7

Electron sums

In 1934 Wigner [17] introduced the concept of an electron gas bathed in a compensating background of positive charge as a model for a metal. He suggested that under certain circumstances the electrons would arrange themselves in a lattice, and that the body-centred lattice would be the most stable of the three common cubic structures. Fuchs [14] appears to have confirmed this in a calculation on copper relying on physical properties of copper. The evaluation of the energy of the three cubic electron lattices under precise conditions was carried out by Coldwell-Horsefall and Maradudin [10] and became the standard form for calculating the energy of static electron lattices, $U(\text{lattice})$. In this model electrons are assumed to be negative point charges located on their lattice sites and surrounded by an equal amount of positive charge uniformly distributed over a cube centered at the lattice point. First one calculates the interaction energy, U_1, of a single electron with all the other electrons on their lattice sites. Then one finds the energy of interaction of an electron with the compensating positive background, U_2. Thus

$$U(\text{lattice}) = U_1 - U_2. \tag{7.0.1}$$

The procedure is outlined here with the simple cubic lattice as its paradigm. Essentially one attempts to evaluate (7.0.1), where

$$U_1 = \frac{e^2}{a_0} \sum{}' \frac{1}{(m^2 + n^2 + p^2)^{1/2}}, \quad U_2 = \frac{e^2}{a_0} \int_0^\infty \int_0^\infty \int_0^\infty \frac{dx\, dy\, dz}{(x^2 + y^2 + z^2)^{1/2}}. \tag{7.0.2}$$

In (7.0.2) e is the charge on an electron, a_0 is the side of the elementary cube of the lattice, and Σ' is the sum over all integers m, n, p from $-\infty$ to ∞ excluding the case when m, n, p are simultaneously zero. Now both U_1 and U_2 are divergent quantities, so the approach is to find ways of evaluating them so that the infinities

cancel. An outline of this procedure is given now; the common factor e^2/a_0 is ignored. The energy U_1 is first expressed as an integral; thus

$$U_1 = \sum{}' \int_0^\infty t^{-1/2} \exp\left[-\pi(m^2+n^2+p^2)t\right] dt.$$

Next, we break the range of integration into two parts, (0,1) and $(1, \infty)$, and define

$$U_{11} = \sum{}' \int_1^\infty t^{-1/2} \exp\left[-\pi(m^2+n^2+p^2)t\right] dt,$$
$$U_{12} = \sum{}' \int_0^1 t^{-1/2} \exp\left[-\pi(m^2+n^2+p^2)t\right] dt.$$

In terms of the auxiliary integrals ϕ_k, which are given by

$$\phi_k(x) = \int_1^\infty t^k e^{-xt}\, dt, \tag{7.0.3}$$

U_{11} can be written as follows:

$$U_{11} = \sum{}' \phi_{-1/2}\left[\pi(m^2+n^2+p^2)\right]. \tag{7.0.4}$$

For U_{12}, remove the restriction on the sum by subtracting the $m = n = p = 0$ term, thus obtaining

$$U_{12} = \int_0^1 \sum t^{-1/2} \exp\left[-\pi(m^2+n^2+p^2)t\right] dt - \int_0^1 t^{-1/2}\, dt. \tag{7.0.5}$$

In (7.0.5) use the Poisson transform

$$\sum_{-\infty}^{\infty} \exp(-\pi m^2 t) = \sum_{-\infty}^{\infty} \frac{1}{\sqrt{t}} \exp\left(\frac{-\pi m^2}{t}\right)$$

and perform the second integral, to obtain

$$U_{12} = \int_0^1 \sum t^{-2} \exp\left[-\frac{\pi}{t}(m^2+n^2+p^2)\right] dt - 2. \tag{7.0.6}$$

In (7.0.6) restore the restriction on the sum by adding back the $m = n = p = 0$ term and, in the remaining integral, substitute $t = 1/u$ to obtain

$$U_{12} = \sum{}' \int_1^\infty \exp\left[-\pi u(m^2+n^2+p^2)\right] du - 2 + \int_0^1 \frac{dt}{t^2}. \tag{7.0.7}$$

On adding U_{11} and U_{12} we get

$$U_1 = \sum{}' \phi_{-1/2}\left[\pi(m^2+n^2+p^2)\right] + \phi_0\left[\pi(m^2+n^2+p^2)\right] - 2 + \int_0^1 \frac{1}{t^2}\, dt, \tag{7.0.8}$$

where, of course, the integral is divergent.

In a similar fashion U_2 can be expressed as the following four-fold integral:

$$U_2 = \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty t^{-1/2} \exp\left[-\pi(x^2+y^2+z^2)t\right] dt\, dx\, dy\, dz. \quad (7.0.9)$$

Changing to polar coordinates and performing the angular integrals leads to

$$U_2 = 4\pi \int_0^\infty \int_0^\infty t^{-1/2} \exp(-\pi t r^2) r^2\, dr\, dt = \int_0^\infty \frac{dt}{t^2} = 1 + \int_0^1 \frac{dt}{t^2}, \quad (7.0.10)$$

where the integral is again divergent. Subtract (7.0.10) from (7.0.8) and 'cancel' the identical divergent integrals; then we get, for the simple cubic lattice,

$$U(\mathrm{SC}) = \sum{}' \phi_{-1/2}\left[\pi(m^2+n^2+p^2)\right] + \phi_0\left[\pi(m^2+n^2+p^2)\right] - 3. \quad (7.0.11)$$

Tables of $\phi_k(x)$ were prepared by Born and Misra [4]. One only needs a few terms of the series, since $\phi_k(x)$ rapidly becomes smaller as x increases. Thus Coldwell-Horsfall and Maradudin [10] found that

$$U(\mathrm{SC}) = -2.837297 \frac{e^2}{a_0}.$$

However, if we look back to Section 1.3, where $a(2s) = \sum{}' 1/(m^2+n^2+p^2)^{2s}$ was treated as the three-dimensional analogue of the Riemann zeta function, we see that $U_1(\mathrm{SC}) = a(1)$ and, by making use of the functional equation coming from analytic continuation, $a(1)$ may be evaluated and is given in Table 1.5. To much surprise it was seen that $U_1(\mathrm{SC})$ found for $a(1)$ by the simple method described in Section 1.3 is equal to the expression $U(\mathrm{SC})$ found by the rather complex method given above. Results for electrons forming face-centred cubic (FCC) and body-centred cubic (BCC) lattices are also found in [10]. It is simple to show that for these lattices the interaction amongst the electrons alone is

$$U_1(\mathrm{FCC}) = a(1) + d(1), \qquad U_1(\mathrm{BCC}) = \tfrac{1}{2}\left[a(1) + 3c(1)\right],$$

and it is equally simple to evaluate them; once again they were found to be equal to the values in [10]. That is,

$$U_1(\mathrm{FCC}) = U(\mathrm{FCC}) = -4.584875 \frac{e^2}{a_0}, \quad U_1(\mathrm{BCC}) = U(\mathrm{BCC}) = -3.639240 \frac{e^2}{a_0}.$$

To find the most stable of these lattices the results have to be expressed in terms of r_s, the radius of a sphere of volume equal to the volume per electron; we have

$$a_0^3 = \tfrac{4}{3}\pi r_s^2(\mathrm{SC}), \quad \tfrac{1}{4}a_0^3 = \tfrac{4}{3}\pi r_s^2(\mathrm{FCC}), \quad \tfrac{1}{2}a_0^3 = \tfrac{4}{3}\pi r_s^2(\mathrm{BCC}),$$

and thus

$$U(\mathrm{SC}) = -1.760119 \frac{e^2}{r_s}, \qquad U(\mathrm{FCC}) = -1.791753 \frac{e^2}{r_s},$$

$$U(\mathrm{BCC}) = -1.791860 \frac{e^2}{r_s},$$

in which the BCC lattice appears as the most stable.

