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Analysis of Certain Lattice Sums*

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1. INTRODUCTION

The genesis of this paper lies in the physical model we now describe. We believe the theorems presented to be of independent mathematical interest. In 1934 Wigner [7] introduced the concept of an electron gas bathed in a compensating background of positive charge as a model for a metal. He stated that in the static case the electrons would form a b.c.c. lattice in the background of positive charge. In 1938 he presented a quantitative treatment of this problem, following a calculation by Fuchs [5], who showed that for a given number density, the b.c.c. lattice was the most stable of the three common cubic structures, namely *s.c.*, *b.c.c.*, and *f.c.c.* lattices—see Coldwell-Horsfall and Maradudin [3]. The evaluation of U (*lattice*)—the energy of an electron in a given lattice—involved finding by some means or other the difference of two divergent quantities. Of these, one term U_1 measures the interaction of an electron with all the other electrons on their lattice sites. The second term U_2 measures the interaction of an electron with the compensating positive background charge. Thus

$$U\,(\text{lattice}) = U_1 - U_2,$$

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where

$$U_1 = \frac{e^2}{a_0} \sum{}' (j^2 + k^2 + l^2)^{-1/2} \tag{1}$$

and

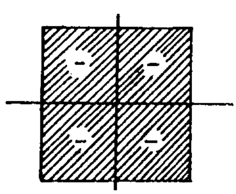
$$U_2 = ne^2 \int_{(\Omega)} (x^2 + y^2 + z^2)^{-1/2} \, dx \, dy \, dz. \tag{2}$$

In (1), a_0 is some lattice parameter and the summation is over all integers (j, k, l) relevant to the given lattice structure. Here and throughout $\sum'$ indicates that undefined (i.e., infinite) terms in the summand are avoided. In (2), n is the number density and Ω is the normalization volume of the given lattice.

In a previous paper (Borwein *et al.* [2]) a new approach to evaluating the static lattice energy of any given Wigner lattice was proposed. The new method is much simpler and faster than the traditional one and, after normalization, consists of computing the value, $\alpha(\frac{1}{2})$, of the analytic continuation of the appropriate three-dimensional zeta function $\alpha(s) := \sum'_{\text{lattice}} (j^2 + k^2 + l^2)^{-s}$. Two-dimensional Wigner lattices can be dealt with in the same manner. The method yields the known value in each case in which traditional techniques have been used.

This leaves open, however, the question of what, if any, underlying direct limiting process produces the same answer? In two dimensions we find our answers correspond to a simple and intuitively plausible way of evaluating the lattice energies (Theorem 1 below). In three dimensions, somewhat surprisingly, we show that this is not the case (Theorem 3 below).

We consider the following model in d-dimensions (in reality $d = 2, 3$). In our model, point charges are located at lattice sites and are surrounded by an equal amount of opposite charge uniformly distributed over d-dimensional cubes centred at the lattice points and of side equal to one lattice spacing. This is illustrated below in two dimensions, where the shaded portion represents positive charge of value equal to the point negative charge but uniformly distributed over a square.



For the simple cubic lattice we shall analyse the behavior of the limit as $N \to \infty$ of

$$\sigma_N(s) := \sum_{-N}^{N} \cdots \sum_{-N}^{N}{}' (n_1^2+n_2^2+\cdots+n_d^2)^{-s}$$
$$- \int_{-(N+1/2)}^{N+1/2} \cdots \int_{-(N+1/2)}^{N+1/2} (x_1^2+x_2^2+\cdots+x_d^2)^{-s}\, dx_1 \cdots dx_d$$

although a priori the limit need not exist. Electrical neutrality is maintained throughout the limiting process. (Using $N+\frac{1}{2}$ is also technically advantageous.) We denote the sum and integral above by $\alpha_N(s)$ and $\beta_N(s)$, respectively.

