

A NOTE ON ALTERNATING SERIES IN SEVERAL DIMENSIONS

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1. Introduction. In the course of a study of chemical lattice sums [1] the authors considered sums such as

$$(1.1) \quad \sum' (-1)^{n+m+k} (n^2 + m^2 + k^2)^{-1/2},$$

the summation being over all non-zero integer triples. Such “sums” occur naturally in the study of crystal potentials. For example, (1.1) is meant to measure the potential at the origin of an infinite cubic crystal with unit Coulomb charges at each integer lattice point. As such the sum is considered to represent an electrochemical constant (Madelung’s constant) for sodium chloride. An excellent account of such lattice sums can be found in Glasser and Zucker’s recent survey [3].

The series in (1.1) is not absolutely convergent and hence its sum is not order independent. Various possible orders suggest themselves. The chemical literature is somewhat vague on this point. As discussed in [1], it is really only appropriate to consider rectangular sums.

We shall consider alternating series of the form

$$(1.2) \quad \sum (-1)^{\bar{m}} f(\bar{m}),$$

where $\bar{m} = (m_1, m_2, \dots, m_N)$ ranges over \mathbb{N}^N , the N -fold product of non-negative integers, $(-1)^{\bar{m}} := (-1)^{m_1 + m_2 + \dots + m_N}$ and $f: \mathbb{N}^N \rightarrow \mathbb{R}$. For $s: \mathbb{N}^N \rightarrow \mathbb{R}$, $s(\bar{n})$ is said to converge to a limit l as \bar{n} increases in \mathbb{N}^N if, given $\varepsilon > 0$, there is an \bar{m} in \mathbb{N}^N such that

$$|s(\bar{n}) - l| < \varepsilon \text{ whenever } \bar{n} \geq \bar{m},$$

the notation $\bar{n} \geq \bar{m}$ or $\bar{m} \leq \bar{n}$ meaning that $n_i \leq m_i$ for $i = 1, 2, \dots, N$. This is equivalent to convergence in the sense of Pringsheim, which requires that $s(\bar{n}) \rightarrow l$ as $\min_{1 \leq i \leq N} n_i \rightarrow \infty$. For discussion of various concepts of convergence, see [2], [4], [5], [6], [7] and the references therein. We shall show that the sum of (1.2) exists under appropriate conditions if it is defined as the limit

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as \bar{n} increases in \mathbb{N}^N of

$$(1.3) \quad \sum_{\bar{0} \leq \bar{m} \leq \bar{n}} (-1)^{\bar{m}} f(\bar{m}).$$

Our main result, Theorem 3.1, is a complete generalization to multiple series of the classical result due to Leibniz, according to which if $\{a_n\}$ is a monotonic sequence of non-negative real numbers converging to zero, then the series $\sum_{n=0}^{\infty} (-1)^n a_n$ converges to s and its sequence of partial sums $\{s_n\}$ satisfies

$$0 \leq s_{2m+1} \leq s_{2m+3} \leq s \leq s_{2n+2} \leq s_{2n} \text{ for all } m, n \text{ in } \mathbb{N}.$$

Theorem 3.1 exhibits order relations between partial sums of the form (1.3) which hold when the function f is fully monotone (as defined in § 2 below); and Lemma 3.1, which plays a key role in the proof of Theorem 3.1, gives precise bounds on the size of these partial sums and also on the difference between them and their limit when it exists (see (3.6) below). To our knowledge neither such order nor such bound results have been considered previously in more than one dimension. There are, however, results available guaranteeing the convergence of non-absolutely convergent multiple dimensional series. Hardy [4] derives a “bounded convergence” test based on Abel partial summation which can be used to establish convergence criteria for series like (1.2) (see also Móricz [6]). Bromwich [2, p. 97] discusses the 2-dimensional version of Hardy’s result. Meyer [5] gives necessary and sufficient conditions for the “diagonal summability” of 2-dimensional monotonic alternating series.

When f is the restriction of an N -times continuously differentiable function, a most satisfactory test involving partial derivatives is given by our Theorem 4.1 for the convergence of the alternating series (1.2). This theorem follows immediately from our Lemma 2.1 which has independent interest as a mean value estimate for general alternating sums.