Results obtained by Bonsall and Maradudin [3] by the traditional method for two-dimensional electron lattices also agreed with closed-form results found by direct evaluation of just the appropriate U_1. Thus for the square and triangular lattices (Bonsall and Maradudin call the latter the hexagonal lattice) we have

$$U_1(\text{sq}) = \sum{}'(m^2+n^2)^{-1/2}, \qquad U_1(\text{tri}) = \sum{}'(m^2+mn+n^2)^{-1/2}.$$

A standard decomposition of these double sums into products of single sums, to be found in Zucker and Robertson [19] and Borwein and Borwein [8], gives

$$U_1(\text{sq}) = 4\zeta(\tfrac{1}{2})L_{-4}(\tfrac{1}{2}) = -3.900\,264\,924,$$
$$U_1(\text{tri}) = 6\zeta(\tfrac{1}{2})L_{-3}(\tfrac{1}{2}) = -4.213\,422\,363$$

in terms of a_0, the side of the square or of the triangle, and it is very simple to calculate these quantities. In terms of r_s, the radius of a circle equal in area to the area per electron, we have

$$a_0^2 = \pi r_s^2(\text{sq}), \qquad \tfrac{\sqrt{3}}{2}a_0^2 = \pi r_s^2(\text{tri}),$$

so that

$$U(\text{sq}) = \frac{-2.200488843e^2}{r_s}, \qquad U(\text{tri}) = \frac{-2.212205173e^2}{r_s}.$$

There were two surprises here. First these numbers could be obtained without going through the long process just described, in particular, avoiding subtracting two infinite integrals. Secondly, why was the actual energy of the lattice given just by the interaction of the electrons alone, calculated in this way? Since it is much easier to evaluate the analytic continuations of the corresponding lattice sums without bothering to subtract divergent integrals 'in the right way', the question arises whether using this method is valid for all Coulomb lattices. An attempt to justify this procedure was explored by Borwein *et al.* [6]. They started by observing that the previous manipulations were not arbitrary, but rather were stable since any answer might be obtained by inappropriate processes. Some regular limiting procedure must be undertaken to guarantee a robust answer. The following principle is proposed: the rearrangements used should depend only on the geometry of the underlying lattice and not on the power s in the law of interaction.

The consequence of this principle is that we look for an appropriate analytic function for $U(\text{lattice} : s)$ and take our answer the value of this function at $s = \frac{1}{2}$. They argue that this forces the answer to be $a_{lat}(1)$ where $a_{lat}(2s)$ is the d-dimensional sum over the lattice sites:

$$a_{lat}(2s) = \sum{}'(l_1^2 + l_2^2 + \cdots + l_d^2)^{-2s},$$

in which the sum represents $a_{lat}(2s)$ for $\text{Re}\, s > \frac{1}{2}d$. This has an analytic continuation for $0 < \text{Re}\, s < \frac{1}{2}d$, which, for the d-dimensional simple cubic lattice, is

obtained via the functional relation

$$\pi^{-s}\Gamma(s)a_{lat}(2s) = \pi^{s-d/2}\Gamma\left(\frac{1}{2}d - s\right)a_{lat}(d-2s).$$

Formally, $U(\text{lattice} : s) = a_{lat}(2s) - U_2(s)$, where

$$U_2 = c\int_{(\Omega)}\cdots\int \frac{dx_1\cdots dx_d}{\left(x_1^2 + x_2^2 \ldots + x_d^2\right)^s},$$

while c is a constant appropriate to the lattice and Ω is some volume in d-dimensional space which gives electrical neutrality. Now split U_2 into the regions inside the unit sphere and outside the unit sphere thus:

$$U_2(s) = U_2^{<}(s) + U_2^{>}(s).$$

Adding on the finite integral $U_2^{<}(s)$ when $0 < \text{Re}\, s < \frac{1}{2}d$ to both sides, we have

$$U(\text{lattice} : s) + U_2^{<}(s) = a_{lat}(2s) - U_2^{>}(s). \tag{7.0.12}$$

Now, $U_2^{<}(s)$ may be integrated to give for $\text{Re}\, s > \frac{1}{2}d$

$$U_2^{<}(s) = \frac{C}{d-2s} \qquad \text{with} \qquad \frac{C = \Omega\, c\, 2\pi^{d/2}}{\Gamma(\frac{1}{2}d)},$$

whereas for $\text{Re}\, s > d/2$ the other integral, $U_2^{>}$, is finite and, by direct computation or by appealing to the central symmetry of the integral, has the value $C/(2s-d)$. Now we argue as follows. The left-hand side of (7.0.12), namely $U(\text{lattice} : s) + C/(d-2s)$, is an analytic continuation of the right-hand side of (7.0.12) for $\text{Re}\, s < \frac{1}{2}d$. Thus, by comparing the two we have

$$U(\text{lattice} : s) = a_{lat}(2s)$$

for $\text{Re}\, s < \frac{1}{2}d$ and hence for $s = \frac{1}{2}$ we have our result. By considering a precise limiting process we shall demonstrate why a unique 'answer' is to be obtained.

The following model in d dimensions will be considered. In this model point charges are located at lattice sites and these are surrounded by an equal amount of opposite charge uniformly distributed over hypercubes centered at the lattice point and of side equal to the lattice spacing. This is illustrated there after in two dimensions, where the shaded portion represents positive charge of value equal to the point negative charge but uniformly distributed over a square.

We shall thus examine the precise limiting procedure

$$\lim_{N\to\infty}\sigma_N(s) = \lim_{N\to\infty}\Bigg[\sum_{-N}^{N}\cdots\sum_{-N}^{N\prime}\left(l_1^2+l_2^2+\cdots+l_d^2\right)^{-s} - \int_{-N+1/2}^{N+1/2}\cdots\int_{-N+1/2}^{N+1/2}\left(x_1^2+x_2^2+\cdots+x_d^2\right)^{-s}dx_1\,dx_2\cdots dx_d\Bigg] = \lim_{N\to\infty}\left[\alpha_N(s)-\beta_N(s)\right],$$

although a priori this limit need not exist. This procedure maintains electrical neutrality throughout the limiting process. Further the model has zero dipole moment and, in three dimensions, zero quadrupole moment as well.