2. Two-Dimensional Lattices

In two dimensions we analyse a more general situation by considering a two-dimensional positive definite quadratic form $Q(x, y) := ax^2 + 2bxy + cy^2$, and examining the behaviour of $\sigma_N(s) := \alpha_N(s) - \beta_N(s)$, where

$$\alpha_N(s) := \sum_{\max(|m|,|n|) \leqslant N}{}' Q(m, n)^{-s},$$

$$\beta_N(s) := \int_{\max(|x|,|y|) \leqslant N+1/2} Q(x, y)^{-2}\, dx\, dy.$$

When $a=1$, $b=0$, $c=1$, this reduces to the two dimensional square case above. Similarly, when $a=1$, $b=\frac{1}{2}$, $c=1$, this yields a triangular lattice sum (see [2]). We write $\sigma(s) := \lim_{N\to\infty} \sigma_N(s)$, $\alpha(s) := \lim_{N\to\infty} \alpha_N(s)$ whenever these limits exist. Note that $\sigma(\frac{1}{2})$ may be viewed as a generalization of Euler's constant.

THEOREM 1. *For any positive definite form Q, $\sigma(s) := \lim_{N\to\infty} \sigma_N(s)$ exists in the strip $0 < \operatorname{re} s < 1$ and coincides therein with the analytic continuation of $\alpha(s)$. In particular, $\lim_{N\to\infty} \sigma_N(\frac{1}{2}) = \alpha(\frac{1}{2})$.*

Proof. Let $\Omega := \{s \mid \operatorname{re} s > \varepsilon > 0,\ |s| < R\}$. All order terms will be uniform with respect to s in the bounded region Ω. For $N \geqslant 1$, we have

$$\delta_N(s) := \sigma_N(s) - \sigma_{N-1}(s)$$
$$= \sum_{\max(|m|,|n|)=N} \int_{\max(|x|,|y|) \leqslant 1/2} (Q(m, n)^{-s} - Q(m+x, n+y)^{-s})\, dx\, dy.$$

Putting $f(x, y) = Q(m+x, n+y)^{-s}$ with $\max(|m|, |n|) = N$ and $\max(|x|, |y|) \leqslant \frac{1}{2}$, we get $f(x, y) - f(0, 0) = xf_x(0, 0) + yf_y(0, 0) + O(N^{-2\varepsilon-2})$, since

$$\begin{aligned} f_{xx} &= s(s+1)\, Q(m+x, n+y)^{-s-2}(2a(m+x) + 2b(n+y))^2 \\ &\quad - 2asQ(m+x, n+y)^{-s-1} \\ &= O(N^{-2\varepsilon-2}) \end{aligned}$$

and likewise f_{xy} and f_{yy} are both $O(N^{-2\varepsilon-2})$. Note that the positive definiteness of Q implies that $Q(m+x, n+y)^{-1} = O(N^{-2})$. It now follows that

$$\begin{aligned} &\int_{\max(|x|, |y|) \leqslant 1/2} (f(0, 0) - f(x, y))\, dx\, dy \\ &\quad = -\int_{\max(|x|, |y|) \leqslant 1/2} (xf_x(0, 0) + yf_y(0, 0))\, dx\, dy + O(N^{-2\varepsilon-2}) \\ &\quad = 0 + O(N^{-2\varepsilon-2}) = O(N^{-2\varepsilon-2}), \end{aligned}$$

and hence that $|\delta_N(s)| \leqslant MN^{-2\varepsilon-1}$, where M is independent of s and N for $s \in \Omega$. Since $\delta_N(s)$ is an entire function it follows, by the Weierstrass M-test, that $\delta(s) := \sum_{N=1}^{\infty} \delta_N(s)$ is analytic in Ω and so in the half-plane $\operatorname{re} s > 0$, and the series is convergent in this half-plane.