We prove all our results for N -dimensions. The interested reader will be able to provide much simpler arguments for the 2-dimensional case as indicated pictorially in § 3 below. The 3-dimensional case, which is of primary interest, is not substantially simpler than the general one. Our vector notation enables us to express N -dimensional results concisely. An explicit treatment of the series (1.1) and its 2-dimensional analogue is given in [1].

2. Preliminaries. Let $\mathbb{N}^N, \mathbb{Z}^N, \mathbb{P}^N, \mathbb{R}^N$ denote respectively the N -fold product of the non-negative integers, the integers, the non-negative real numbers, and the real numbers. We denote by $\bar{1}$ the vector in \mathbb{R}^N with every component 1, and by \bar{e}_j the vector with j th component 1 and every other component 0. For

$$\bar{a} = (a_1, a_2, \dots, a_N), \bar{b} = (b_1, b_2, \dots, b_N) \text{ in } \mathbb{R}^N,$$

we define

$$|\bar{a}| := \max_{1 \leq i \leq n} |a_i|, \quad \bar{a} \cdot \bar{b} := a_1 b_1 + a_2 b_2 + \dots + a_n b_n, \quad \bar{a}\bar{b} := (a_1 b_1, a_2 b_2, \dots, a_N b_N);$$

and for $\bar{s} = (s_1, s_2, \dots, s_N)$ in \mathbb{Z}^N , we define

$$(-1)^{\bar{s}} := (-1)^{\bar{1} \cdot \bar{s}} = (-1)^{s_1 + s_2 + \dots + s_N}.$$

A function $f: \mathbb{N}^N \rightarrow \mathbb{R}$ is said to be $(N -)$ monotone (decreasing) if

$$(2.1) \quad \sum_{\substack{|\bar{s}| \leq 1 \\ \bar{s} \in \mathbb{N}^N}} (-1)^{\bar{s}} f(\bar{m} + \bar{s}) \geq 0$$

for all \bar{m} in \mathbb{N}^N . We shall say that f is *fully monotone* if f and all its coordinate restrictions are monotone. Then 1-monotonicity means that $f(m) \geq f(m + 1)$ for m in \mathbb{N} ; 2-monotonicity requires that

$$f(m, n) + f(m + 1, n + 1) \geq f(m, n + 1) + f(m + 1, n) \text{ for } m, n \text{ in } \mathbb{N};$$

and in general N -monotonicity of f requires the alternating sum (1.2) over any unit N -cube to have the same sign as $(-1)^m$ at the corner nearest the origin. Note that any linear functional Φ on \mathbb{R}^N is N -monotone for $N > 1$, but Φ is fully monotone only if $\Phi \leq 0$ on \mathbb{P}^N .

We prove a lemma useful for obtaining criteria for monotonicity in which subscripts denote partial derivatives taken in order of the subscripts and

$$\mathbb{P}_*^N := \{ \bar{x} \in \mathbb{P}^N | x_i > 0 \text{ for } i = 1, 2, \dots, N \}.$$

LEMMA 2.1. (a) Let the function $f: \mathbb{P}_*^N \rightarrow \mathbb{R}$ have partial derivatives $f_{12\dots N}$ throughout \mathbb{P}_*^N . Then, for $\bar{x} \in \mathbb{P}_*^N, \bar{a} \in \mathbb{P}^N$,

$$(2.2) \quad \sum_{\substack{|\bar{s}| \leq 1 \\ \bar{s} \in \mathbb{N}^N}} (-1)^{\bar{s}} f(\bar{x} + \bar{a}\bar{s}) = (-1)^N a_1 a_2 \cdots a_N f_{12\dots N}(\bar{c})$$

for some \bar{c} between \bar{x} and $\bar{x} + \bar{a}$.

(b) Let the function $\psi: \mathbb{P}_* \rightarrow \mathbb{R}$ be N -times differentiable. Then, for $x > 0, \bar{a} \in \mathbb{P}^N$,

$$(2.3) \quad \sum_{\substack{|\bar{s}| \leq 1 \\ \bar{s} \in \mathbb{N}^N}} (-1)^{\bar{s}} \psi(x + \bar{a} \cdot \bar{s}) = (-1)^N a_1 a_2 \cdots a_N \psi^{(N)}(c)$$

for some c between x and $x + a_1 + a_2 + \cdots + a_N$.