Consider first the multidimensional integral $\beta_N(s)$. Writing $x_j = (N+\frac{1}{2})X_j$, we have

$$\frac{\beta_N(s)}{(N+\frac{1}{2})^{d-2s}} = I(s) = \int_{-1}^{1}\cdots\int_{-1}^{1}\left(X_1^2+\cdots+X_d^2\right)dX_1\cdots dX_d. \quad (7.0.13)$$

Now, $I(s)$ may be rewritten as follows:

$$I(s) = 2d\int\cdots\int_{W_d}\frac{dX_1\cdots dX_d}{(X_1^2+\cdots+X_d^2)^s},$$

where W_d is the pyramidal region $|X_i|\le X_d\le 1$. Making the substitution $X_i = X_d x_i$, we have

$$I(s) = 2d\int_0^1 X_d^{d-1-2s}dX_d\int_{-1}^{1}\cdots\int_{-1}^{1}\frac{dx_1\cdots dx_{d-1}}{(1+x_1^2+\cdots x_{d-1}^2)^s} = \frac{2d}{d-2s}C(s),$$

where

$$C(s) = \int_{-1}^{1}\cdots\int_{-1}^{1}\frac{dx_1\cdots dx_{d-1}}{(1+x_1^2+\cdots x_{d-1}^2)^s},$$

and this integral clearly converges for Re $s>0$. Thus

$$\sigma_N(s) = \alpha_N(s) - (N+\tfrac{1}{2})^{d-2s}\frac{2d}{d-2s}C(s), \quad (7.0.14)$$

and the whole of the right-hand side of (7.0.14) is meromorphic for Re $s>0$, with a single simple pole at $s=\frac{1}{2}d$. Note that

$$\beta_0(s) = 2^{2s-d}\frac{2dC(s)}{(d-2s)} \quad (7.0.15)$$

gives an analytic continuation of the integral inside the unit hypercube. For Re $s>\frac{1}{2}d$, $\sigma_N(s)$ is infinite since its defining integral is infinite. Then, for Re $s>\frac{1}{2}d$,

$$\lim_{N\to\infty}\sigma_N(s)+\beta_0(s) = \lim_{N\to\infty}\alpha_N(s)+\beta_0(s) = a_{lat}(2s)+\beta_0(s), \quad (7.0.16)$$

since $\beta_N(s)$ tends to zero. We can use (7.0.15) to see that $a_{lat}(2s) + \beta_0(s)$ is analytic in Re $s > 0$. The principle of analytic continuation allows us to conclude that (7.0.16) continues to hold in any half-plane in which the left-hand side exists and is known to be analytic. However, for $0 <$ Re $s < \frac{1}{2}d$, $\beta_0(s)$ is a finite integral. Thus, in the appropriate strip, $\lim_{N\to\infty} \sigma_N(s) = a_{1at}(2s)$ for the particular limiting process we have undertaken – if it is, in fact, true that $\lim_{N\to\infty} \sigma_N(s) + \beta_0(s)$ exists and is analytic in the appropriate half-plane (or at least for $\frac{1}{2} <$ Re $s < \frac{1}{2}d$ with continuity at $\frac{1}{2}$).

Now, for all lattices in two dimensions, $\sigma_N(s) + \beta_0(s)$ can be shown to tend to an analytic limit in the right half-plane. This was proved for the square lattice in Borwein *et al.* [6]. While it might seem reasonable to presume that it holds generally, that is in fact false. Considerations similar to those given there show that, for the simple cubic lattice in three dimensions, the limit is analytic for $\frac{1}{2} <$ Re $s < \frac{3}{2}$ but is discontinuous at $\frac{1}{2}$. Indeed $\lim_{s\to 1/2+} \lim_{N\to\infty} \sigma_N(s) = a_{lat}(2s)$, the correct answer, but this differs by $\pi/6$ from $\lim_{N\to\infty} \sigma_N(\frac{1}{2})$ (the rectangular limit). This is discussed more fully in a further paper by Borwein *et al.* [5].

In addition, in two dimensions one can also show that the limit over expanding circles, namely the limit as $N \to \infty$ of

$$\tau_N(s) = \sum_{1\le(m^2+n^2)\le N} (m^2+n^2)^{-s} - \int\int_{1\le(m^2+n^2)\le N} (x^2+y^2)^{-s}\,dx\,dy$$

is analytic for Re $s > \frac{1}{3}$. As a consequence, when the integral inside the unit circle is reintroduced, the corresponding limiting value at $s = \frac{1}{2}$ is also $4\zeta(\frac{1}{2})L_{-4}(\frac{1}{2})$.

Granted the general applicability of the previous meta-principle – which we have illustrated already for SC, FCC, BCC, square, and triangular lamina lattices – we can easily determine U(lattice) for many other lattices. Thus other three-dimensional lattices were investigated; in particular, various types of hexagonal lattice were considered. A simple hexagonal lattice is a structure formed by stacking planes of two-dimensional triangular lattices directly above each other. The direction of stacking is known as the c axis and the separation of planes in terms of the nearest neighbour distance, R, in the triangular lattice is called the axial ratio, c. If particles on such a lattice interact with an r^{-s} potential, it is simple to show that the appropriate lattice sums are given by

$$H(2s:c) = {\sum}'(m^2+3n^2+c^2p^2)^{-s} + \sum\left[(m-\tfrac{1}{2})^2+3(n-\tfrac{1}{2})^2+c^2p^2\right]^{-s}.$$

Using our principle that the energy of a such a lattice of electrons in a compensating positive background is given in terms of e^2/R by

$$H(\text{hex}) = H(1:c),$$

methods of converting such sums into rapidly converging cosech sums have been previously described in Section 1.3 and, after some detailed algebra, $H(1:c)$ can be converted to rapidly converging sums and double sums of cosech functions:

$$
\begin{aligned}
&H(1:c)\\
&= -\frac{16\log 2}{3c} - \frac{\sqrt{3}\pi c}{18} + \frac{\sqrt{3}}{3}\Bigg[2\sum_1^\infty \frac{\operatorname{cosech}(c\pi m)}{m}\\
&\quad + 2\sum_1^\infty \frac{\sqrt{3}\operatorname{cosech}(c\pi m/\sqrt{3})}{m} + 4\sum_1^\infty\sum_1^\infty \frac{\sqrt{3}\operatorname{cosech} c\pi\sqrt{m^2+n^2/3}}{\sqrt{3m^2+n^2}}\Bigg]\\
&\quad + \frac{4\sqrt{3}}{3c}\Bigg[2\sum_1^\infty \frac{\operatorname{cosech}(2\pi m/c)}{2m/c} + 4\sum_1^\infty\sum_1^\infty \frac{4\operatorname{cosech}\pi\sqrt{4m^2/3+4n^2/c^2}}{\sqrt{4m^2/3+4n^2/c^2}}\Bigg]\\
&\quad + \frac{4\sqrt{3}}{c}\Bigg[2\sum_1^\infty \frac{\operatorname{cosech}(\sqrt{12}\pi m/c)}{\sqrt{12m}/c}\\
&\qquad\qquad + 4\sum_1^\infty\sum_1^\infty \frac{4\operatorname{cosech}\pi\sqrt{12m^2/3+12n^2/c^2}}{\sqrt{12m^2+12n^2/c^2}}\Bigg]\\
&\quad - \frac{\sqrt{3}}{c}\Bigg[2\sum_1^\infty \frac{(-1)^m\operatorname{cosech}(\sqrt{3}\pi m/c)}{\sqrt{3}m/c}\\
&\qquad\qquad + 4\sum_1^\infty\sum_1^\infty \frac{(-1)^{m+n}\operatorname{cosech}\pi\sqrt{(3m^2/3+3n^2/c^2)}}{\sqrt{3m^2+3n^2/c^2}}\Bigg]. \qquad (7.0.17)
\end{aligned}
$$

