Convergence of lattice sums and Madelung’s constant

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The lattice sums involved in the definition of Madelung’s constant of an NaCl-type crystal lattice in two or three dimensions are investigated. The formal mathematical questions of convergence and uniqueness of the sum of these, not absolutely convergent, series are considered. It is shown that some of the simplest direct sum methods converge and some do not converge. In particular, the very common method of expressing Madelung’s constant by a series obtained from expanding spheres does not converge. The concept of analytic continuation of a complex function to provide a basis for an unambiguous definition of Madelung’s constant is introduced. By these means, the simple intuitive direct sum methods and the powerful integral transformation methods, which are based on theta function identities and the Mellin transform, are brought to a brief analysis of a hexagonal lattice is also given.

I. INTRODUCTION

Lattice sums have played a role in physics for many years and have received a great deal of attention on both practical and abstract levels. The term lattice sum is not a precisely defined concept; it refers generally to the addition of the elements of an infinite set of real numbers, which are indexed by the points of some lattice in N-dimensional space. A method of performing a lattice sum involves accumulating the contributions of all these elements in some sequence order. Unfortunately, the elements of the set are not in general, absolutely summable so the sequential order chosen can affect the answer. In this paper we are concerned with the particular lattice sums involved in Madelung’s constant. Indeed, attaining specificity in the definition of Madelung’s constant is our primary motive. Although we are dealing with purely mathematical questions it is our belief that the results presented here may shed some light on the physics of crystals. Other researchers have expressed concern about the ambiguities involved in summing a nonabsolutely convergent series in a different manner, but it appears that no one has confronted it fully.

Let \( L \) be a lattice in \( N \)-dimensional space and let \( A_i = \{a_i, \ldots, \} \) be a set of real numbers indexed by \( L \). There are two basic approaches to summing the elements of \( A_i \): by direct summation or by integral transformations. The major factors involved in choosing a method are physical meaningfulness and speed of convergence. The direct summation methods involve an orderly grouping of the elements of \( A_i \) into sequentially indexed finite subsets increasing in size to eventually include any element of \( A_i \). Sometimes fractions of elements are included in the subsets to maintain a physical principal such as electrical neutrality. Two commonly used direct summation methods are due to Ehrenfest and Hajdudahl.

The most commonly used integral transformation method is known as the Ewald method. More recently the Mellin transformation applied to theta functions has been used to put the integral transformation methods in a general context. An excellent review article by Glasser and Zucker gives a development of these methods and an extensive bibliography.

In this paper we deal primarily with NaCl-type ionic crystals in two or three dimensions. This is for two main reasons: the ease of notation and the fact that almost every textbook introduces Madelung’s constant on this crystal first. From a mathematical and physical point of view there are two very reasonable simple direct summation methods that could be applied to give Madelung’s constant for an NaCl-type ionic crystal. One could take a basic cube centered at the reference ion with sides parallel to the basic vectors and let the cube expand as the contributions from all lattice points within the cube are accumulated. Alternately one could use expanding spheres centered at the reference ion. This latter method is intuitively appealing since all ions are an equal distance from the reference ion are given equal treatment. Thus, many textbooks (and some research articles) write down the resulting infinite series (6 – 12/2 + 8/3 – 6/4 + ...) as giving Madelung’s constant for an NaCl-type ionic crystal. Unfortunately, this infinite series does not converge. This was proven by Eversheim and, in light of the fact that most people are unaware of this divergence, we include a short elementary proof in Theorem 3.

Section II is devoted to the two-dimensional square lattice while Section III contains the above-mentioned result on expanding spheres. In Theorem 4 we prove that the method of expanding cubes converges. In Section IV, the mathematical tools become more sophisticated as we consider integral transformation methods and their relation to the direct sum-
II. TWO DIMENSIONS

It is convenient to introduce the notation in the two-dimensional case of a simple lattice in the plane with unit charges located at integer lattice points (j,k) and of signs (-1)^{j+k}. The potential energy at the origin due to the charge at (j,k) is (1 - (-1)^{j+k})/j^2+k^2. If we want the total potential energy at the origin due to all other charges, then we must sum all the numbers in the following set:

\[ A = \{(-1)^{j+k}/j^2+k^2 \} \text{ for } (j,k) \in \mathbb{Z}^2 \setminus \{(0,0)\} \]

where \( \mathbb{Z} \) denotes the integers. Because the elements of the subset of \( A \) with \( j \neq k \) form a set of positive numbers with divergent sum, it is clear that the value of the sum is highly dependent on the order in which the elements of \( A \) are added. It is not immediately clear that any reasonable method will produce a convergent series. In addition, for the model to be physically relevant, all "reasonable" methods should converge to the same number. Here are two very reasonable methods.