Proof. (a) The result is true for $N = 1$. Suppose inductively that it is true with $N - 1$ in place of N . The left-hand side of (2.2) is evidently equal to

$$\sum_{\substack{|\bar{s}| \leq 1 \\ \bar{s} \in \mathbb{N}^{N-1}}} (-1)^{\bar{s}} g(x_1 + a_1 s_1, x_2 + a_2 s_2, \dots, x_{N-1} + a_{N-1} s_{N-1}),$$

where $g: \mathbb{P}_*^{N-1} \rightarrow \mathbb{R}$ is defined by

$$g(\bar{t}) := f(\bar{t}, x_N) - f(\bar{t}, x_N + a_N).$$

Hence, by the inductive hypothesis and the mean value theorem, the left-hand side of (2.2) equals

$$\begin{aligned} & (-1)^{N-1} a_1 a_2 \cdots a_{N-1} g_{12\dots N-1}(c_1, c_2, \dots, c_{N-1}) \\ & = (-1)^N a_1 a_2 \cdots a_N f_{12\dots N}(c_1, c_2, \dots, c_N), \end{aligned}$$

where $x_i \leq c_i \leq x_i + a_i$ for $i = 1, 2, \dots, N$.

(b) Define $f: \mathbb{P}_*^N \rightarrow \mathbb{R}$ by $f(\bar{t}) := \psi(t_1 + t_2 + \cdots + t_N)$. Then, with $\bar{x} := (x, x, \dots, x)/N$, we have

$$f(\bar{x} + \bar{a}\bar{s}) = \psi(x + \bar{a} \cdot \bar{s});$$

and (2.3) follows from (2.2). \square

The following lemma yields a stock of fully monotone functions.

LEMMA 2.2. Let the function $\psi: \mathbb{P} \rightarrow \mathbb{R}$ be continuous and satisfy

$$(2.4) \quad (-1)^n \psi^{(n)}(x) \geq 0 \text{ for all } x > 0 \text{ and } n = 1, 2, \dots, N.$$

Then

(a) for $x \geq 0, \bar{a} \in \mathbb{P}^N$,

$$(2.5) \quad \sum_{\substack{|\bar{s}| \leq 1 \\ \bar{s} \in \mathbb{N}^N}} (-1)^{\bar{s}} \psi(x + \bar{a} \cdot \bar{s}) \geq 0;$$

(b) given non-decreasing functions $g_i: \mathbb{N} \rightarrow \mathbb{N}, i = 1, 2, \dots, N$, the function $f: \mathbb{N}^N \rightarrow \mathbb{R}$ defined by

$$(2.6) \quad f(\bar{m}) := \psi \left(\sum_{i=1}^N g_i(m_i) \right)$$

is fully monotone on \mathbb{N}^N .

Proof. (a) It follows from (2.3) that (2.5) holds for $x > 0$. By continuity it also holds for $x = 0$.

(b) We have

$$\sum_{|\bar{s}| \leq 1} (-1)^{\bar{s}} f(\bar{m} + \bar{s}) = \sum_{|\bar{s}| \leq 1} (-1)^{\bar{s}} \psi \left(\sum_{i=1}^N g_i(m_i) + \sum_{i=1}^N s_i (g_i(m_i + 1) - g_i(m_i)) \right) \geq 0$$

by part (a), since $g_i(m_i + 1) - g_i(m_i) \geq 0$ and $\sum_{i=1}^N g_i(m_i) \geq 0$. Thus f is N -monotone. Since the argument applies with some of the g_i constant, it follows that f is in fact fully monotone. \square

EXAMPLE 2.1. (a) Let

$$\|\bar{m}\|_p := \left(\sum_{i=1}^N |m_i|^p \right)^{1/p} \quad (p > 0).$$

Then

$$f(\bar{m}) := \|\bar{1} + \bar{m}\|_p^{-q} \quad (q > 0)$$

is fully monotone, by Lemma 2.2(b) with

$$\psi(x) := (N + x)^{-q/p}$$

and each $g_i(x) := (1 + x)^p - 1$. Note that with $\|\bar{m}\|_\infty := |\bar{m}|$ the function f is still fully monotone for $p = \infty$.