Evaluations of $H(1:c)$ for several values of c are given below. The only corresponding results we know in the literature are those given by Hund [15, 16] for $c=2$ and $c=\sqrt{\frac{8}{3}}$. The latter value for c is the so-called ideal ratio. Hund's values were calculated by the traditional Ewald method and the numerical accuracy was low. He gave

$$H\left(1:\sqrt{\tfrac{8}{3}}\right) = -2.238, \qquad H(1:2) = -1.796.$$

As in the case of the three cubic lattices, we convert the values in terms of e^2/R into values in terms of e^2/r_s. For the simple hexagonal lattice the volume of a unit cell is $3\sqrt{3}cR^3/2$, and with three electrons per cell the volume per electron is $\sqrt{3}cR^3/2$. Hence

$$\sqrt{3}cR^3/2 = 4\pi r_s^3/3 \qquad \text{and} \qquad r_s/R = (3\sqrt{3}c/8\pi)^{1/3}.$$

Multiplying $H(1:c)$ by $(3\sqrt{3}c/8\pi)^{1/3}$ yields $U(\text{hex})$ in terms of e^2/r_s, as in Table 7.1. It is so simple to evaluate $H(1:c)$ via (7.0.17) that numerically the minimum was located at $c=0.9284$ with

$$\frac{U(\text{hex})}{e^2/r_s} = -1.774642655.$$

We have also evaluated U for the hexagonal close-packed (HCP) structure, which may be regarded as two equal interpenetrating hexagonal crystals with ideal

Table 7.1

c^2	$U(\text{hex})/(e^2/R)$	$U(\text{hex})/(e^2/r_s)$
$\frac{1}{4}$	−3.263230504	−1.531505030
$\frac{9}{16}$	−3.253618321	−1.747971578
$\frac{3}{4}$	−3.143633242	−1.771826683
1	−2.995711953	−1.771389474
$\frac{3}{2}$	−2.730799747	−1.727636634
2	−2.502936140	−1.661251716
$\frac{8}{3}$	−2.238722127	−1.558866728
4	−1.795017494	−1.337291317

axial ratios, one lattice based at the origin (0, 0, 0) and the other at $\left(\frac{1}{2}, \frac{1}{3}, \frac{1}{2}\right)$. The lattice sums for such a structure in terms of R may be written

$$\text{HCP}(2s) = H\left(2s : \sqrt{\tfrac{8}{3}}\right) + H^*(2s),$$

where

$$H^*(2s) = \sum\left[(m-\tfrac{1}{2})^2 + 3(n-\tfrac{1}{3})^2 + \tfrac{8}{3}(p-\tfrac{1}{2})^2\right]^{-s} + \sum\left[m^2 + 3(n-\tfrac{1}{6})^2 + \tfrac{8}{3}(p-\tfrac{1}{2})^2\right]^{-s}.$$

For the HCP structure the volume of a hexagonal cell is $3\sqrt{2}R^3$, but there are six electrons per cell. Hence we have

$$\sqrt{2}R^3/2 = 4\pi r_s^3/3 \qquad \text{and} \qquad r_s/R = (3\sqrt{2}/8\pi)^{1/3},$$

and we obtain

$$U(\text{HCP}) = -3.241858662e^2/R = -1.791676267e^2/r_s.$$

Foldy [12] found by the traditional method that $U(\text{HCP}) = -1.79167624e^2/r_s$ and noted that if the axial ratio is 1.0016 times the ideal value then the last two figures read 90 instead of 24, and he claims this is the real minimum.

As a final example, the result for the diamond lattice is given. The diamond lattice may be considered as two equal interpenetrating FCC lattices, one based on (0, 0, 0) and the other on $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. In terms of the cube side of an FCC lattice, the diamond lattice sums are easily shown to be

$$\text{di}(2s) = \text{FCC}(2s) + 2^{2s-1}\left[\text{BCC}(2s) - \text{SC}(2s)\right],$$

and again the principle gives $U(\text{di}) = \text{di}(l)$ in terms of e^2/a_0. Using previous results,

$$\text{di}(1) = \frac{1}{2}[a(1) + 3c(1) + 2d(1)] = -5.386789045.$$

For the diamond lattice, the volume of a cubic cell is U and this has eight electrons per cell. Hence $a_0^3/8 = 4\pi r_s^3/3$ and $r_s/a_0 = (3/32\pi)^{1/3}$, and we obtain

$$U(\text{di}) = -1.670851406e/r_s,$$

in complete agreement with Foldy's 1978 value, obtained conventionally.

It should, however, be pointed out that in all the previous calculations the structures were either Bravais lattices or contained a basis of energy equivalent sites. With more complex lattices where this is not the case, ignoring this point has led to incorrect results for the fluorite, perovskite, and spinel lattices – see Zucker [18]. This was noted by Cockayne [9], who found the correct results by the conventional Ewald approach. Baldereschi *et al.* [2] showed that by correctly superimposing the component Bravais lattices with the right weightings, the method used here gives the correct values. Thus the perovskite lattice is a simple cubic lattice with a five-fold basis, with the general formula ABX_3. The A sites are the corners of the cube, the B sites the centres of the cube and the X sites the faces of the cube. The X sites, though energetically equivalent to each other, are not equivalent to the A and B sites. One has to evaluate the interaction of each site with the others and weight them accordingly. Thus the perovskite lattice may be taken to be made up of the A lattice, an SC lattice based at the origin (0, 0, 0), the B lattice, an SC lattice based on $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, and three X lattices, i.e. SC lattices based on the equivalent sites $(0, \frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, 0, \frac{1}{2})$, and $(\frac{1}{2}, \frac{1}{2}, 0)$. So, the interaction of A with the other sites may be written, in the notation of Section 1.3, as

$$\psi_A = \psi(0,0,0) + \psi(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) + 3\psi(0,\tfrac{1}{2},\tfrac{1}{2}) = a(1) + \tfrac{1}{2}[3c(1) - a(1)] + d(1).$$

Similarly, we have

$$\psi_B = \psi(0,0,0) + \psi(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) + 3\psi(0,0,\tfrac{1}{2}) = a(1) + \tfrac{1}{2}[3c(1) - a(1)] + \frac{1}{2}[3b(1) - d(1)],$$

and

$$\psi_X = \psi(0,0,0) + 3\psi(0,\tfrac{1}{2},\tfrac{1}{2}) + \psi(0,0,\tfrac{1}{2}) = a(1) + f(1) + \tfrac{1}{6}[3b(1) - d(1)].$$

To obtain the correct electronic interaction we require to weight these terms correctly:

$$U_P = \tfrac{1}{5}(\psi_A + \psi_B + 3\psi_X) = \tfrac{1}{5}\Big[7b(1) + 7c(1) + \tfrac{1}{3}13d(1)\Big] = 4.671242310\frac{e^2}{a_0}.$$

Since there are five electrons per cube, in terms of r_s this becomes $1.694\,648\,083e^2/r_s$, in complete agreement with Cockayne's result. Similarly, for the fluorite lattice AB_2, A is an FCC lattice based on $(0, 0, 0)$ and the two B lattices are FCC lattices based on the equivalent sites $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ and $(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$. As before,

$$\psi_A = \psi_{FCC}(0, 0, 0) + 2\psi_{FCC}\left(\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}\right) = a(1) + d(1) + 3c(1) - a(1)$$

and

$$\begin{aligned}\psi_B &= \psi_{FCC}(0, 0, 0) + \psi_{FCC}\left(\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}\right) + \psi_{FCC}\left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right)\\ &= a(1) + d(1) + \frac{1}{3}[3c(1) - a(1)] + a(1) - d(1).\end{aligned}$$

Hence

$$U_{\text{Fluorite}} = \frac{1}{12}(4\psi_A + 8\psi_B) = \frac{1}{3}[3b(1) + 9c(1) + 2d(1)] = 6.380598623\frac{e^2}{a_0}.$$

Since there are 12 electrons per cube, in terms of r_s this becomes $1.728906369e^2/r_s$, again in complete agreement with Cockayne's result. Of all the three-dimensional structures considered, the BCC remains energetically the most stable.

