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Weak "Phase Transitions" in Asymptotic Properties of Lattice Sums

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Two classes of n-dimensional lattice sums are shown to exhibit a weak form of a "phase transition" in their asymptotic properties. Both classes depend on two parameters such that the leading term in an asymptotic limit of one parameter is independent of the structure of the lattice in one domain of the second parameter and dependent on the structure in an adjacent domain, with a "boundary point," or "transition temperature," between the two domains.

KEY WORDS: Phase transitions; lattice sums; theta functions; Ewald's summation methods; theta function method.

1. INTRODUCTION

Perhaps some insight into the mathematics of phase transitions in realistic models may be found by studying tractable mathematical systems that possess properties weakly analogous to those of a phase transition. With this purpose, we have studied several classes of n-dimensional lattice sums that exhibit a weak form of a "phase transition" in their asymptotic properties. In this paper we report on two quite different classes and show a relationship between the two classes. For our purposes, a lattice sum depending on two positive parameters is said to possess a *weak phase transition* if the leading term in an asymptotic limit of one parameter is independent of the structure

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of the lattice in one domain of the other parameter and dependent on the structure in an adjacent domain, with a "boundary point" between the two domains.

Let $\{\tau\}$ and $\{\gamma\}$ be two mutually reciprocal, unit, Bravais lattices in an n-dimensional Euclidean space. Earlier we reported[1,2] some of the asymptotic properties of the sums

$$S(q) = \sum_{\gamma}{}' \gamma^{-2l}(\gamma^2 + q^2)^{-j}, \qquad 0 < l, j, \quad 2l + 2j > n \tag{1}$$

for large q values, and more recently we investigated the asymptotic properties of the sums[3]

$$J(a) = \sum_{\gamma}{}' \tau^{-2k} \exp(-a\tau^2), \qquad 0 < a, k \tag{2}$$

for a small a values. When k is a positive integer, the $J(a)$ are Chaba–Pathria[4] sums. With the theta function method (TFM) of Ewald,[5] Born and co-workers,[6] and others,[7] the $S(q)$ may be evaluated for all $0 \leqslant q < \infty$ and $J(a)$ for $0 < a < \infty$ if $0 < 2k \leqslant n$ and for $0 \leqslant a$ if $2k > n$. For positive, integral k values the methods of Chaba and Pathria[4] may be used to study $J(a)$.

In this paper we show that the asymptotic properties of the $S(q)$ follow easily from those of the $J(a)$. Then we shall discuss the weak phase transitions possessed by $S(q)$ and $J(a)$.

Using the TFM, one easily finds[3] for $J(a)$ that

$$J(a \ll 1) = \begin{cases} \pi^{n/2}[\Gamma(k)(n/2 - k)a^{(n/2)-k}]^{-1}, & 0 < 2k < n \\ \pi^{n/2}\Gamma(k)^{-1} \ln(1/a), & 2k = n \\ \sum_{\tau}' \tau^{-2k}, & 2k > n \end{cases} \tag{3}$$

Using these properties $J(a \ll 1)$, we shall show here that

$$S(q \gg 1) = \begin{cases} \dfrac{\pi^{n/2}\Gamma(j + l - n/2)}{(n/2 - l)\Gamma(l)\Gamma(j)q^{2l+2j-n}}, & 0 < 2l < n \\ \dfrac{2\pi^{n/2} \ln q}{\Gamma(k)q^{2j}}, & 2l = n \\ \sum_{\gamma}' \gamma^{-2l}q^{-2j}, & 2l > n \end{cases} \tag{4}$$

Thus the asymptotic properties of $S(q)$ for large q follow from the asymptotic properties of $J(a)$ for small a. In our earlier reports[1,2] on the asymptotic properties of $S(q)$, we used the TFM directly without first applying it to investigate $J(a)$; the present procedure is somewhat shorter than the earlier one, and it is simpler at the boundary point of Eq. (4) given by $2l = n$.

2. RELATION BETWEEN ASYMPTOTIC PROPERTIES

By the TFM we write

$$S(q) = \frac{1}{\Gamma(j)} \sum_{\gamma}' \int_0^\infty t^{j-1} \exp(-q^2 t) \frac{\exp(-\gamma^2 t)}{\gamma^{2k}} \, dt \qquad (5)$$

Then, knowing the results of Eq. (3), we are able to apply the Lebesgue dominated convergence theorem[8] and write

$$S(q) = \frac{1}{\Gamma(j)} \int_0^\infty t^{j-1} \exp(-q^2 t) \sum_{\gamma}' \frac{\exp(-\gamma^2 t)}{\gamma^{2k}} \, dt \qquad (6)$$

To secure the leading term in $S(q \gg 1)$ we use Eq. (3) with $a = t$ and (with a change of lattice identification) substitute into Eq. (6), except for the case $2k = n$, where we integrate only from zero to $t = 1$. The results are given in Eq. (4). This procedure is justified by examining the functional form of the entire integrand of Eq. (6).

3. DISCUSSION

A "temperature" T may be defined for $S(q \gg 1)$ by setting $T = (2l)^{-1}$ with a critical temperature $T_c = 1/n$, and for $J(a \ll 1)$ a temperature T may be defined by $T = (2k)^{-1}$ with $T_c = 1/n$. Then $S(q \gg 1)$ and $J(a \ll 1)$ are independent of the lattice structure for $T \geqslant T_c$ and are dependent on the lattice structure for $T < T_c$. To see if further analogy can be developed with phase transitions, let us examine $S(q \gg 1)$ in more detail.

Excluding the point $T = T_c$, write

$$S(q \gg 1) \simeq C(T)/q^{P(T)} \qquad (7)$$

The $P(T)$, when sketched as a function of T, acts a little like an order parameter and $C(T)$ acts a little like a specific heat. Although the analogy with a true phase transition is weak, it is rather surprising that this much exists when one considers the simple form of the summand in the defining Eq. (1) for $S(q)$. This encourages search for other lattice sums for which the analogy may be more complete and more instructive without the sums being intractable.

For $T > T_c$ two points should be made: (1) the $J(a \ll 1)$ diverge as $a \to 0$, whereas the $S(q \gg 1)$ converge (albeit to zero) as $q \to \infty$. (2) The leading term for both classes arises in a manner similar to the "collapse of the lattice" of Greenspoon and Pathria.[9]

At $T = T_c$, the properties of $S(q)$ are, we feel, somewhat more unexpected than those of $J(a)$. Viewing Eq. (2) with $2k = n$, one sees immediately that $J(a)$ diverges as $a \to 0$, and one expects quite different behavior of

$J(a)$ for $2k < n$ and $2k > n$. In contrast, since $S(q)$ converges for $2l = n$ provided $j > 0$, one might not expect the properties of $S(q)$ to vary so markedly for $2l < n$ and $2l > n$.

A subset of the class $J(a)$ has been of considerable interest recently in several areas of physics, as discussed by Chaba and Pathria.[4] For $n = 3$ and $j = 2$, the $S(q)$ sums arose in calculations by Plaskett and Hall[2] for $l = 1$ (energy) and $l = 2$ (effective mass). Additionally, Plaskett[10] has found relationships between the sums ($n = 3$)

$$\sum_{\tau}{}' \tau^{-1} \exp(-q\tau) \tag{8}$$

and

$$\sum_{\gamma}{}' \gamma^{-2}(\gamma^2 + q^2)^{-1} \tag{9}$$

which are useful for evaluating the former when $0 < q \ll 1$. Accordingly, the sums $S(q)$ for $0 \leqslant q < \infty$ are not without interest in physics.

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