-1)^l[l!T(k-l)]^{-1}\sum_\gamma{}'(\P^2\gamma^2/a)^{k-l-1}\Gamma(1+l-k,\P^2\gamma^2/a),
\end{aligned}\tag{10}$$

where

$$A(k,2)=\sum_{l=0}^{\infty}(-1)^{l-1}\binom{k-1}{l}(k-l-1)^{-1}=\P/\sin(k\P). \tag{11}$$

2.1.2. m = 3. When k is an integer, say $k=n\geqslant 1$, we proceed parallel to the corresponding two-dimensional case. During the process, we use (A7) with $p=1$ and finally obtain

$$J_\tau(a,n,3)=\sum_{l=0}^{n}(-1)^l(l!)^{-1}J_\tau(0,n-l,3)a^l+\P^{3/2}[(n-1)!]^{-1}A(n,3)a^{n-3/2}-\P^{3/2}a^{n-3/2}$$
$$\times\sum_{l=0}^{n-1}(-1)^l[l!(n-l-1)!]^{-1}\sum_\gamma{}'(\P^2\gamma^2/a)^{n-l-3/2}\Gamma(3/2+l-n,\P^2\gamma^2/a), \tag{12}$$

where

$$A(n,3)=\sum_{l=0}^{n-1}(-1)^{l-1}\binom{n-1}{l}(n-l-3/2)^{-1}=B(n,3/2-n), \tag{13}$$

$B(m,n)$ being the beta function. Note that, for a simple cubic lattice (I), $J(0,1,3)=C_3=-8{\cdot}913\,633$.

When k is not an integer, the procedure is similar to, but somewhat more involved than, the case of two dimensions. One has to split the sum appearing on the right-hand side of the three-dimensional counterpart of equation (3), depending on whether $(k-n)$ is greater than, equal to or less than $\frac{1}{2}$. During the process, use is also made of equations (A7) and (A10). We obtain (for $k-n\neq\frac{1}{2}$)

$$J_\tau(a,k,3)=\sum_{l=0}^{\infty}(-1)^l(l!)^{-1}J_\tau(0,k-l,3)a^l+\P^{3/2}A(k,3)\Gamma^{-1}(k)a^{k-3/2}-\P^{3/2}a^{k-3/2}$$
$$\times\sum_{l=0}^{\infty}(-1)^l[l!\Gamma(k-l)]^{-1}\sum_\gamma{}'(\P^2\gamma^2/a)^{k-l-3/2}\Gamma(3/2+l-k,\P^2\gamma^2/a), \tag{14}$$

where

$$A(k,3)=\sum_{l=0}^{\infty}(-1)^{l-1}\binom{k-1}{l}(k-l-3/2)^{-1}=-\P\Gamma(k)[\Gamma(3/2)\Gamma(k-1/2)]^{-1}/\cos(k\P) \tag{15}$$

and (for $k-n=\frac{1}{2}$)

$$J_\tau(a,k,3)=\sum_{l=0}^{\infty}(-1)^l(l!)^{-1}J_\tau(0,k-l,3)a^l+\P^{3/2}\Gamma^{-1}(k)A(k,3)a^{k-3/2}$$
$$+(-1)^{n-1}[(n-1)!]^{-1}2\P a^{n-1}\ln(1/a)-\P^{3/2}a^{k-3/2}\sum_{l=0}^{\infty}(-1)^l$$
$$\times[l!\Gamma(k-l)]^{-1}\sum_\gamma{}'(\P^2\gamma^2/a)^{k-l-3/2}\Gamma[3/2+l-k,\P^2\gamma^2/a], \tag{16}$$

where

$$A(k,3)=\sum_{l=0}^{\infty}{}'(-1)^{l-1}\binom{k-1}{l}(k-l-3/2)^{-1}$$
$$=(-1)^{n-1}2\Gamma(k)[\P^{1/2}\Gamma(n)]^{-1}[\psi(k-1/2)-\psi(3/2)]; \tag{17}$$

the primed summation here implies the exclusion of the term for which the denominator vanishes. In fact, this definition is comparatively more general and, for $(k-n)\neq\frac{1}{2}$, reduces to the one in (15).