(b) Similarly the functions

$$f(\bar{m}) := -\log \left(\sum_{i=1}^N e^{a_i m_i} \right) \quad (a_i > 0)$$

and

$$f(\bar{m}) := \prod_{i=1}^N (1 + m_i)^{-1/N} = \exp \left(-\frac{1}{N} \sum_{i=1}^N \log(1 + m_i) \right)$$

are fully monotone. \square

3. Alternating sums over rectangles. Before proceeding to the main results it is convenient to prove the following lemma.

LEMMA 3.1. *Let $f: \mathbb{N}^N \rightarrow \mathbb{P}$ be fully monotone. Then*

$$(3.1) \quad 0 \leq (-1)^{\bar{a}} \sum_{\bar{a} \leq \bar{m} \leq \bar{n}} (-1)^{\bar{m}} f(\bar{m}) \leq f(\bar{a})$$

whenever $\bar{a}, \bar{n} \in \mathbb{N}^N$ and $\bar{a} \leq \bar{n}$.

Proof. It suffices to prove (3.1) for the case $\bar{a} = \bar{0}$, since the general case follows from this case with $f(\bar{m})$ replaced by $f(\bar{m} + \bar{a})$. We establish the first inequality in (3.1) by induction. Clearly it holds for $N = 1$. Suppose it holds with $N - 1$ in place of N . Observe that, for $\bar{n} = (n_1, n_2, \dots, n_N) \in \mathbb{N}^N$,

$$\sum_{\bar{0} \leq \bar{m} \leq \bar{n}} (-1)^{\bar{m}} f(\bar{m}) = S_1 + S_2$$

with

$$S_1 := \sum_{\bar{0} \leq 2\bar{k} \leq \bar{n}} (-1)^{2\bar{k}} \sum_{\bar{0} \leq \bar{s} \leq \bar{1}} (-1)^{\bar{s}} f(2\bar{k} + \bar{s}),$$

$$S_2 := \sum_{i \in E} \sum_{\substack{m_i = n_i \\ \bar{0} \leq \bar{m} \leq \bar{a}_i}} (-1)^{\bar{m}} f(\bar{m}),$$

where $E := \{i | n_i \text{ even}\}$, and $\bar{a}_i := (\alpha_1, \alpha_2, \dots, \alpha_N)$ with

$$\alpha_j := \begin{cases} n_j - 1 & \text{if } j < i, j \in E \text{ and } n_j \neq 0, \\ n_j & \text{otherwise.} \end{cases}$$

Now $S_1 \geq 0$ because of the N -monotonicity of f and $S_2 \geq 0$ by the inductive hypothesis. The validity of the first inequality in (3.1) for every $N \geq 1$ follows.

To establish the second inequality in (3.1), we observe that

$$\sum_{\bar{0} \leq \bar{m} \leq \bar{n}} (-1)^{\bar{m}} f(\bar{m}) - f(\bar{0}) = - \sum_{\substack{\bar{0} \leq \bar{s} \leq 1 \\ \bar{s} \neq \bar{0}}} (-1)^{\bar{s}} \sum_{\bar{s} \leq \bar{m} \leq \bar{n}} (-1)^{\bar{m}} f(\bar{m}) \leq 0$$

by the first inequality in (3.1). □

In what follows we use the notation:

$$(3.2) \quad t_{\bar{n}} := t_{\bar{n}}(f) := \sum_{\bar{0} \leq \bar{m} \leq \bar{n}} (-1)^{\bar{m}} f(\bar{m}),$$

where $\bar{m}, \bar{n} \in \mathbb{N}^N$.

THEOREM 3.1 (Alternating series test). *If $f: \mathbb{N}^N \rightarrow \mathbb{P}$ is fully monotone, $\bar{n}, \bar{r} \in \mathbb{N}^N$ and $\bar{n} \leq \bar{r}$, then*

- (i) $t_{2\bar{n}} \geq t_{2\bar{r}} \geq 0$,
- (ii) $t_{2\bar{r} + \bar{1}} \geq t_{2\bar{n} + \bar{1}} \geq 0$,
- (iii) $t_{2\bar{n}} \geq t_{2\bar{n} + \bar{1}}$.