Now let

$$I_1(s) := \int_{Q(x, y) < 1} Q(x, y)^{-s}\, dx\, dy, \quad I_2(s) := \int_{Q(x, y) > 1} Q(x, y)^{-s}\, dx\, dy.$$

Then, for $\operatorname{re} s < 1$,

$$\begin{aligned} I_1(s) &= |Q|^{-1/2} \int_{x^2+y^2<1} (x^2+y^2)^{-s}\, dx\, dy \\ &= |Q|^{-1/2} \int_0^{2\pi} d\theta \int_0^1 r^{1-2s}\, dr \\ &= |Q|^{-1/2}\, \pi/(1-s), \qquad \text{where} \quad |Q| = ac - b^2; \end{aligned} \tag{3}$$

and, for $\operatorname{re} s > 1$,

$$I_2(s) = |Q|^{-1/2}\, \pi/(s-1). \tag{4}$$

Thus $I_1(s)$ and $I_2(s)$ extend analytically to the whole plane and $I_1(s) = -I_2(s)$ therein. Now, for re $s < 1$,

$$\sigma(s) + I_1(s) = \lim_{N \to \infty} \sigma_N(s) + I_1(s) = \delta(s) - \beta_0(s) + I_1(s),$$

which is analytic for re $s > 0$. Further, for re $s < 1$,

$$\beta_N(s) - I_1(s) = \int_{\substack{\max(|x|,|y|) \leqslant N+1/2 \\ Q(x,y) > 1}} Q(x, y)^{-s} \, dx \, dy$$

and the final integral is an entire function which tends to $I_2(s)$ in the half-plane re $s > 1$, though $\beta_N(s)$ itself is infinite therein. Hence, for re $s > 1$,

$$\sigma(s) + I_1(s) = \lim_{N \to \infty} \alpha_N(s) - I_2(s) = \alpha(s) + I_1(s).$$

It follows that $\alpha(s)$ has an analytic continuation to the half-plane re $s > 0$—see also [4, Vol. 3, pp. 42 and 129]. Consequently $\sigma(s) = \alpha(s)$ for $0 < \text{re}\, s < 1$. ∎

Remarks. In effect the integral plays no role in the final answer. The theorem shows that for two dimensional Wigner lattices, the answer obtained by analytic continuation—or by classical methods—coincides with that given by a simple direct limiting process. In addition, the last two equations in the proof of the theorem actually provide a physically based analytic continuation of $\alpha(s)$ to the right half-plane.

EXAMPLE. (a) For the square lattice $\alpha(s) = 4\zeta(s)\,\xi(s)$ with

$$\zeta(s) := 1 + 2^{-s} + 3^{-s} + 4^{-s} + \cdots \qquad (\text{re}\, s > 1)$$

$$= \frac{1}{1 - 2^{1-s}} (1 - 2^{-s} + 3^{-s} - 4^{-s} + \cdots) \qquad (\text{re}\, s > 0)$$

and

$$\xi(s) := 1 - 3^{-s} + 5^{-s} - 7^{-s} + \cdots \qquad (\text{re}\, s > 0).$$

Thus we have that

$$\sigma(\tfrac{1}{2}) = 4\zeta(\tfrac{1}{2})\,\xi(\tfrac{1}{2}) = -3.900264924 \cdots.$$

(b) For the triangular lattice $\alpha(s) = 6\zeta(s)\,\eta(s)$, where

$$\eta(s) := 1 - 2^{-s} + 4^{-s} - 5^{-s} + \cdots \qquad (\text{re}\, s > 0).$$

Thus we have that

$$\sigma(\tfrac{1}{2}) := 6\zeta(\tfrac{1}{2})\,\eta(\tfrac{1}{2}) = -4.2134227006\cdots. \quad \blacksquare$$

The factorization of α in these cases is discussed in detail in [2]. The cases have been dealt with by the traditional methods by Bonsall and Maradudin [1], who considered a more general Bravais–Wigner model also covered by Theorem 1.