2.1.3. General m. The above procedure can readily be extended to the case of general dimensionality as well. Of course, one has to study two cases separately: (i) when m is even, in which case calculations proceed parallel to the case of $m=2$, and (ii) when m is odd, in which case one proceeds parallel to the case of $m=3$. The result for any positive k, integral or not, can be written in the form

$$J_\tau(a,k,m)=\sum_{l=0}^{\infty}(-1)^l(l!)^{-1}J_\tau(0,k-l,m)a^l+¶^{m/2}\Gamma^{-1}(k)A(k,m)a^{k-m/2}$$
$$+(-1)^p¶^{m/2}[\Gamma(m/2)\Gamma(p+1)]^{-1}a^p\ln(1/a)\delta_{k-m/2,p}-¶^{m/2}a^{k-m/2}$$
$$\times\sum_{l=0}^{\infty}(-1)^l[l!\Gamma(k-l)]^{-1}\sum_{\gamma}{}'(¶^2\gamma^2/a)^{k-l-m/2}\Gamma(l-k+m/2,¶^2\gamma^2/a), \tag{18}$$

where p occurring as one of the arguments of the Kronecker delta is zero or a positive integer, and

$$A(k,m)\equiv\sum_{l=0}^{\infty}{}'(-1)^{l-1}\binom{k-1}{l}(k-l-m/2)^{-1}. \tag{19}$$

As before, the primed summation implies the exclusion of the term, if any, for which the denominator vanishes. If k is an integer, say n, the sum in (19) goes only up to $l=n-1$. Noting that (Gradshteyn and Ryzhik 1965)

$$B(x,y)=\sum_{n=0}^{\infty}(-1)^n(y-1)(y-2)\dots(y-n)/[n!(x-n)] \qquad y>0, \tag{20}$$

we have, in the case when $(k-m/2)$ is not equal to zero or a positive integer,

$$A(k,m)=B(k,m/2-k), \tag{21}$$

and, in the case when $(k-m/2)=p$ is zero or a positive integer, it can be shown, using equation (20), that

$$A(k,m)=(-1)^p\Gamma(k)[\Gamma(m/2)\Gamma(p+1)]^{-1}[\psi(p+1)-\psi(m/2)]. \tag{22}$$

All the definitions and results, such as in equations (8), (11), (13), (15) and (17), are special cases of equations (19), (21) and (22). When k is an integer (equal to n), the first sum in (18) is cut off at $l=n$, because $J_\tau(0,p,m)=0$ when p is a negative integer, and the last sum is truncated at $l=(n-1)$, because $\Gamma(p)=\infty$ when p is zero or a negative integer. For $k=1$, equation (18) reduces to

$$J_\tau(a,1,m)=\sum_{\tau}{}'\exp(-a\tau^2)/\tau^2=J_\tau(0,1,m)+a+¶^{m/2}A(1,m)a^{1-m/2}$$
$$-¶\ln a\,\delta_{m,2}-¶^{2-m/2}\sum_{\gamma}{}'\gamma^{2-m}\Gamma(-1+m/2,¶^2\gamma^2/a), \tag{23}$$

which is quite similar to equation I(5) and is, in fact, its generalisation when applied to an arbitrary lattice τ.

We may now comment on the structure of the result in (18). If $(k-m/2)$ is zero or a positive integer, there occurs a term of the type $a^{k-m/2}\ln(1/a)$. In addition, when k is an integer, there occurs a polynominal of degree n in a, a term in $a^{k-m/2}$ and a finite number of terms in the summation over l involving incomplete gamma functions. When k is not an integer, the first and the last summations over l extend to infinity. It is important to notice that the two terms after the first summation are independent of the structure of the lattice, while the coefficients $J_\tau(0, k-l, m)$ in the first summation are structure-dependent, except for the special case of $J_\tau(0, 0, m)$ which is identically equal to -1.

2.2. *When k is zero or a negative number, $k \leqslant 0$*

We start from equation (18) for $J_\tau(a, r, m)$ with $0 < r \leqslant 1$, differentiate both sides with respect to a n_1 times ($n_1 \geqslant 1$) and put $r - n_1 = k$ so that $k \leqslant 0$ and $n_1 = [-k]+1$. We obtain

$$J_\tau(a, k, m) = \sum_\tau{}' \exp(-a\tau^2)/\tau^{2k} = \sum_{l=0}^{\infty} (-1)^l (l!)^{-1} J_\tau(0, k-l, m) a^l$$

$$+ \pi^{m/2} A(k, m) \Gamma^{-1}(k) a^{k-m/2} - \pi^{m/2} a^{k-m/2} \sum_{i=0}^{n_1} (-1)^i \binom{n_1}{i} \Gamma(m/2-k)$$