If in addition $\lim_{n \rightarrow \infty} f(n\bar{e}_i) = 0$ for $i = 1, 2, \dots, N$, then $t_{\bar{n}}$ converges to a limit t as \bar{n} increases, $t_{2\bar{n}} \geq t \geq t_{2\bar{n} + \bar{1}}$ for each $\bar{n} \in \mathbb{N}^N$, and consequently

$$(3.3) \quad t = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \dots \sum_{m_N=0}^{\infty} (-1)^{\bar{m}} f(\bar{m}).$$

Proof. To establish (i) and (ii) it suffices to consider $\bar{r} := \bar{n} + \bar{e}_j, 1 \leq j \leq N$. We then have

$$t_{2\bar{r}} - t_{2\bar{n}} = \sum_{\bar{a} \leq \bar{m} \leq 2\bar{r}} (-1)^{\bar{m}} f(\bar{m}) \quad \text{with } \bar{a} := (2n_j + 1)\bar{e}_j,$$

and

$$t_{2\bar{r} + \bar{1}} - t_{2\bar{n} + \bar{1}} = \sum_{\bar{b} \leq \bar{m} \leq 2\bar{r} + \bar{1}} (-1)^{\bar{m}} f(\bar{m}) \quad \text{with } \bar{b} := (2n_j + 2)\bar{e}_j.$$

Since $(-1)^{\bar{a}} = -1$ and $(-1)^{\bar{b}} = 1$, (i) and (ii) follow by Lemma 3.1. Next, by an “inclusion-exclusion” counting argument, we have

$$t_{2\bar{n} + \bar{1}} - t_{2\bar{n}} = - \sum_{i=1}^{2^N - 1} (-1)^{\bar{a}_i} \sum_{\bar{a}_i \leq \bar{m} \leq 2\bar{n} + \bar{1}} (-1)^{\bar{m}} f(\bar{m}),$$

each \bar{a}_j being of the form $(\alpha_1, \alpha_2, \dots, \alpha_N) \neq \bar{0}$ with every α_j either 0 or $2n_j + 1$. Lemma 3.1 now yields (iii).

It follows from (i) that $t_{2\bar{n}}$ converges (to $\inf_{\bar{n} \in \mathbb{N}^N} t_{2\bar{n}}$) as \bar{n} increases in \mathbb{N}^N . Hence to establish the convergence of $t_{\bar{n}}$ as \bar{n} increases in \mathbb{N}^N , it suffices to show that, for fixed \bar{k} in \mathbb{N}^N , $t_{\bar{n}+\bar{k}} - t_{\bar{n}} \rightarrow 0$ as \bar{n} increases, and for this it is enough to consider $\bar{k} := \bar{e}_j$. We then have

$$t_{\bar{n}+\bar{k}} - t_{\bar{n}} = \sum_{\bar{c} \leq \bar{m} \leq \bar{n}+\bar{k}} (-1)^{\bar{m}} f(\bar{m}) \quad \text{with } \bar{c} := (n_j + 1)\bar{e}_j,$$

and hence, by Lemma 3.1,

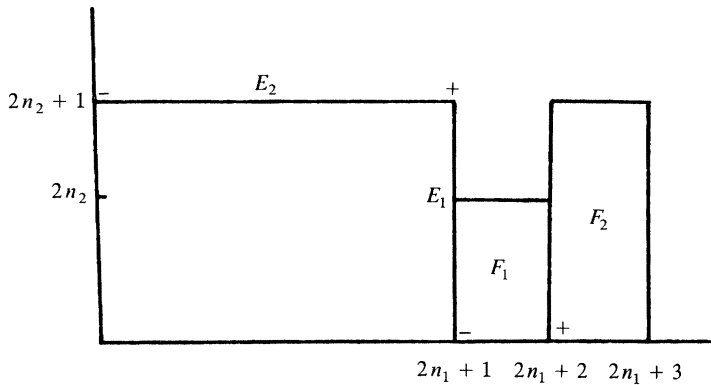
$$(3.4) \quad |t_{\bar{n}+\bar{k}} - t_{\bar{n}}| \leq f(\bar{c})$$

which tends to 0 as \bar{n} increases.