First, consider the total potential due to all the charges within a circle of radius \( r \) about the origin and let \( r \to \infty \). This leads to the series

\[ S_2(r) = \sum (-1)^{j+k}/j^2+k^2 - \pi \cdot \text{arc sin} \frac{r}{\sqrt{2}} \]

where \( S_2(r) \) is the number of ways of writing \( n \) as a sum of two squares of integers (positive, negative, or zero). By deriving (1), use the fact that \( (-1)^{j+k} = (-1)^{j+k} = 1 \), and for any \( j,k \in \mathbb{Z} \) with \( j^2+k^2 = n \). We refer to (1) as the method of expanding squares.

Second, there is the method of expanding series. This is intuitively appealing, as a perfect crystal grows by expansion of the shape of a basic unit cell. For each natural number \( n \), let

\[ S_3(n) = \sum (-1)^{j+k}/j^2+k^2 - \pi \cdot \text{arc sin} \frac{r}{\sqrt{2}} \]

Then

\[ \lim_{n \to \infty} S_3(n) = \pi \cdot \text{arc sin} \frac{r}{\sqrt{2}} \]

is a way of expressing the series obtained by expanding squares.

It turns out that both these methods converge as we will now show.

Theorem 1: The series in (1) converges.

Proof: To carry out the proof that the series in (1) converges, we introduce some notation and standard facts from number theory. For any sequence of real numbers \( \{a_n\}_{n=1}^{\infty} \) and \( \beta > 0 \) we write \( a_n = O(\beta^n) \) if the sequence \( \{a_n\}_{n=1}^{\infty} \) is bounded. Let \( A = \sum (-1)^{j+k}/j^2+k^2 \) for each natural number \( n \). Then \( A_n \) denotes the number of nonzero lattice points inside or on a circle of radius \( n^{1/2} \). It is fairly easy to see that \( A_n \) should be approximately \( \pi n \), in fact, the reader can easily show that \( A_n = \pi n - O(n^{3/2}) \). However, this is not quite enough for us here so we quote a stronger result, which can be found in Dickson's[2].

\[ A_n = \pi n + \text{error terms} \]

for some \( \epsilon \). Thus, we have

\[ \sum (-1)^{j+k}/j^2+k^2 = \pi \cdot \text{arc sin} \frac{r}{\sqrt{2}} \]

This together with Theorem 315 of Hardy and Wright[1] implies that

\[ S_2(r) = \pi \cdot \text{arc sin} \frac{r}{\sqrt{2}} \]

for any \( r > 0 \).

Note that, \( A_n = \pi n + \text{error terms} \), for \( n = 1, 2, \ldots, 3n \).

Thus \( S_2(r) = \pi \cdot \text{arc sin} \frac{r}{\sqrt{2}} \), for all natural numbers \( n \).

Let \( B_n = \sum (-1)^{j+k}/j^2+k^2 \).

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\[ = \sum (-1)^{j+k}/j^2+k^2 - \pi \cdot \text{arc sin} \frac{r}{\sqrt{2}} \]

(1)

Using (1),

\[ B_n = A_n - \pi \cdot \text{arc sin} \frac{r}{\sqrt{2}} \]

From (1) and (2), we have that, with \( A_n = \pi n + \text{error terms} \) in (3),

\[ B_n = C_2(2n+1) = O(n^{3/2}) \]

Furthermore, this along with (4) implies that

\[ B_n = A_n = C_2(2n+1) = O(n^{3/2}) \]

Therefore,

\[ B_n = O(n^{3/2}) \]

Now consider the partial sums of the series in (1)

\[ T_n = \sum (-1)^{j+k}/j^2+k^2 - \pi \cdot \text{arc sin} \frac{r}{\sqrt{2}} \]

\[ \sum (-1)^{j+k}/j^2+k^2 - \pi \cdot \text{arc sin} \frac{r}{\sqrt{2}} = O(n^{3/2}) \]

and therefore

\[ B_n = A_n = C_2(2n+1) = O(n^{3/2}) \]

By the mean value theorem, \( |B_k| = (1 - k^{-1/2}) \) and (5) converges.

Theorem 2: The limit in (2) exists.

Proof: We apply the lemma to \( f_{2n} \) with \( g_j = j^2+k^2 \) and \( z = j \). Then, if \( j > 0 \) and \( k > 0 \) with \( j > k \), we have

\[ f_{2n}(j^2+k^2) = f_{2j}(j^2+k^2) + \frac{1}{2} \]

Explicitly this is

\[ (j^2+k^2)^{-1/2} - (j^2+k^2)^{-1/2} = (j^2+k^2)^{-1/2} \]

Thus \( B_n = O(n^{3/2}) \).