To illustrate the robustness of taking an analytic limit we provide another limiting procedure for the square lattice. We consider

$$\psi_N(s) := \sum_{1 \leqslant m^2+n^2 \leqslant N} (m^2+n^2)^{-s} - \int_{x^2+y^2 \leqslant N} (x^2+y^2)^{-s}\,dx\,dy.$$

THEOREM 2. *The limit* $\psi(s) := \lim_{N\to\infty} \psi_N(s)$ *exists in the strip* $\frac{1}{3} < \operatorname{re} s < 1$ *and coincides therein with the analytic continuation of* $\alpha(s)$. *In particular*, $\lim_{N\to\infty} \psi_N(\frac{1}{2}) = \psi(\frac{1}{2}) = \alpha(\frac{1}{2}) = 4\zeta(\frac{1}{2})\,\xi(\frac{1}{2})$.

Proof. Let $\Omega := \{s \mid \operatorname{re} s > \frac{1}{3}, |s| < R\}$. All order terms will be uniform with respect to s in the bounded region Ω. Let

$$\psi_N^*(s) := \sum_{1 \leqslant m^2+n^2 \leqslant N} (m^2+n^2)^{-s} - \int_{1 \leqslant x^2+y^2 \leqslant N} (x^2+y^2)^{-s}\,dx\,dy.$$

Then

$$\psi_N^*(s) = \sum_{n=1}^{N} r(n)\,n^{-s} - \int_0^{2\pi} d\theta \int_1^{\sqrt{N}} r^{1-2s}\,dr = \sum_{n=1}^{N} r(n)\,n^{-s} - \pi \int_1^N u^{-s}\,du,$$

where $r(n)$ is the number of ways of expressing n as a sum of two integer squares. Let $t_n = r(1) + r(2) + \cdots + r(n)$. It is known that $t_n = \pi n + O(n^\gamma)$, where $\frac{1}{4} \leqslant \gamma < \frac{1}{3}$ [6, p. 272; 4, Vol. 2, pp. 253 and 257]. Hence, for $s \in \Omega$ and $M > N \to \infty$,

$$\begin{aligned}
&\psi_M^*(s) - \psi_{N-1}^*(s)\\
&\quad= \sum_{n=N}^{M} r(n)\,n^{-s} - \pi \int_N^M u^{-s}\,du\\
&\quad= \sum_{n=N}^{M} t_n(n^{-s} - (n+1)^{-s}) + t_M(M+1)^{-s} - t_{N-1}N^{-s} - \pi \int_N^M u^{-s}\,du\\
&\quad= \sum_{n=N}^{M} t_n n^{-s-1}(s + O(1/n)) + \pi(M^{1-s} - N^{1-s}) - \pi \int_N^M u^{-s}\,du + o(1)
\end{aligned}$$

$$= \pi s \sum_{n=N}^{M} n^{-s} + \sum_{n=N}^{M} O(n^{\gamma-4/3}) + \pi(M^{1-s} - N^{1-s}) - \pi \int_N^M u^{-s}\, du + o(1)$$

$$= \pi s \int_N^M u^{-s}\, du + \sum_{n=N}^{M} O(n^{\gamma-4/3}) + \pi(M^{1-s} - N^{1-s}) - \pi \int_N^M u^{-s}\, du + o(1)$$

$$= \pi(M^{1-s} - N^{1-s}) - \pi(s-1) \int_N^M u^{-s}\, du + \sum_{n=N}^{M} O(n^{\gamma-4/3}) + o(1)$$

$$= \sum_{n=N}^{M} O(n^{\gamma-4/3}) + o(1) = o(1).$$

Thus $\psi_N^*(s)$ tends uniformly in Ω to $\psi^*(s)$ say. Since $\psi_N^*(s)$ is entire, $\psi^*(s)$ is analytic in Ω and therefore in the half-plane $\operatorname{re} s > \frac{1}{3}$. Further, for $\operatorname{re} s > 1$,