Since f is fully monotone, an inductive argument shows that the sums implicit in (3.3) exist and that the identity holds. \square

The convergence conclusion also follows from Hardy’s “bounded series” test which also requires full monotonicity without so naming it. Hardy’s result, however, does not yield the alternation information expressed by (i), (ii) and (iii).

To indicate the underlying geometric simplicity of our proof we show pictorially why (i), (ii) and (iii) hold in the two-dimensional case when $\bar{n} = (n_1, n_2)$ and $\bar{r} = (n_1 + 1, n_2)$.



$$\begin{aligned} t_{2\bar{r}} - t_{2\bar{n}} &= F_1 \leq 0; \\ t_{2\bar{r}+\bar{1}} - t_{2\bar{n}+\bar{1}} &= F_2 \geq 0; \\ t_{2\bar{n}+\bar{1}} - t_{2\bar{n}} &= E_1 + E_2 - f(2\bar{n} + \bar{1}) \\ E_1 &\leq 0, E_2 \leq 0. \end{aligned}$$

Here F_i represents the sum over the enclosed rectangle and E_i the sum over the adjacent edge.

The next theorem is a special case of Theorem 3.1. We use the notation:

$$(3.5) \quad t_n := t_n(f) := \sum_{|\bar{m}| \leq n} (-1)^{\bar{m}} f(\bar{m}),$$

where $\bar{m} \in \mathbb{N}^N$ and $n \in \mathbb{N}$. Observe that $t_n = t_{n\bar{1}}$.

THEOREM 3.2. *If $f: \mathbb{N}^N \rightarrow \mathbb{P}$ is fully monotone, then, for $m, n \in \mathbb{N}$,*

$$0 \leq t_{2m+1} \leq t_{2m+3} \leq t_{2n+2} \leq t_{2n}.$$

If in addition $\lim_{n \rightarrow \infty} f(n\bar{e}_i) = 0$ for $i = 1, 2, \dots, N$, then t_n converges to a limit t as $n \rightarrow \infty$, and $t_{2n} \geq t \geq t_{2n+1}$ for each $n \in \mathbb{N}$.

COROLLARY 3.3. For $0 < p \leq \infty, q > 0, \bar{n} \in \mathbb{N}^N,$

$$S_{\bar{n}}^N := \sum_{\bar{1} \leq \bar{m} \leq \bar{n}} (-1)^{\bar{m}} \|\bar{m}\|_p^{-q}$$

converges as \bar{n} increases.

Proof. We have

$$S_{\bar{n}+\bar{1}}^N = (-1)^N \sum_{\bar{0} \leq \bar{m} \leq \bar{n}} (-1)^{\bar{m}} \|\bar{1} + \bar{m}\|_p^{-q}$$

and Theorem 3.1 applied to Example 2.1 (a) yields the required convergence. \square

COROLLARY 3.4. For $0 < p \leq \infty, q > 0, \bar{n} \in \mathbb{N}^N,$

$$A_{\bar{n}}^N := \sum_{\substack{-\bar{n} \leq \bar{m} \leq \bar{n} \\ \bar{m} \in \mathbb{Z}^N \setminus \{\bar{0}\}}} (-1)^{\bar{m}} \|\bar{m}\|_p^{-q}$$

converges as \bar{n} increases.

Proof. Observe that

$$A_{\bar{n}}^N = 2^N S_{\bar{n}}^N + R,$$

where R is the sum of a number of finite series each of the same general form as $A_{\bar{n}}^N$ but of lower dimension. The desired result follows by induction. \square

Similarly we have:

COROLLARY 3.5. For $0 < p \leq \infty, q > 0, \bar{a} \in \mathbb{R}^N, \bar{n} \in \mathbb{N}^N,$

$$\sum_{\substack{-\bar{n} \leq \bar{m} \leq \bar{n} \\ \bar{m} \in \mathbb{Z}^N \setminus \{\bar{0}\}}} (-1)^{\bar{m}} \|\bar{a}\bar{m}\|_p^{-q}$$

converges as \bar{n} increases.