(10)

Let \( g(j,k) \) denote the left-hand side of (10). Then \( 1 \leq j \leq k \leq n \) and \( g(j,k) \) is the contribution to the potential at the origin due to a basic cell of four adjacent ions with the closest ion \( (j,k) \). Inequality (10) says that the contribution always has the same sign as that of the nearest ion.

Rewrite \( S_3(n) \) using the symmetries to get

\[ S_3(n) = 4q(n) + 4n \]

where

\[ q(n) = \sum (-1)^{j+k}/j^2+k^2 \]

\[ X(n) = \sum (-1)^{j+k}/j^2+k^2 \]

Since \( \lim_{n \to \infty} X(n) = -2 \), we prove that \( \lim_{n \to \infty} Q(n) \) exists, then the limit in (2) will exist. We will establish a number of properties of the sequence \( \{Q(n)\}_{n=1}^{\infty} \), which will be used to prove in convergence.

Property 1.

\[ Q(2n) = Q(2n+2) - 0 \]

That is, the even indexed elements increase. To see this we group the terms of \( Q(2n) \) into basic cells of \( 4^2 \), as is illustrated in Fig. 1(a) for \( Q(8) \) and (4), thus

\[ Q(2n) = Q(2n+2) \]

\[ = \sum g(2n+2,2n+1) + \sum g(2n+2,2n+1) \]

\[ = \sum g(2n+2,2n+1) + \sum g(2n+2,2n+1) \]

where as before, \( g(j,k) \) denotes the left-hand side of (10). So property 1 holds.

Property 2.

\[ Q(2n) = Q(2n+2) - 0 \]

That is, the odd indexed elements decrease. Referring to Fig. 1(b) and correcting for the overlap at the (2n+2) point we get the following grouping:

\[ Q(2n+1) = Q(2n+3) \]

\[ \sum g(2n+2,2n+1) - \sum g(2n+2,2n+1) \]

Thus \( Q(2n+1) \) satisfies the property 2.

Q.E.D.

We now turn to the limit in (2). We need an easy lemma from calculus that will be left to the reader to verify. This lemma will also be used in the proof of Theorem 4.

FIG. 1. Illustrations of property 1 and its property 2.
\[ S = \sum_{n \geq 1} (-1)^{C(n)} \frac{C(n)}{\pi} \sqrt{n} \]

In fact, the contributions of individual spherical shells do not tend to zero.

So it is not at all appropriate to define Madelung's constant via the method of expanding spheres. We turn to the method of expanding cubes. Let

\[ S_n = \sum_{j,k,l \geq 1} \frac{(-1)^{j+k+l}}{(j^3 + k^3 + l^3)^{1/3}} \]

Notice that the inequalities are reversed from those of properties 1 and 2 in the two-dimensional case. To get the analogues of properties 3 and 4 for the \( P(m) \) we need to refer to the lemma one final time. For \( n, j, k, l \geq 1 \),

\[ h_{2j,2k,l} = \frac{(2j)^{1/3} + (2k)^{1/3} - (2l)^{1/3}}{2} \sum_{j,k,l \geq 1} \frac{(-1)^{j+k+l}}{(j^3 + k^3 + l^3)^{1/3}} \]

Finally, we have

\[ Q(n) = \sum_{j,k,l \geq 1} \frac{(-1)^{j+k+l}}{(j^3 + k^3 + l^3)^{1/3}} \]

Since each of the terms on the right-hand side of (19) approach a limit as \( n \to \infty \), we have that \( \lim_{n \to \infty} S_n \) exists.

\[ \left( \frac{j}{k} \right) \left( \frac{k}{l} \right) \left( \frac{l}{j} \right) = -1 \]

If \( \left( \frac{j}{k} \right) \left( \frac{k}{l} \right) \left( \frac{l}{j} \right) = 1 \), then

\[ \left( \frac{j}{k} \right) \left( \frac{k}{l} \right) \left( \frac{l}{j} \right) = -1 \]

These leads to the following property:

\[ P(2n+1) + P(2n) = -3 \sum_{j=1}^{n} \left( \frac{j}{j+1} \right)^{2/3} \]

To verify (17) let

\[ x_j = \frac{(-1)^{j+1}}{\sqrt{j+1}} \]

Then

\[ \sum_{j=1}^{n} x_j = \frac{n(n+1)}{4} \]

Note that \( x_j \) itself is an alternating sum of decreasing terms, so the sign of \( x_j \) is \( (-1)^j \). With (18), this implies that

\[ x_j > 1 \]

\[ \left( \frac{j}{k} \right) \left( \frac{k}{l} \right) \left( \frac{l}{j} \right) = 1 \]

Theorem 4 states that the series in (11) diverges.