$$\begin{aligned}
\psi^*(s) &= \lim_{N\to\infty} \sum_{1 \leqslant m^2+n^2 \leqslant N} (m^2+n^2)^{-s} \\
&\quad - \lim_{N\to\infty} \int_{1 \leqslant x^2+y^2 \leqslant N} (x^2+y^2)^{-s}\, dx\, dy \\
&= \alpha(s) - \lim_{N\to\infty} \pi \int_1^N u^{-s}\, du \qquad \text{(using (4))} \\
&= \alpha(s) - \pi/(s-1);
\end{aligned}$$

and so $\alpha(s) = \psi^*(s) - \pi/(1-s)$ for $\operatorname{re} s > \frac{1}{3}$. On the other hand, for $\frac{1}{3} < \operatorname{re} s < 1$,

$$\begin{aligned}
\psi_N(s) &= \psi_N^*(s) - \int_{x^2+y^2 \leqslant 1} (x^2+y^2)^{-s}\, dx\, dy \\
&= \psi_N^*(s) - \pi/(1-s) \qquad \text{(using (3))}
\end{aligned}$$

so that $\psi(s) = \psi^*(s) - \pi/(1-s)$. Hence $\psi(s) = \alpha(s)$ for $\frac{1}{3} < \operatorname{re} s < 1$. ∎

3. Three-Dimensional Lattices

We turn now to three dimensions. We show that, even when we restrict attention to the simple cubic lattice, a curious anomaly occurs. We consider $\sigma_N(s) = \alpha_N(s) - \beta_N(s)$, where

$$\alpha_N(s) := \sum_{\max(|m|,|n|,|p|) \leqslant N}{}' (m^2+n^2+p^2)^{-s},$$

$$\beta_N(s) := \int_{\max(|x|,|y|,|z|) \leqslant N+1/2} (x^2+y^2+z^2)^{-s}\, dx\, dy\, dz.$$

As before we write $\sigma(s) := \lim_{N\to\infty} \sigma_N(s)$, $\alpha(s) := \lim_{N\to\infty} \alpha_N(s)$ whenever these limits exist. Though in general we use the same symbol to denote a function and its analytic continuation, in any case where a defined function value differs from the value of its analytic continuation we give precedence to the defined function value (as with $\sigma(s)$ at $s = \frac{1}{2}$ in the following theorem).

THEOREM 3. *The limit* $\sigma(s) := \lim_{N\to\infty} \sigma_N(s)$ *exists exactly for* $\frac{1}{2} < \operatorname{re} s < \frac{3}{2}$ *and for* $s = \frac{1}{2}$. *For* $\frac{1}{2} < \operatorname{re} s < \frac{3}{2}$, $\sigma(s)$ *coincides with the analytic continuation of* $\alpha(s)$, *but* $\sigma(s)$ *is discontinuous at* $\frac{1}{2}$. *Indeed,*

$$\sigma(\tfrac{1}{2}) - \pi/6 = \alpha(\tfrac{1}{2}) = -2.837297\cdots = \lim_{s\to 1/2+} \sigma(s).$$

Proof. Let $\Omega := \{s \mid \operatorname{re} s > \varepsilon > 0, |s| < R\}$. All order terms will be uniform with respect to s in the bounded region Ω. For $N \geqslant 1$, we have $\delta_N(s) := \sigma_N(s) - \sigma_{N-1}(s) = \sum_{\max(|m|,|n|,|p|)=N} I(m, n, p)$, where

$$I(m, n, p) = \int_{\max(|x|,|y|,|z|) \leqslant 1/2} \{(m^2 + n^2 + p^2)^{-s} - ((m+x)^2 + (n+y)^2 + (p+z)^2)^{-s}\}\, dx\, dy\, dz.$$