In particular Madelung’s constant exists for any rectilinear lattice in \mathbb{R}^N if defined as

$$M^N(\bar{a}) := \lim_{n \rightarrow \infty} \sum_{\substack{|\bar{m}| \leq n \\ \bar{m} \in \mathbb{Z}^N \setminus \{\bar{0}\}}} (-1)^{\bar{m}} \|\bar{a}\bar{m}\|_2^{-1}.$$

By virtue of the underlying alternation it is easy to obtain a good error bound for $t - t_{\bar{n}}$, when $t, t_{\bar{n}}$ are as in Theorem 3.1. If $f: \mathbb{N}^N \rightarrow \mathbb{R}$ is fully monotone and $t_{\bar{n}}$ converges to t as \bar{n} increases, then, letting $\bar{n}_0 := \bar{n}$ and $\bar{n}_j := \bar{n}_{j-1} + \bar{e}_j$ for $j = 1, 2, \dots, N$, we have

$$(3.6) \quad |t - t_{\bar{n}}| \leq |t_{\bar{n}+\bar{1}} - t_{\bar{n}}| \leq \sum_{j=1}^N |t_{\bar{n}_j} - t_{\bar{n}_{j-1}}| \leq \sum_{j=1}^N f((n_j + 1)\bar{e}_j),$$

on repeated application of (3.4). For the series in (1.1) the difference between

$$\sum_{\substack{|\bar{m}| \leq n \\ \bar{m} \in \mathbb{Z}^N \setminus \{\bar{0}\}}} (-1)^{\bar{m}} \|\bar{m}\|_2^{-1}$$

and the limit is at most $N/(n + 1)$. Thus, to compute 15 digits of Madelung’s constant for NaCl directly would appear to take around 10^{45} calculations! No wonder indirect transform techniques are used in practice [3]. Actually only a few digits seem to be used in applications. The NaCl crystal would have to be galaxy sized for a 15 digit approximation to have physical significance. This indicates the limited utility of using an infinite model for a finite crystal.

By virtue of Example 2.1 (b) and Theorem 3.1,

$$\sum_{\bar{1} \leq \bar{m} \leq \bar{n}} (-1)^{\bar{m}} \left(\prod_{i=1}^N m_i \right)^{-1/N}$$

converges as \bar{n} increases in \mathbb{N}^N . This is the limiting case as $p \rightarrow 0$ of Corollary 3.3 with $q = 1$. In fact the sum is just

$$\left(\sum_{m=1}^{\infty} (-1)^m m^{-1/N} \right)^N.$$

More generally, in view of Lemma 2.2, Theorem 3.1 applies to $f(\bar{m}) := \prod_{i=1}^N g_i(m_i)$ whenever each $g_i: \mathbb{N} \rightarrow \mathbb{R}$ decreases to zero. In this case, of course,

$$\sum_{\bar{0} \leq \bar{m} \leq \bar{n}} (-1)^{\bar{m}} \prod_{i=1}^N g_i(m_i)$$

converges to

$$\prod_{i=1}^N \sum_{m=0}^{\infty} (-1)^m g_i(m)$$

as \bar{n} increases in \mathbb{N}^N .

4. A characterization involving partial derivatives. We define a function $f: \mathbb{P}^N \rightarrow \mathbb{R}$ to be (N -) *monotone* if

$$(4.1) \quad \sum_{\substack{|\bar{s}| \leq 1 \\ \bar{s} \in \mathbb{N}^N}} (-1)^{\bar{s}} f(\bar{x} + \bar{a}\bar{s}) \geq 0$$

whenever $\bar{x}, \bar{a} \in \mathbb{P}^N$. We shall say that f is *fully monotone* on \mathbb{P}^N if f and all its coordinate restrictions are monotone. Then Lemma 2.2 (b) has an obvious analogue. More importantly, we have the following characterization of full monotonicity on \mathbb{P}^N in which subscripts denote partial derivatives.

THEOREM 4.1. *Let $f: \mathbb{P}^N \rightarrow \mathbb{R}$ have continuous partial derivatives of order N . Then*

- (a) f is monotone on \mathbb{P}^N if and only if $(-1)^N f_{12\dots N} \geq 0$, and
- (b) f is fully monotone on \mathbb{P}^N if and only if, for $1 \leq k \leq N$,

$$(4.2) \quad (-1)^k f_{i_1 i_2 \dots i_k} \geq 0$$

whenever i_1, i_2, \dots, i_k are distinct integers in $\{1, 2, \dots, N\}$.