$$\times \Gamma^{-1}(m/2 - k + i - n_1) \sum_{l=0}^{\infty} (-1)^l [l! \Gamma(k-l+n_1)]^{-1} \sum_\gamma{}' (\pi^2\gamma^2/a)^{k-l+n_1-m/2}$$

$$\times \Gamma(l-k-n_1+i+m/2, \pi^2\gamma^2/a). \qquad (24)$$

Here, for $k \leqslant 0$, $A(k, m)$ is defined by the relation

$$A(k, m)\Gamma^{-1}(k) \equiv \Gamma(m/2-k)\Gamma^{-1}(m/2). \qquad (25)$$

Also for $k < 0$, the prime on the sum Σ'_τ is unnecessary. For $k = 0$, equation (24) just gives back Poisson's summation formula. For $k = -n_2$, where n_2 is a positive integer or zero, equation (24) gives

$$J_\tau(a, -n_2, m) = \sum_\tau{}' \tau^{2n_2} \exp(-a\tau^2) = -\delta_{n_2,0} + \pi^{m/2}\Gamma(n_2 + m/2)\Gamma^{-1}(m/2) a^{-n_2-m/2}$$

$$+ \pi^{m/2} a^{-n_2-m/2} \sum_{i=0}^{n_2} (-1)^i \binom{n_2}{i} \Gamma(n_2+m/2)\Gamma^{-1}(i+m/2)$$

$$\times \sum_\gamma{}' (\pi^2\gamma^2/a)^i \exp(-\pi^2\gamma^2/a), \qquad (26)$$

which could be directly obtained by differentiating the PSF n_2 times.

2.3. *When k is any real number*

We can write equations (18) and (24) together, for any real k:

$$\sum_\tau{}' \exp(-a\tau^2)/\tau^{2k}$$

$$= \sum_{l=0}^{\infty} (-1)^l (l!)^{-1} J_\tau(0, k-l, m) a^l + \pi^{m/2} A(k, m) \Gamma^{-1}(k) a^{k-m/2}$$

$$+(-1)^p[\Gamma(m/2)\Gamma(p+1)]^{-1}\P^{m/2}a^p\ln(1/a)\delta_{k-m/2,p}-\P^{m/2}a^{k-m/2}\sum_{i=0}^{n_1}(-1)^i$$

$$\times\binom{n_1}{i}\Gamma(m/2-k)\Gamma^{-1}(m/2-k+i-n_1)\sum_{l=0}^{\infty}(-1)^l[l!\Gamma(k-l+n_1)]^{-1}$$

$$\times\sum_{\gamma}{}'(\P^2\gamma^2/a)^{k-l+n_1-m/2}\Gamma(l-k-n_1+i+m/2,\P^2\gamma^2/a), \tag{27}$$

where n_1 is now defined to be

$$n_1=\begin{cases}[-k]+1 & \text{when } k\leqslant 0\\ 0 & \text{when } k>0.\end{cases} \tag{28}$$

Equation (27) is formally the same as equation (18), except for the additional terms involving incomplete gamma functions in the last part of the right-hand side, which occur in the case when $k\leqslant 0$.

2.4. *Asymptotic results for $J_\tau(a, k, m)$ and discussion*

From equation (27) it follows that, for $a \ll \P$, the sum $J_\tau(a, k, m)$ has the following asymptotic forms:

$$J_\tau(a,k,m)=\begin{cases}\P^{m/2}\Gamma^{-1}(k)A(k,m)a^{k-m/2} & (k<m/2) \quad (29a)\\ \P^{m/2}\Gamma^{-1}(k)\ln(1/a) & (k=m/2) \quad (29b)\\ \sum_\tau{}'\,\tau^{-2k} & (k>m/2). \quad (29c)\end{cases}$$

Thus, insofar as the asymptotic behaviour of $J_\tau(a, k, m)$, in the limit $a\to 0$, is concerned, the discreteness of the sum is unimportant for $k\leqslant m/2$ and is quite important for $k>m/2$. The case $k=m/2$ defines the boundary separating the two regions and, in this case, our sum displays a logarithmic divergence. These results are in complete agreement with those of Hall, except that there exists a slight error in his result for $k<m/2$. Looking at the summation for $A(k, m)$ in equation (19) and equation (29a), we observe that Hall's result amounts to keeping only the $(l=0)$ term of this sum.

In passing, we would like to mention that the asymptotic results in (29) could also be obtained directly by replacing the summation over τ by an integration when $k\leqslant m/2$. For $k>m/2$, the sum is convergent for all values of a, so the desired asymptotic result is obtained simply by putting $a=0$ in the summand.