Notice that the inequalities are reversed from those of properties 1 and 2 in the two-dimensional case. To get the analogues of properties 3 and 4 for the \( P(m) \) we need to refer to the lemma one final time. For \( n, j, k, l \geq 1 \),

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Since each of the terms on the right-hand side of (19) approach a limit as \( n \to \infty \), we have that \( \lim_{n \to \infty} S_n \) exists.

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Since each of the terms on the right-hand side of (19) approach a limit as \( n \to \infty \), we have that \( \lim_{n \to \infty} S_n \) exists.

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These leads to the following property:

\[ P(2n+1) + P(2n) = -3 \sum_{j=1}^{n} \left( \frac{j}{j+1} \right)^{2/3} \]

To verify (17) let

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\[ x_j > 1 \]
IV. INTEGRAL TRANSFORMATIONS AND ANALYTICITY

Our purpose in this section is to establish a firm connection between the elementary direct summation methods discussed above and the integral transformation methods, which are described by Glasser and Zucker in their survey article. One major consequence of this connection is that we can give a definition of Madelung's constant, which has firm mathematical foundation and is unique in a strong enough sense to indicate why diverse methods of performing the lattice sums lead to the same number. We begin with general discussion of analyticity of certain lattice sums in a multidimensional space. Of course, the case of 2 and 3 are the most interesting cases, but the general notation is just as convenient. For a complex number $s$, let $Re$ denote the real part of $s$ and let

$$A(s) = \left(\frac{-1}{1 + \nu} - \left(1 - \frac{1}{1 + \nu}\right)^{-2}\right)\nu,$$

where $\nu = \left[\frac{1}{1 - \nu}\right]$, $\frac{1}{1 - \nu}$, and $\nu = 1, 2, 3, 4$. We also use the notations

$$n = \left|n_1, n_2, n_3, n_4\right|, \quad \nu(n) = 2, \quad \nu(n_1, n_2, n_3, n_4) = 2 + n_1 + n_2 + n_3 + n_4.$$

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V. BACK TO TWO DIMENSIONS

In this section we consider the analyticity of various methods of summation of the sets \( A_k = (\{ -1 \}^j \times \{ 0 \}^i \times \{ k \}^l \}).\)

From Theorem 6, it follows that the method of expanding squares leads to \( d_0^{(2)} \), which is analytic for \( Re z > 0 \). In fact, expanding rectangles of any shape with sides parallel to the axes lead to \( d_0^{(2)} \). In Theorem 7, we showed that the method of expanding circles converges when \( z = 1 \), but there is no reason to believe that \( d_1^{(2)} \) is obtained unless one shows that the appropriate function is analytic. Using the notation of Sec. II, let

\[
G(z) = \sum_{n \geq 1} \frac{(-1)^n}{n^s} C(n)
\]

whenever the right-hand side converges. Then \( G(z) \) is the sum of the elements of \( A_k \), obtained by expanding circles.

Theorem 7: The function \( G(z) \) exists and is analytic for \( Re z > 0 \). Thus, \( G(z) = d_0^{(2)} \) if \( z > 1 \), in particular, \( d_2(z) = \sum_{n \geq 1} \frac{(-1)^n}{n^z} C(n) e^{-\pi n} \).

Proof: As in the proof of Theorem 1, let \( B_k = \sum_{n \geq 1} \frac{(-1)^n}{n^z} C(n). \) By (8), \( B_k = 0 \) for \( n \neq k \). For each \( n \geq 1 \), let \( A_n = \frac{(-1)^n}{n^z} C(n) \).

\[
G(z) = \sum_{n \geq 1} \frac{(-1)^n}{n^z} C(n)
\]

where \( z \) is a complex number. Note that \( A_n \) counts the contributions within the diamond \( \{ |z| = 1 \} \). Now, let \( \Sigma_k = \lim_{s \to +\infty} \sum_{n \geq 1} \frac{1}{n^k} e^{-\pi n} \) and \( \eta \) is known to be analytic for \( Re z > 0 \). Therefore, in order to determine for which \( z \) the limit of the \( A_n \) exists and is analytic, it is sufficient to analyze \( \Sigma_k \). We begin by estimating a number of facts about the sequence of \( \delta_k \).

Proposition 2: (a) \( \lim_{s \to +\infty} \delta_k \) exists and is analytic for \( Re z > 0 \).