Proof. (a) By Lemma 2.1 (a), for $\bar{x} \in \mathbb{P}_*^N, \bar{a} \in \mathbb{P}^N$,

$$(4.3) \quad \sum_{|\bar{s}| \leq 1} (-1)^{\bar{s}} f(\bar{x} + \bar{a}\bar{s}) = (-1)^N a_1 a_2 \cdots a_N f_{12\dots N}(\bar{c}),$$

where $\bar{x} \leq \bar{c} \leq \bar{x} + \bar{a}$. In view of the continuity of f and $f_{12\dots N}$ on \mathbb{P}^N , conclusion (a) follows from (4.3).

(b) This follows from (a) by consideration of coordinate restrictions. \square

Note that (4.3) shows that if $(-1)^N f_{12\dots N} > 0$ on \mathbb{P}^N , then f is strictly N -monotone. Further, since full monotonicity on \mathbb{P}^N implies full monotonicity on \mathbb{N}^N , (4.2) yields a simple test for full monotonicity on \mathbb{N}^N . Let $\mathbb{R}_{\bar{c}}^N := \{\bar{x} \in \mathbb{R}^N \mid \bar{x} \geq \bar{c}\}$ and say that f is N -monotone or fully monotone on $\mathbb{R}_{\bar{c}}^N$ if $f(\bar{x} - \bar{c})$ is similarly monotone on $\mathbb{R}_0^N = \mathbb{P}^N$.

EXAMPLE 4.2. (a) Let $f(x, y, z) := (x^2 + y^2 + z^2)^{-q}$ for $q > 0$ and $(x, y, z) \in \mathbb{R}_+^3$. Then

$$f_1 = -2xq(x^2 + y^2 + z^2)^{-q-1} < 0, \quad f_{12} = 4xyq(q+1)(x^2 + y^2 + z^2)^{-q-2} > 0,$$

and

$$f_{123} = -8xyzq(q + 1)(q + 2)(x^2 + y^2 + z^2)^{-q-3} < 0$$

on \mathbb{R}_1^3 . By symmetry this suffices to show that f is (strictly) fully monotone on \mathbb{R}_1^3 . The N -dimensional case can be treated similarly, as can the function in Example 2.1 (a).

(b) Consider the two-dimensional lattice sum

$$(4.4) \quad \sum_{m, n=1}^{\infty} (-1)^{m+n} \left((a_1 m + b_1 n)^2 + (a_2 m + b_2 n)^2 \right)^{-q},$$

where $q > 0$ and a_1, a_2, b_1, b_2 are real numbers. This corresponds to summing over the cone of vectors of the form $m\bar{a} + n\bar{b}$ for $m \geq 1, n \geq 1$, where $\bar{a} := (a_1, a_2), \bar{b} := (b_1, b_2)$. Let

$$A := a_1^2 + a_2^2, \quad B := b_1^2 + b_2^2, \quad C := \bar{a} \cdot \bar{b} = a_1 b_1 + a_2 b_2,$$

and

$$D := D(x, y) = (a_1 x + b_1 y)^2 + (a_2 x + b_2 y)^2.$$

Then $f(x, y) := D^{-q}(x, y)$ satisfies

$$\begin{aligned} f_1 &= -2q(Ax + Cy)D^{-q-1}, \quad f_2 = -2q(Cx + By)D^{-q-1}, \\ f_{12} &= 4q(q + 1)(Ax + Cy)(Cx + By)D^{-q-2} - 2qCD^{-q-1} \\ &= 2qD^{-q-2} \left((2q + 1)(Ax^2 + By^2)C + 2xy(qC^2 + (q + 1)AB) \right). \end{aligned}$$

We see that $f_{12} \geq 0$ while $f_1 \leq 0$ and $f_2 \leq 0$ on \mathbb{R}_1^2 if and only if $C \geq 0$. Thus f is fully monotone on \mathbb{R}_1^2 if and only if the angle between \bar{a} and \bar{b} is acute, and in this case the series in (4.4) converges in the sense of Theorem 3.1 or Theorem 3.2. \square

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MISCELLANEA

Too long for haiku!
Truly marvellous the proof
Of Fermat’s theorem.

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