Although our aim was to determine the dependence of $J_\tau(a, k, m)$ on a, as has been found in equation (27), we may indicate how one can determine, numerically, the constants $J_\tau(0, k, m)$ which appear in that equation. For $k>m/2$, as we said before, $J_\tau(0, k, m)=\Sigma_\tau'\,\tau^{-2k}$ and can be determined for a given value of k and for a given lattice, using a machine. For $k\leqslant m/2$, one can determine $J_\tau(0, k, m)$, in principle, by using its definition in equation (5) along with the expressions in equations (29a) and (29b), and using smaller and smaller values of a until the result is independent of it. Perhaps one could develop relatively faster methods of calculating $J_\tau(0, k, m)$, especially when k is a positive integer (see, for example, Chaba and Pathria (1975a) for the determination of C_3), but we shall not pursue it here.

3. Evaluation of sums $S_\gamma(q, l, j, m)$

3.1. *Exact results for $S_\gamma(q, l, j, m)$*

Following Hall (1976b), we can write $S_\gamma(q, l, j, m)$ as

$$S_\gamma(q, l, j, m) = \Gamma^{-1}(j) \int_0^\infty \mathrm{d}t\, t^{j-1} \exp(-q^2 t) \sum_\gamma{}' \exp(-\gamma^2 t)/\gamma^{2l} \qquad j>0. \tag{30}$$

For the summation over γ that occurs in equation (30), we use the result in equation (27) and obtain, for $(2l+2j)>m$,

$$\begin{aligned} S_\gamma(q, l, j, m) = {} & \sum_{l_1=0}^{\infty} (-1)^{l_1}\Gamma(j+l_1)[l_1!\Gamma(j)]^{-1} J_\gamma(0, l-l_1, m) q^{-2j-2l_1} \\ & + \P^{m/2}\Gamma(j+l-m/2)[\Gamma(l)\Gamma(j)]^{-1} A(l, m) q^{-2j-2l+m} - (-1)^p \P^{m/2}\Gamma(p+j) \\ & \times [\Gamma(m/2)\Gamma(p+1)\Gamma(j)]^{-1}[\psi(p+j) - 2\ln q] q^{-2p-2j}\, \delta_{l-m/2,p} \\ & - \P^{m/2}\Gamma^{-1}(j) \sum_{i=0}^{n_3} (-1)^i \binom{n_3}{i} \Gamma(m/2-l)\Gamma^{-1}(m/2-l+i-n_3) \\ & \times \sum_{l_1=0}^{\infty} (-1)^{l_1}[l_1!\Gamma(l-l_1+n_3)]^{-1} \sum_\tau{}' (\P^2\tau^2)^{l-l_1+n_3-m/2} I, \end{aligned} \tag{31}$$

where

$$n_3 = \begin{cases} [-l]+1 & \text{when } l \leqslant 0 \\ 0 & \text{when } l > 0 \end{cases} \tag{32}$$

and

$$I = \int_0^\infty \mathrm{d}t\, t^{j+l_1-n_3-1} \exp(-q^2 t) \Gamma(l_1 - l - n_3 + i + m/2, \P^2\tau^2/t). \tag{33}$$

When j is a positive integer, this integral can be performed and gives

$$\begin{aligned} & (\P^2\tau^2)^{l-l_1+n_3-m/2} I \\ & \quad = 2(\P^2\tau^2)^i \sum_{i_1=1}^{j+l_1-n_3} \Gamma(j+l_1-n_3)\Gamma^{-1}(j+l_1-n_3-i_1+1) \\ & \quad \times q^{-2i_1}(\P\tau/q)^{j+l-i-i_1-m/2} K_{j+l-i-i_1-m/2}(2\P q\tau). \end{aligned} \tag{34}$$

For $l=1$, $j=1$ and $m=2$, equation (31) with (34) leads to

$$\sum_\gamma{}' \gamma^{-2}(\gamma^2+q^2)^{-1} = (2\P/q^2)\ln q + [\P C + J_\gamma(0, 1, 2)]/q^2 + (1/q^4) - (2\P/q^2) \sum_\tau{}' K_0(2\P q\tau), \tag{35}$$

which is the generalisation of equation I(14) when applied to an arbitrary lattice.