7.1 Commentary: Wigner sums as limits

We now describe an analysis from [5], as follows. The authors investigated the limit as $N \to \infty$ of the d-dimensional quantity

$$\sigma_N(s) := \alpha_N(s) - \beta_N(s),$$

where

$$\alpha_N(s) = \sum_{-N}^{N} \cdots \sum_{-N}^{N} \left[f(n_1, n_2, \ldots, n_d)\right]^s, \tag{7.1.1}$$

$$\beta_N(s) = \int_{-(N+1/2)}^{N+1/2} \cdots \int_{-(N+1/2)}^{N+1/2} \left[f(x_1, x_2, \ldots, x_d)\right]^s \, dx_1 \cdots dx_d$$

for various particular functions f. Two instances were studied in detail.

(1) First, the two-dimensional case where f is given by a positive definite binary quadratic form $Q(x, y) := ax^2 + bxy + cy^2$ was analyzed in [5, Theorem 1].

Namely, for any positive definite form Q, the quantity $\sigma(s) := \lim_{N\to\infty} \sigma_N(s)$ exists in the strip $0 < \text{Re } s < 1$ and coincides therein with the analytic continuation of $\alpha(s)$.

Thus, the integral $\beta_N(s)$ plays no role in the final answer. This is very tidy for two-dimensional lattices.

(2) The authors of [5] then investigated the three-dimensional case for the simple cubic lattice, namely $Q(x, y, z) := x^2 + y^2 + z^2$ and came to a similar conclusion as before, for the strip $\frac{1}{2} < \mathrm{Re}\, s < \frac{3}{2}$. However, at $s = \frac{1}{2}$, $\sigma(s)$ is discontinuous and

$$\sigma\left(\tfrac{1}{2}\right) = \alpha\left(\tfrac{1}{2}\right) + \tfrac{1}{6}\pi. \tag{7.1.2}$$

The physicist's method of finding $\lim_{N\to\infty} \sigma_N(\frac{1}{2})$ always alights on $\alpha(\frac{1}{2})$; why this so is not fully understood but some heuristic explanations – regarding analytic continuations—are to be found in [6].

We leave an open question:

Can a similar analysis be done for the four-dimensional simple cubic lattice? Presumably, there is a strip for which $\sigma(s) = \alpha(s)$ but will $s = \frac{1}{2}$ lie within this strip?

In four dimensions the closed form is known for α in the simple cubic case:

$$\alpha(s) = -8\Big(1 - 2^{2-s}\Big)\Big(1 - 2^{1-s}\Big)\zeta(s)\zeta(s-1);$$

see [8, (9.2.5)].

7.2 Commentary: Sums related to the Poisson equation

In a recent treatment of 'natural' Madelung constants [11], it is pointed out that the Poisson equation for an n-dimensional point-charge source,

$$\nabla^2 \Phi_n(\mathbf{r}) \;=\; -\delta(\mathbf{r}), \tag{7.2.1}$$

gives rise to an electrostatic potential – we call it the *bare-charge potential* – of the form

$$\Phi_n(\mathbf{r}) = \frac{\Gamma(\frac{n}{2} - 1)}{4\pi^{n/2}} \frac{1}{r^{n-2}} \;=:\; \frac{C_n}{r^{n-2}} \qquad \text{if } n \neq 2, \tag{7.2.2}$$

$$\Phi_2(\mathbf{r}) = -\frac{1}{2\pi} \log r \;=:\; C_2 \log r, \tag{7.2.3}$$

where $r := |\mathbf{r}|$. Since this Poisson solution generally behaves as r^{2-n}, [11] defines a 'natural' Madelung constant $\mathcal{N}_n$ as (here, $m := |\mathbf{m}|$):

$$\mathcal{N}_n := C_n \sum_{\mathbf{m}\in\mathbb{Z}^n}{}' \frac{(-1)^{\mathbf{1}\cdot\mathbf{m}}}{m^{n-2}} \quad \text{if } n \neq 2, \tag{7.2.4}$$

$$\mathcal{N}_2 := C_2 \sum_{\mathbf{m}\in\mathbb{Z}^n}{}' (-1)^{\mathbf{1}\cdot\mathbf{m}} \log m,$$

where, in cases such as this log sum, one must infer an analytic continuation [11] as the literal sum is quite non-convergent. This $\mathcal{N}_n$ coincides with the classical Madelung constant

$$\mathcal{M}_n \;:=\; {\sum_{\mathbf{m}\in\mathbb{Z}^n}}' \frac{(-1)^{\mathbf{1}\cdot\mathbf{m}}}{m} \tag{7.2.5}$$

only for $n = 3$ dimensions, in which case $\mathcal{N}_3 = \frac{1}{4\pi}\mathcal{M}_3$. In all other dimensions there is no obvious $\mathcal{M}, \mathcal{N}$ relation.

A method for gleaning information about $\mathcal{N}_n$ is to contemplate the Poisson equation with a crystal charge source, modelled on NaCl (salt) in the sense of alternating lattice charges:

$$\nabla^2\phi_n(\mathbf{r}) \;=\; -\sum_{\mathbf{m}\in\mathbb{Z}^n}(-1)^{\mathbf{1}\cdot\mathbf{m}}\delta(\mathbf{m}-\mathbf{r}). \tag{7.2.6}$$

Accordingly – on the basis of the Poisson equation (7.2.1) – solutions ϕ_n can be written in terms of the respective bare-charge functions Φ_n as

$$\phi_n(\mathbf{r}) \;=\; \sum_{\mathbf{m}\in\mathbb{Z}^n}(-1)^{\mathbf{1}\cdot\mathbf{m}}\Phi_n(\mathbf{r}-\mathbf{m}). \tag{7.2.7}$$

7.2.1 Madelung variants

We have defined the classical Madelung constants (7.2.5) and the 'natural' Madelung constants (7.2.4). Following [11] we define a *Madelung potential*, now depending on a complex s and spatial point $\mathbf{r} \in \mathbb{Z}^n$:

$$\mathcal{M}_n(s,\mathbf{r}) \;:=\; {\sum_{\mathbf{p}\in\mathbb{Z}^n}}' \frac{(-1)^{\mathbf{1}\cdot\mathbf{p}}}{|\mathbf{p}-\mathbf{r}|^s}, \tag{7.2.8}$$

We can write limit formulae for our Madelung variants, first the classical Madelung constant,

$$\mathcal{M}_n := \lim_{\mathbf{r}\to\mathbf{0}}\left[\mathcal{M}_n(1,\mathbf{r}) - \frac{1}{r}\right] \tag{7.2.9}$$

$$= {\sum_{\mathbf{p}\in\mathbb{Z}^n}}' \frac{(-1)^{\mathbf{1}\cdot\mathbf{p}}}{p}, \tag{7.2.10}$$

and then the 'natural' Madelung constant,

$$\mathcal{N}_n := \lim_{\mathbf{r}\to\mathbf{0}}\left[\phi(\mathbf{r}) - \Phi(r)\right] \tag{7.2.11}$$

$$= C_n {\sum_{\mathbf{p}\in\mathbb{Z}^n}}' \frac{(-1)^{\mathbf{1}\cdot\mathbf{p}}}{p^{n-2}}. \tag{7.2.12}$$