Putting $f(x, y, z) = ((m+x)^2 + (n+y)^2 + (p+z)^2)^{-s}$ with $\max(|m|, |n|, |p|) = N$ and $\max(|x|, |y|, |z|) \leqslant \frac{1}{2}$, we get, much as in the proof of Theorem 1,

$$f(x, y, z) - f(0, 0, 0) = \left(x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} + z\frac{\partial}{\partial z}\right) f + \frac{1}{2}\left(x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} + z\frac{\partial}{\partial z}\right)^2 f + O(N^{-2\varepsilon-3}),$$

the partial derivatives being evaluated at $x = y = z = 0$. Integrating over the unit cube $\max(|x|, |y|, |z|) \leqslant \frac{1}{2}$ eliminates terms of odd order in x, y, or z to yield

$$\begin{aligned} I(m, n, p) &= \int_{\max(|x|,|y|,|z|) \leqslant 1/2} (f(0,0,0) - f(x, y, z))\, dx\, dy\, dz \\ &= -\frac{1}{2} \int_{\max(|x|,|y|,|z|) \leqslant 1/2} (ax^2 + by^2 + cz^2)\, dx\, dy\, dz + O(N^{-2\varepsilon-3}) \\ &= -\frac{1}{24}(a + b + c) + O(N^{-2\varepsilon-3}), \end{aligned}$$

where $a = f_{xx}(0, 0, 0)$, $b = f_{yy}(0, 0, 0)$, $c = f_{zz}(0, 0, 0)$. It is easily verified that $a + b + c = 2s(2s - 1)(m^2 + n^2 + p^2)^{-s-1}$ and hence

$$\begin{aligned}\delta_N(s) &= \frac{1}{12} s(1-2s) \sum_{\max(|m|,|n|,|p|)=N} (m^2+n^2+p^2)^{-s-1} + O(N^{-2\varepsilon-1})\\ &= \frac{1}{2} s(1-2s)\, N^{-2s} V_N(s) + O(N^{-2\varepsilon-1}),\end{aligned}$$

where

$$\begin{aligned}V_N(s) &:= \frac{1}{N^2} \sum_{\substack{-N \leqslant m < N\\ -N \leqslant n < N}} (1 + (m/N)^2 + (n/N)^2)^{-s-1}\\ &= \frac{1}{6N^2} \sum_{\max(|m|,|n|,|p|)=N} ((m/N)^2 + (n/N)^2 + (p/N)^2)^{-s-1} + O(N^{-1}).\end{aligned}$$

Now let

$$V(s) := \int_{\max(|x|,|y|) \leqslant 1} (1 + x^2 + y^2)^{-s-1}\, dx\, dy.$$

Then, for $\operatorname{re} s \geqslant -2$,

$$\begin{aligned}&|V_N(s) - V(s)|\\ &\quad = \left| \sum_{\substack{-N \leqslant m < N\\ -N \leqslant n < N}} \int_{\substack{m \leqslant Nx \leqslant m+1\\ n \leqslant Ny \leqslant n+1}} \{(1 + (m/N)^2 + (n/N)^2)^{-s-1} \right.\\ &\qquad \left. - (1 + x^2 + y^2)^{-s-1}\}\, dx\, dy \right|\\ &\quad \leqslant \sum_{\substack{-N \leqslant m < N\\ -N \leqslant n < N}} 4|s+1|\, N^{-3} = 16|s+1|\, N^{-1}.\end{aligned}$$

It follows that

$$\delta_N(s) = \tfrac{1}{2} s(1-2s)\, N^{-2s} V(s) + W_N(s), \tag{5}$$

where $V(s)$ and $W_N(s)$ are entire functions and $W_N(s) = O(N^{-2\varepsilon-1})$ in Ω. Thus, by the Weierstrass M-test,

$$\delta(s) := \sum_{n=1}^{\infty} \delta_n(s) = \frac{1}{2} s(1-2s)\, \zeta(2s)\, V(s) + W(s)$$

in the half-plane $\operatorname{re} s > \frac{1}{2}$; the series being convergent therein, and $W(s) := \sum_{n=1}^{\infty} W_n(s)$ is analytic in Ω and hence for $re\, s > 0$. Since $\zeta(2s)$ has a simple pole with residue 1 at $s = \frac{1}{2}$, it follows that

$$\lim_{s \to 1/2+} \delta(s) = W(\tfrac{1}{2}) - \tfrac{1}{4} V(\tfrac{1}{2}).$$