3.2. *Asymptotic results for $S_\gamma(q, l, j, m)$ and discussion*

From equation (31), it follows that, for $q \gg 1$, the sum $S_\gamma(q, l, j, m)$ has the following asymptotic forms:

$$S_\gamma(q, l, j, m) = \begin{cases} \pi^{m/2}\Gamma(l+j-m/2)[\Gamma(l)\Gamma(j)]^{-1}A(l, m)q^{-2l-2j+m} & l < m/2, \quad (36a) \\ 2\pi^{m/2}\Gamma^{-1}(m/2)q^{-2j}\ln q & l = m/2, \quad (36b) \\ (1/q^{2j})\sum_{\gamma}{}' \gamma^{-2l} & l > m/2. \quad (36c) \end{cases}$$

Again, we notice that, so far as the asymptotic behaviour of $S_\gamma(q, l, j, m)$ in the limit $q \to \infty$ is concerned, the discreteness of the sum is unimportant for $l \leqslant m/2$ and is quite important for $l > m/2$. These results also agree with those of Hall (1976b), except that there exists a slight error in his result for $l < m/2$. Looking at equation (19) and equation (36*a*), we observe that Hall's result amounts to keeping only the ($l = 0$) term of the sum in equation (19) for $A(k, m)$.

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Appendix

Writing the Poisson summation formula in two dimensions as

$$\sum_{\gamma}{}' \exp(-a\tau^2) = \pi/a - 1 + (\pi/a)\sum_{\gamma}{}' \exp(-\pi^2\gamma^2/a), \tag{A1}$$

and integrating with respect to a, we obtain

$$\sum_{\tau}{}' \exp(-a\tau^2)/\tau^2 = -\pi\ln a + J_\tau(0, 1, 2) + a - \pi\sum_{\gamma}{}' \Gamma(0, \pi^2\gamma^2/a). \tag{A2}$$

However, multiplying (A1) by a^{s-1} and then integrating with respect to a, we obtain (for $s \neq 0, 1$)

$$\sum_{\tau}{}' \Gamma(s, a\tau^2)/\tau^{2s} = a^s/s - \pi a^{s-1}/(s-1)D_\tau(s) - \pi^{2s-1}\sum_{\gamma}{}' \gamma^{2s-2}\Gamma(1-s, \pi^2\gamma^2/a). \tag{A3}$$

Note that equation (A2) is the counterpart of (A3) for $s = 0$ or 1; hence (A2) and (A3) are complementary to each other.

Interchanging a and (π^2/a), τ and γ, s and $(1-s)$, we obtain from (A3) the elegant relation

$$D_\tau(s)/\pi^s = D_\gamma(1-s)/\pi^{1-s}. \tag{A4}$$

Also letting $a \to 0$ in (A3), we find that

$$D_\tau(s) = \Gamma(s)J_\tau(0, s, 2). \tag{A5}$$

Combining (A4) and (A5), we may write

$$\Gamma(s)J_\tau(0, s, 2)/\pi^s = \Gamma(1-s)J_\gamma(0, 1-s, 2)/\pi^{1-s} \tag{A6}$$

(cf equation (2.16) of Zucker (1976) which is a special case of (A6), as applied to a square lattice). Further, we notice that, since $D_\tau(s)$ is a finite constant, $J_\tau(0, s, 2) = 0$ whenever s is a negative integer.

Similarly, starting from the PSF in three dimensions, we obtain the following relationship (for $s \neq 0, \frac{3}{2}$):

$$\sum_\tau{}' \Gamma(s, a\tau^2)/\tau^{2s}$$

$$= a^s/s + \P^{3/2}a^{s-3/2}/(3/2-s) + E_\tau(s) - \P^{2s-3/2} \sum_\gamma{}' \gamma^{2s-3}\Gamma(3/2-s, \P^2\gamma^2/a), \tag{A7}$$

where

$$E_\tau(s)/\P^s = E_\gamma(3/2-s)/\P^{3/2-s} \tag{A8}$$

and

$$\Gamma(s)J_\tau(0, s, 3)/\P^s = \Gamma(3/2-s)J_\gamma(0, 3/2-s, 3)/\P^{3/2-s} \tag{A9}$$

and (for $s = 0$ or $\frac{3}{2}$)

$$\sum_\tau{}' \Gamma(3/2, a\tau^2)/\tau^3 = 2a^{3/2}/3 - \P^{3/2} \ln a + E_\tau(3/2) - \P^{3/2} \sum_\gamma{}' \Gamma(0, \P^2\gamma^2/a). \tag{A10}$$

We may remark that (A3) and (A7) are generalisations of equations (46) and (64) of Chaba and Pathria (1976), when applied to arbitrary lattices.

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