For small even n, this last sum is evaluable. For example, from [8, (9.2.5)] we have

$$\sum_{\mathbf{p}\in\mathbb{Z}^4}{}' \frac{(-1)^{\mathbf{1}\cdot\mathbf{p}}}{p^{2s}} = (1-2^{2-s})(1-2^{1-s})\zeta(s)\zeta(s-1), \tag{7.2.13}$$

which with $s=1$ yields

$$\mathcal{N}_4 = -\frac{1}{\pi^2}\log 2.$$

Similarly, from [8, Exercise 4b, p. 292] we have

$$\sum_{\mathbf{p}\in\mathbb{Z}^8}{}' \frac{(-1)^{\mathbf{1}\cdot\mathbf{p}}}{p^{2s}} = -16(1-2^{4-s})\zeta(s)\zeta(s-3), \tag{7.2.14}$$

which with $s=3$ determines that

$$\mathcal{N}_8 = -\frac{4}{\pi^4}\,\zeta(3).$$

Generally, via the Mellin transform $M_s\theta_4^{2n}(q)$ (see below), values of $\mathcal{N}_{2n}$ for small n are similarly susceptible. For instance, if G denotes Catalan's constant, we have

$$\mathcal{N}_6 = -\frac{1}{24\pi} - \frac{2G}{\pi^3},$$

as in [11]. The more complex value $\mathcal{N}_2$ is presented in (7.2.21), below.

7.2.2 Relation between crystal solutions ϕ_n and Madelung potentials

From (7.2.2), (7.2.7), and (7.2.8) we have the general relation, for dimension $n \neq 2$,

$$\phi_n(\mathbf{r}) \;=\; C_n\mathcal{M}_n(n-2,\mathbf{r}). \tag{7.2.15}$$

Note that, for the case $n = 3$, the solution ϕ_3 coincides with the classical Madelung potential $\mathcal{M}_3(1,\mathbf{r})$ in the sense that

$$\phi_3(\mathbf{r}) \;=\; \frac{1}{4\pi}\mathcal{M}_3(1,\mathbf{r}),$$

because $C_3 = 1/(4\pi)$. Likewise, the 'natural' and classical Madelung constants are related by $4\pi\,\mathcal{N}_3 = \mathcal{M}_3$. The whole idea of introducing 'natural' Madelung constants $\mathcal{N}_n$ is that this coincidence of radial powers for ϕ and $\mathcal{M}$ potentials holds *only* in three dimensions. For example, in $n=5$ dimensions, the summands for ϕ_5 and $\mathcal{M}_5(1,\cdot)$ involve radial powers $1/r^3$, as in

$$\phi_5(\mathbf{r}) \;=\; \frac{1}{8\pi^2}\mathcal{M}_5(3,\mathbf{r}).$$

In [11] it is argued that a solution to (7.2.6) is

$$\phi_n(\mathbf{r}) \;=\; \frac{1}{\pi^2} \sum_{\mathbf{m}\,\in\,\mathbb{O}^n} \frac{\prod_{k=1}^{n} \cos\,\pi m_k r_k}{m^2}, \tag{7.2.16}$$

where $\mathbb{O}$ denotes the odd integers (including negative odds). These ϕ_n give the potential within the appropriate n-dimensional crystal, in that ϕ_n vanishes on the surface of the cube $[-\frac{1}{2}, \frac{1}{2}]^n$, as is required via symmetry within an NaCl-type crystal of any dimension. To render this representation more explicit and efficient, we could write equivalently

$$\phi_n(\mathbf{r}) \;=\; \frac{2^n}{\pi^2} \sum_{m_1,\ldots,m_n\,>\,0,\ \text{odd}} \frac{\cos\,\pi m_1 r_1 \cdots \cos\,\pi m_n r_n}{m_1^2 + \cdots + m_n^2}.$$

It is also useful that – owing to the symmetry arising because the summation indices are odd – we can replace in a cavalier way the cosine product in (7.2.16) with a simple exponential:

$$\phi_n(\mathbf{r}) \;=\; \frac{1}{\pi^2} \sum_{\mathbf{m}\,\in\,\mathbb{O}^n} \frac{e^{i\pi\mathbf{m}\cdot\mathbf{r}}}{m^2}. \tag{7.2.17}$$

7.2.3 Fast series for ϕ_n

From previous work [11] we know a computational series

$$\phi_n(\mathbf{r}) \;=\; \frac{1}{2\pi} \sum_{\mathbf{R}\,\in\,\mathbb{O}^{n-1}} \frac{\sinh[\pi R(1/2 - |r_1|] \prod_{k=1}^{n-1} \cos\,\pi R_k r_{k+1}}{R\cosh(\pi R/2)}, \tag{7.2.18}$$

suitable for any nonzero vector $\mathbf{r} \in [-\frac{1}{2}, \frac{1}{2}]^n$. The work [11] also gives an improvement in the case of $n = 2$ dimensions, namely the following form (see Fig. 7.1) for which the logarithmic singularity at the origin has been siphoned off:

$$\phi_2(x, y) \;=\; \frac{1}{4\pi} \log \frac{\cosh\,\pi x + \cos\,\pi y}{\cosh\,\pi x - \cos\,\pi y} - \frac{2}{\pi} \sum_{\mathbf{m}\,\in\,\mathbb{O}^+} \frac{\cosh\,\pi m x \cos\,\pi m y}{m(1 + e^{\pi m})}. \tag{7.2.19}$$

These series, (7.2.18) and (7.2.19) are valid, respectively, for $r_1, x \in [-1, 1]$. For clarification, we give here the fast series for $n = 3$ dimensions:

$$\phi_3(x, y, z) \;=\; \frac{2}{\pi} \sum_{p,q\,>\,0,\ \text{odd}} \frac{\sinh\left[\frac{\pi}{2}\sqrt{p^2+q^2}\ (1 - 2|x|)\right] \cos\,\pi p y \cos\,\pi q z}{\sqrt{p^2+q^2}\cosh\left(\frac{\pi}{2}\sqrt{p^2+q^2}\right)}. \tag{7.2.20}$$

7.2.4 Closed form for the 'natural' Madelung constant $\mathcal{N}_2$

The natural Madelung constant for $n = 2$ dimensions has also been found, on the basis of (7.2.19) (see [11]), to take the value

$$\mathcal{N}_2 \;=\; \frac{1}{4\pi}\log\frac{4\,\Gamma^3(\frac{3}{4})}{\pi^3}. \tag{7.2.21}$$

We remind ourselves that this closed form was achieved by contemplating the limiting process $\mathbf{r} \to \mathbf{0}$ and hence by Coulomb-singularity removal. The derivation of the above $\mathcal{N}_2$ form depends on the relation

$$\frac{4\,\Gamma^3\left(\frac{3}{4}\right)}{\pi^3} \;=\; \frac{\sqrt{2}}{\mathrm{K}^{3/2}\left(\frac{1}{\sqrt{2}}\right)\pi^{3/4}}.$$