On the other hand, by (5), $\delta_n(\frac{1}{2}) = W_n(\frac{1}{2})$ and so

$$\sum_{n=1}^{\infty} \delta_n\left(\frac{1}{2}\right) = W\left(\frac{1}{2}\right) = \lim_{s \to 1/2+} \delta(s) + \frac{1}{4} V\left(\frac{1}{2}\right). \tag{6}$$

Observe now that, for $\operatorname{re} s < \frac{3}{2}$,

$$\begin{aligned}
\beta_N(s) &= (N+1/2)^{3-2s} \int_{\max(|x|,|y|,|z|) \leqslant 1} (x^2+y^2+z^2)^{-s}\, dx\, dy\, dz \\
&= 2(N+1/2)^{3-2s} \int_0^1 dz \int_{\max(|x|,|y|) \leqslant 1} (x^2+y^2+z^2)^{-s}\, dx\, dy \\
&= 6(N+1/2)^{3-2s} \int_0^1 dz \int_{\max(|x|,|y|) \leqslant z} (x^2+y^2+z^2)^{-s}\, dx\, dy \\
&= 6(N+1/2)^{3-2s} \int_0^1 z^{2-2s}\, dz \int_{\max(|x|,|y|) \leqslant 1} (1+x^2+y^2)^{-s}\, dx\, dy \\
&= 6(N+1/2)^{3-2s} V(s-1)/(3-2s).
\end{aligned}$$

It follows that, for $\frac{1}{2} < \operatorname{re} s < \frac{3}{2}$,

$$\begin{aligned}
\sigma(s) := \lim_{N \to \infty} \sigma_N(s) &= \delta(s) + \sigma_0(s) = \delta(s) - \beta_0(s) \\
&= \delta(s) + 3\, \frac{4^{s-1}}{2s-3}\, V(s-1) \\
&= \frac{1}{2}\, s(1-2s)\, \zeta(2s)\, V(s) + W(s) + 3\, \frac{4^{s-1}}{2s-3}\, V(s-1),
\end{aligned} \tag{7}$$

which is meromorphic in the half-plane $\operatorname{re} s > 0$ with a simple pole at $s = \frac{3}{2}$. Further, for $\operatorname{re} s < \frac{3}{2}$,

$$\beta_N(s) - \beta_0(s) = 3\, \frac{2(N+1/2)^{3-2s} - 4^{s-1}}{3-2s}\, V(s-1),$$

which is entire. Thus $\beta_N(s) - \beta_0(s) = \beta_N(s) + 3 \cdot 4^{s-1} V(s-1)/(2s-3)$ which is defined for $\operatorname{re} s < \frac{3}{2}$ and extends to an entire function which tends to

$3 \cdot 4^{s-1} V(s-1)/(2s-3)$ in the half-plane $\operatorname{re} s > \frac{3}{2}$, though $\beta_N(s)$ itself is infinite therein. Hence, for $\operatorname{re} s > \frac{3}{2}$,

$$\begin{aligned}\delta(s) &= \sigma(s) - 3\,\frac{4^{s-1}}{2s-3}\,V(s-1)\\ &= \lim_{N\to\infty} \alpha_N(s) - 3\,\frac{4^{s-1}}{2s-3}\,V(s-1)\\ &= \alpha(s) - 3\,\frac{4^{s-1}}{2s-3}\,V(s-1)\end{aligned}\tag{8}$$

and $\alpha(s)$ is known to have an analytic continuation to the half-plane $\operatorname{re} s > 0$. In (8), $\sigma(s)$ is the analytic continuation afforded by (7) of $\sigma(s)$ from the strip $\frac{1}{2} < \operatorname{re} s < \frac{3}{2}$. It follows that $\sigma(s) = \alpha(s)$ for $\frac{1}{2} < \operatorname{re} s < \frac{3}{2}$ and that