(b) For real \( z > 0 \), \( \delta_k \) is real and \( \delta_k = 2 \lambda_k \) for \( k = 2, 3, 4, \ldots \).

(c) \( \Sigma_k \) is not analytic for \( Re z > 0 \).

Proof: (a) \( \delta_k = \sum_{n \geq 1} \frac{(k + 1)^{n-1}}{n^{k+1}} \) diverges.

(b) For real \( z > 0 \), \( \delta_k \) is real and \( \delta_k = 2 \lambda_k \) for \( k = 2, 3, 4, \ldots \).

(c) \( \Sigma_k \) is not analytic for \( Re z > 0 \).

We now describe the behavior of the diamond sums.

Theorem 8: For each complex number \( z \) with \( Re z > 0 \) and each \( n \geq 1 \), let

\[
\delta_k = \sum_{n \geq 1} \frac{(k + 1)^{n-1}}{n^{k+1}}
\]

is divergent, it is Cesàro summable or Abel summable to \( d_1(z) \).


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The diamond sums provide a nice illustration of how a method of summing the elements of $A_i$ can be analytic in a for $Re \; s$ large, then with decreasing $Re \; s$, this analyticity fails at a specific point. With the diamond sums it happens to be at $\frac{1}{8}$ with expanding squares or rectangles it is at $0$. It is not clear where the expanding circles fails; it is at a point somewhere less than $\frac{1}{8}$. In three dimensions the method of expanding spheres fails at some point greater than $\frac{1}{8}$.

VI. THE HEXAGONAL LATTICE

As an illustration of what is obtained when one studies other crystal lattices in the above manner, we include a brief summary of results on the hexagonal lattice as a two-dimen-
sional regular hexagonal lattice with ions of alternating unit charge. In order to obtain a tractable expression for the terms appearing in the lattice sum, choose a coordinate system with an angle of $\phi = \pi/3$ between the positive axes. Then an arbitrary site in the lattice has coordinates $(n, m)$ with $n$ and $m$ integers. A charge of $+1$, $-1$, or 0 is attached to that site in a regular fashion (see Fig. 2). By considering the two parallelograms indicated in Fig. 2, one can see that this charge may be expressed by $\eta(n, m) = \left[ \sin(n \theta) \sin[(m - 1) \theta] + \sin(m \theta + 1) \sin[(n + 1) \theta] \right] / \theta$, $\theta = 2 \pi / 3$. The distance of the point $(n, m)$ from the origin is given by $(n, m) = \left[ (n + m + 1/2)^2 + 3(m/2)^2 \right]^{1/2}$. The set of numbers to be summed in this case is $C_6 = \{ (n, m) | (n, m) \}^{1/2}$, $(n, m, 2 \pi \theta / 3, 0)$. For $Re > 0$.

As before, the elements of $C_6$ are absolutely summable for $Re > 1$ and we wish an analytic continuation of their sum to a region which includes $s = 1$. Arguments, like those used for the diamond sums, will show that direct summation by expanding shells of hexagons will converge analytically for $Re > 1$ and even have a limit as $s$ approaches $1$ from the right. However, for precise calculation purposes an analytic continuation via the integral transform method is far superior. Let $H_2(n, m) = \sum \left\{ \frac{(n, m) \cos(m \theta)}{(n, m) \sin(\theta)} \right\}^{1/2, (0, 0)}$, for $Re > 1$. Then $H_2(n, m)$ is an analytic function of $s$ and the series converges absolutely. Substituting the expression for $\eta(n, m)$ and using elementary trigonometric identities yields $H_2(n, m) = \frac{1}{2} \left[ \frac{1}{2} \cos(n \theta) \right]^{1/2, (0, 0)}$, where $\Sigma$ indicates the sum is over $(n, m, 2 \pi \theta / 3, 0)$. By symmetry considerations, the second term in the right-hand side of (38) is zero. Further manipulation of theta functions (using the modular equation of order 3) produces a rectangular sum.

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We have provided a unity to the concept of Madelung's constant by the use of analytic continuation of a complex function. Thus, although conditionally convergent when summed by expanding squares (or cubes), other methods of summation will provide the same answer provided that they are "analytic" in the correct sense. We have provided an analysis of the expanding circles and expanding diamonds methods in two dimensions to illustrate this point.

Perhaps the most important results are those in Sec. IV, rationalizing the integral transformation methods with the direct summation methods. These integral transform methods are the most useful in practice as they lead to very rapidly convergent series.

In the course of these investigations we have encountered many curious facts, most of which are probably known to experts in the area. However, the formulas (42) and (43) seem to be unknown and may be of sufficient interest to have been included; at least, as an illustration that the techniques of analytic continuation are applicable to other lattices.