We also record the following numerically effective Mellin transform for $n > 2$:

$$\mathcal{N}_n \;=-\frac{1}{4\pi}\int_0^\infty \left[1-\theta_4^n\left(\mathrm{e}^{-\pi x}\right)\right] x^{n/2-2}\,dx \;<0, \tag{7.2.22}$$

where the integral is positive since $0 < \theta_4(q) < 1$ for $0 \le q \le 1$. From this the large-n behavior of $\mathcal{N}_n$ may be estimated as

$$\mathcal{N}_n \asymp -\frac{\Gamma(\frac{1}{2}n-1)}{\pi^{n/2}}\cdot\left[\frac{n}{2}-\frac{n(n-1)}{2^{n/2}}+\cdots\right], \tag{7.2.23}$$

on making the approximations

$$\theta_4\,(q) = 1-2q+O\left(q^4\right)$$

and

$$1-x^n = -n(x-1)+\frac{n(n-1)}{2}\,(x-1)^2+O\big((x-1)^3\big)$$

and then integrating term by term. For instance, from (7.2.22) we compute

$$N_{100} = -8.6175767047403040779\ldots\times 10^{37}$$

while the asymptotic (7.2.23) gives

$$\mathcal{N}_{100} \asymp -8.6175767047403038\ldots\times 10^{37}.$$

7.2.5 Closed forms for the ϕ_2-potential

Theorem 7.1 *It can be proved that*

$$\phi_2(\tfrac{1}{3}, \tfrac{1}{3}) = \frac{1}{8\pi} \log\left(1 + \frac{2}{\sqrt{3}}\right), \tag{7.2.24}$$

$$\phi_2(\tfrac{1}{4}, \tfrac{1}{4}) = \frac{1}{4\pi} \log(1 + \sqrt{2}), \tag{7.2.25}$$

$$\phi_2(\tfrac{1}{3}, 0) = \frac{1}{8\pi} \log(3 + 2\sqrt{3}). \tag{7.2.26}$$

Proof Consider, for $s > 0$,

$$V_2(x, y; s) := \sum_{m,n=-\infty}^{\infty} \frac{\cos \pi(2m+1)x \cos \pi(2n+1)y}{[(2m+1)^2 + (2n+1)^2]^s}. \tag{7.2.27}$$

This V_2-function is related to ϕ_2 by $V_2(x, y; 1) = \pi^2 \phi_2(x, y)$. Treating it as a general lattice sum [8], we derive (with a difficulty)

$$V_2\left(\tfrac{1}{3}, \tfrac{1}{3}; s\right) = 2^{-1-s}\Big[-(1 - 2^{-s})(1 - 3^{2-2s})L_1(s)L_{-4}(s) + 3(1 + 2^{-s})L_{-3}(s)L_{12}(s)\Big]. \tag{7.2.28}$$

The L-functions in (7.2.28) are various Dirichlet series; L_1 is the Riemann ζ-function. Note that $1 - 3^{2-2s}$ factors as $(1 + 3^{1-s})(1 - 3^{1-s})$, that $\lim_{s\to 1} (1 - 3^{1-s})L_1(s) = \log 3$, and that

$$L_{-4}(1) = \frac{\pi}{4}, \qquad L_{-3}(1) = \frac{\sqrt{3}\pi}{9}, \qquad L_{12}(1) = \frac{1}{\sqrt{3}} \log(2 + \sqrt{3}). \tag{7.2.29}$$

After gathering everything together we have

$$\phi_2(\tfrac{1}{3}, \tfrac{1}{3}) = \tfrac{1}{\pi^2} V_2(\tfrac{1}{3}, \tfrac{1}{3}, 1) = \tfrac{1}{8\pi} \log\left(\tfrac{3+2\sqrt{3}}{3}\right),$$

which is (7.2.24).

We find more easily that

$$V_2(\tfrac{1}{4}, \tfrac{1}{4}; s) = 2\sum_{m,n=-\infty}^{\infty} \tfrac{(-1)^{m+n}}{[(4m-1)^2+(4n-1)^2]^s} = 2^{1-s} L_{-8}(s)L_8(s) \tag{7.2.30}$$

is a familiar lattice sum [8]. So, with

$$L_{-8}(1) = \frac{\pi}{2\sqrt{2}} \qquad \text{and} \qquad L_8(1) = \frac{1}{\sqrt{2}} \log(1 + \sqrt{2}), \tag{7.2.31}$$

we derive

$$\phi_2(\tfrac{1}{4}, \tfrac{1}{4}) = \tfrac{1}{4\pi} \log(1 + \sqrt{2}),$$

which is (7.2.25). Likewise

$$V_2\left(\tfrac{1}{3}, 0; s\right) = 2^{-1-s}\Big[(1 - 2^{-s})(1 - 3^{2-2s})L_1(s)L_{-4}(s) + 3(1 + 2^{-s})L_{-3}(s)L_{12}(s)\Big], \tag{7.2.32}$$

which yields

$$\phi_2\left(0, \tfrac{1}{3}\right) = \frac{1}{16\pi} \log\left[3(2+\sqrt{3})^2\right] = \frac{\pi}{8} \log(3+2\sqrt{3}),$$

which is (7.2.26). □

Remark: The V_2 lattice sum can be given as a fast series:

$$V_2(x, y; s) := \sum_{m,n \in \mathbb{O}} \frac{\cos \pi m x \cos \pi n y}{(m^2+n^2)^s} \tag{7.2.33}$$

$$= \frac{2^{3/2-s}\pi^s}{\Gamma(s)} \sum_{\substack{n \in \mathbb{O}^+ \\ u \in \mathbb{Z}}} (-1)^u \left(\frac{|u+x|}{n}\right)^{s-1/2} K_{1/2-s}(\pi n|u+x|) \cos \pi n y,$$

where K_ν is a standard modified Bessel function. For $s = 1$ this series collapses further into π^2 times our series (7.2.19) for the Poisson potential ϕ_2.

Using the *integer relation method* PSLQ [7] to hunt for results of the form

$$\exp\left[\pi \phi_2(x, y)\right] \stackrel{?}{=} \alpha, \tag{7.2.34}$$

for α algebraic, we may obtain and further simplify many results such as the following.

Conjecture 7.1 Empirically,

$$\phi_2\left(\tfrac{1}{4}, 0\right) \stackrel{?}{=} \frac{1}{4\pi} \log \alpha \quad \text{where} \quad \frac{\alpha + 1/\alpha}{2} = \sqrt{2}+1,$$

$$\phi_2\left(\tfrac{1}{5}, \tfrac{1}{5}\right) \stackrel{?}{=} \frac{1}{8\pi} \log\left(3 + 2\sqrt{5} + 2\sqrt{5+2\sqrt{5}}\right),$$

$$\phi_2\left(\tfrac{1}{6}, \tfrac{1}{6}\right) \stackrel{?}{=} \frac{1}{4\pi} \log \gamma \quad \text{where} \quad \frac{\gamma + 1/\gamma}{2} = \sqrt{3}+1,$$

$$\phi_2\left(\tfrac{1}{3}, \tfrac{1}{6}\right) \stackrel{?}{=} \frac{1}{4\pi} \log \tau \quad \text{where} \quad \frac{\tau - 1/\tau}{2} = (2\sqrt{3}-3)^{1/4},$$

$$\phi_2\left(\tfrac{1}{8}, \tfrac{1}{8}\right) \stackrel{?}{=} \frac{1}{4\pi} \log\left(\frac{1+\sqrt{2-\sqrt{2}}}{\sqrt[4]{2}-1}\right),$$

$$\phi_2\left(\tfrac{1}{10}, \tfrac{1}{10}\right) \stackrel{?}{=} \frac{1}{4\pi} \log \mu \quad \text{where} \quad \frac{\mu + 1/\mu}{2} = 2+\sqrt{5}+\sqrt{5+2\sqrt{5}};$$

the notation $\stackrel{?}{=}$ indicates that we have only experimental (i.e., extreme-precision numerical) evidence of an equality.