$$\alpha(1/2) = \lim_{s\to 1/2+} \sigma(s).$$

On the other hand, by (6),

$$\begin{aligned}&\lim_{N\to\infty} \sigma_N(\tfrac{1}{2}) - \lim_{s\to 1/2+} \sigma(s)\\ &\quad = \sigma(\tfrac{1}{2}) - \lim_{s\to 1/2+} \sigma(s)\\ &\quad \sum_{n=1}^{\infty} \delta_n(\tfrac{1}{2}) - \lim_{s\to 1/2+} \delta(s) = \tfrac{1}{4} V(\tfrac{1}{2}).\end{aligned}$$

Further, $\sigma(s)$ is defined as a direct limit only in the strip $\frac{1}{2} < \operatorname{re} s < \frac{3}{2}$ and at the point $s = \frac{1}{2}$, because $\sum_{n=1}^{\infty} n^{-2s}$ is divergent when $\operatorname{re} s \leqslant \frac{1}{2}$ and $\int_{\max(|x|,|y|,|z|) \leqslant N+1/2} (x^2+y^2+z^2)^{-s}\,dx\,dy\,dz$ is divergent when $\operatorname{re} s \geqslant \frac{3}{2}$.

It remain only to prove that $V(\frac{1}{2}) = 2\pi/3$, and this can be done as follows. Changing to polar coordinates we have

$$V(s) = 4\int_0^{\pi/4} d\theta \int_0^{\sec\theta} 2r(1+r^2)^{-s-1}\,dr = \frac{4}{s}\left(\frac{\pi}{4} - J(s)\right),$$

where

$$\begin{aligned}J(s) &= \int_0^{\pi/4} (1+\sec^2\theta)^{-s}\,d\theta = \int_0^{\pi/4} (2-\sin^2\theta)^{-s}(\cos\theta)^{2s}\,d\theta\\ &= \int_0^{1/\sqrt{2}} (2-t^2)^{-s}(1-t^2)^{s-1/2}\,dt \qquad (\sin\theta = t)\\ &= 2^{-s+1/2}\int_0^{\pi/6} (\cos u)^{1-2s}(1-2\sin^2 u)^{s-1/2}\,du \qquad (t = \sqrt{2}\sin u).\end{aligned}$$

Hence $J(\frac{1}{2}) = \pi/6$ and so $V(\frac{1}{2}) = 2\pi/3$. In addition, it is now easy to show that $V(-\frac{1}{2}) = 4\log(2+\sqrt{3}) - 2\pi/3$. ∎

Similar arguments establish the analyticity of $\sigma(s)$ in the strip $\frac{1}{2} < \operatorname{re} s < \frac{3}{2}$ for more general three dimensional quadratic forms.

The accepted value of the electron energy (normalized) for the simple cubic lattice is $-2.837297...$, while that obtained by taking the direct limit is $-2.313698....$ If one computes the direct limit for real s infinitesimally larger than $\frac{1}{2}$ one will obtain the accepted value to any desired degree of accuracy. This begs the obvious question as to why $-2.837297...$ is a "better" value than $-2.313698....$ The effect on the calculation of the relative stability on the three common cubic structures is as follows. Originally one had, after a more appropriate normalization than the one mentioned above,

$$U(\text{s.c.}) = -1.76012.., \qquad U(\text{f.c.c.}) = -1.79175..., \qquad U(\text{b.c.c.}) = -1.79186...,$$

while now, working exactly as indicated in [2], but taking the $\pi/6$ shift into account in appropriate parts of the calculations, one obtains

$$U(\text{s.c.}) = -1.43530..., \; U(\text{f.c.c.}) = -1.58713..., \; U(\text{b.c.c.}) = -1.66296....$$

Thus the relative stability of the three structures remains the same, but their separation becomes much more substantial.

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