Such hunts are made entirely practicable by (7.2.19). Note that for general x and y we have $\phi_2(y, x) = \phi_2(x, y) = -\phi_2(x, 1-y)$, so we can restrict searches to $\frac{1}{2} > x \geq y > 0$, as illustrated in Figure 7.1. Indeed computations by Glasser and Crandall given in [11] were precipitated from such experiments and led to the following result.

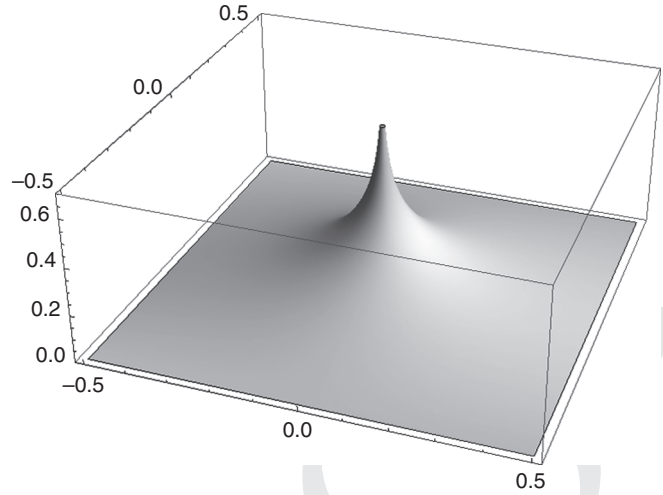

Figure 7.1 High-precision plot of the Monge surface $z = \phi_2(x, y)$, via the fast series (7.2.19), showing the logarithmic singularity at the origin (the plot is adapted from [11]). In this plot, x, y range over the 2-cube $[-\frac{1}{2}, \frac{1}{2}]^2$; from symmetry one need know the ϕ_2 surface only over the octant $\frac{1}{2} > x \geq y > 0$. We are able to establish closed forms for the heights on this surface above certain rational pairs (x, y). As just one example, $\phi_2(\frac{1}{4}, \frac{1}{4}) = \frac{1}{4\pi} \log(1 + \sqrt{2}) \approx 0.0701$.

Theorem 7.2 *For* $z := \dfrac{\pi}{2}(y + ix)$,

$$\phi_2(x, y) = \frac{1}{2\pi} \log \left| \frac{\theta_2(z, q)\theta_4(z, q)}{\theta_1(z, q)\theta_3(z, q)} \right| = \frac{1}{4\pi} \log \left| \frac{1 - \lambda(z)/\sqrt{2}}{1 - 1/[\lambda(z)\sqrt{2}]} \right|, \quad (7.2.35)$$

where

$$\lambda(z) = \frac{\theta_4^2(z, e^{-\pi})}{\theta_3^2(z, e^{-\pi})} = \prod_{n=1}^{\infty} \frac{(1 - 2\cos\, 2z\, q^{2n-1} + q^{4n-2})^2}{(1 + 2\cos\, 2z\, q^{2n-1} + q^{4n-2})^2}, \quad (7.2.36)$$

with $q := e^{-\pi}$.

Hence, the presumption that, for rational x, y, (7.2.34) is always algebraic is equivalent to the provable conjecture that, for all $z = \frac{\pi}{2}(y+ix)$ with x, y rational, $\lambda(z)$ in (7.2.36) is algebraic, and this is proved in [1, Theorem 10]. How to provide computationally assisted proofs of results such as those of Conjecture 7.1 is also discussed in [1].

7.2.6 Closed forms for $n = 3, 4$ dimensions

The only nontrivial closed-form evaluation of ϕ_3 of which we are aware is that of Forrester and Glasser [8, 13]. Namely,

$$4\pi\phi_3(\mathbf{1/6}) \;=\; \mathcal{M}_3(1, \mathbf{1/6}) \;=\; \sum_{\mathbf{m}\in\mathbb{Z}^3} \frac{(-1)^{\mathbf{1}\cdot\mathbf{m}}}{|\mathbf{m}-\mathbf{1/6}|} = \sqrt{3}.$$

References

[1] D. H. Bailey, J. M. Borwein, R. E. Crandall, and I. J. Zucker. Lattice sums arising from the Poisson equation. 2012. Preprint.

[2] A. Baldereschi, G. Senatore, and I. Oriani. Madelung energy of the Wigner crystal on lattices with non-equivalent sites. *Solid State Commum.*, 81:21–22, 1992.

[3] L. Bonsall and A. A. Maradudin. Some static and dynamical properties of a two-dimensional Wigner crystal. *Phys. Rev. B*, 15:1959–1973, 1977.

[4] M. Born and R. D. Misra. On the stability of crystal lattices. IV. *Proc. Camb. Phil. Soc.*, 36:466–478, 1940.

[5] D. Borwein, J. M. Borwein, and R. Shail. Analysis of certain lattice sums. *J. Math. Anal. Appl.*, 143:126–137, 1989.

[6] D. Borwein, J. M. Borwein, R. Shail, and I. J. Zucker. Energy of static electron lattices. *J. Phys. A: Math. Gen.*, 21:1519–1531, 1988.

[7] J. M. Borwein and D. H. Bailey. *Mathematics by Experiment: Plausible Reasoning in the 21st Century, 2nd edition*. A. K. Peters, 2008.

[8] J. M. Borwein and P. B. Borwein. *Pi and the AGM – A Study in Analytic Number Theory and Computational Complexity*. Wiley, New York, 1987.

[9] E. Cockayne. Comment on 'stability of the Wigner electron crystal on the perovskite lattice'. *J. Phys. Condens. Matter*, 3:8757, 1991.

[10] R. A. Coldwell-Horsfall and A. A. Maradudin. Zero point energy of an electron lattice. *J. Math. Phys.*, 1:395–404, 1960.

[11] R. E. Crandall. The Poisson equation and 'natural' Madelung constants. 2012. Preprint.

[12] L. L. Foldy. Electrostatic stability of Wigner and Wigner–Dyson lattices. *Phys. Rev. B*, 17:4889–4894, 1978.

[13] P. J. Forrester and M. L. Glasser. Some new lattice sums including an exact result for the electrostatic potential within the NaCl lattice. *J. Phys. A*, 15:911–914, 1982.

[14] K. Fuchs. A quantum mechanical investigation of the cohesive forces of metallic copper. *Proc. Roy. Soc. London A*, 151:585–602, 1935.

[15] F. Hund. Versuch einer Ableitung der Gittertypen aus der Vorstellung des isotropen polarisierbaren Ions. *Z. Phys.*, 34:833–857, 1925.

[16] F. Hund. Vergleich der elektrostatischen Energien einiger Ionengitter. *Z. Phys.*, 94:11–21, 1935.

[17] E. P. Wigner. On the interaction of electrons in metals. *Phys. Rev.*, 46:1002–1011, 1934.

[18] I. J. Zucker. Stability of the Wigner electron crystal on the perovskite lattice. *J. Phys. Condens. Matter*, 3:2595–2596, 1991.

[19] I. J. Zucker and M. M. Robertson. Systematic approach to the evaluation of $\sum_{(m,n\neq 0,0)}(am^2+bmn+cn^2)^{-s}$. *J. Phys. A*, 9:1215–1225, 1976.