

BCC optimality for the three-dimensional Coulomb lattice energy

C. B. Muratov* M. Novaga*

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Abstract

We prove that the body-centered cubic lattice uniquely minimizes the renormalized Coulomb energy among three-dimensional Bravais lattices of fixed covolume, up to orthogonal transformations. Using Ewald summation, we write the energy, to within an additive constant, as a sum of two positive, rapidly convergent series in real and reciprocal space. Their positivity provides finite lower bounds for all competitors. A passage to the dual lattice reduces the problem to a face-centered cubic comparison. A short basis vector estimate, a certified local Hessian, and interval bounds on a compact five-dimensional domain complete the computer-assisted proof.

1 Introduction

In 1934, in his quantum mechanical treatment of an interacting electron gas in a uniform neutralizing background, Wigner posited that when the electron density becomes sufficiently low, the system's ground state should transform from a weakly interacting gas in which the electrons are delocalized to a crystal in which the electrons are strongly localized [37]. More precisely, Wigner conjectured that at densities for which the average inter-electron distance much exceeds the Bohr radius the ground state energy must be dominated by the potential energy of the Coulombic repulsion of the electrons, favoring a densely packed crystalline lattice. While Wigner hypothesized that such a ground state would be given by a body-centered cubic (BCC) lattice of electrons, it was Fuchs who demonstrated numerically that another candidate in the form of a close-packed lattice – the face-centered cubic (FCC) lattice – has a slightly higher energy, confirming Wigner's claim among BCC, FCC and simple cubic lattices [19].

In practice, the assumption of a uniform neutralizing background (jellium) is quite unrealistic for typical solids. In fact, in his calculation of the electrostatic energy of a lattice Fuchs considered the energy of positive *ions* in the negative uniform background of electrons [19]. While nowadays such an assumption would also be considered too crude for ordinary metals, it is actually quite a reasonable one in an entirely different context, namely, that of nuclear matter in the crust of neutron stars or other astrophysical situations [32]. Perhaps the simplest model of such dense nuclear matter would be a variant of Gamow's liquid drop model specified in a macroscopically large volume with a fixed charge density. Here the ultrarelativistic electrons provide the uniform negative charge background, while nuclear matter arranges itself into small proton-rich droplets corresponding to individual atomic nuclei.

*Dipartimento di Matematica, Università di Pisa, Largo Bruno Pontecorvo 5, 56127 Pisa, Italy

An analysis of the above energy at low volume fraction of proton-rich matter in three space dimensions reveals a limiting energy in which the droplet shapes are determined by the competition of surface tension with Coulombic self-energy of the droplets [13, 23], while the spatial arrangement of the droplets minimizes the repulsive energy of point charges in a neutralizing background [18]. Recently, the problem associated with the optimal droplet shape has been fully settled, with the help of AI tools [9], yielding an implication that all the droplets in the low density regime are asymptotically identical balls that minimize the droplet energy per unit volume. In that case the arrangement of the droplets reduces to that of the zero temperature Coulomb gas in a uniform neutralizing background [35], which is mathematically equivalent to the Wigner crystal.

Whether the above system forms a crystalline ground state, either as a charged nuclear liquid or a zero temperature Coulomb gas is a very difficult and fundamental unsolved problem in mathematical physics [1, 5, 26, 35] (for a recent preprint by OpenAI in two space dimensions, see [31]). Therefore, studies of this and other such systems typically assume an a priori periodicity of the ground state and then attempt to calculate the lowest energy state among a greatly reduced configuration space of periodic lattices with a fixed macroscopic particle density. For Coulombic systems, this amounts to computing the Madelung constant of the charges [8, 26, 27, 29], a dimensionless quantity characterizing the Coulombic interaction energy per unit volume in a charge neutral periodic lattice. In the case of a single unit charge per Wigner-Seitz cell $\Omega_L \subset \mathbb{R}^3$ [22, 26] of a Bravais lattice

$$L = \{m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2 + m_3 \mathbf{a}_3 \in \mathbb{R}^3 : (m_1, m_2, m_3) \in \mathbb{Z}^3\}, \quad (1)$$

where $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3 \in \mathbb{R}^3$ are three linearly independent lattice vectors, the Madelung constant is most naturally defined as (using the normalization of [10, 19])

$$K_L := \frac{R_{\text{WS}}}{2} \lim_{x \rightarrow 0} \left(v(x) - \frac{1}{|x|} \right), \quad (2)$$

where $R_{\text{WS}} := \sqrt[3]{3|\Omega_L|/(4\pi)}$ is the spherical Wigner-Seitz cell radius. Here the electrostatic potential v is the unique mean zero L -periodic solution of

$$-\Delta v = 4\pi \left(\sum_{p \in L} \delta_p - |\Omega_L|^{-1} \right) \quad \text{in } \mathcal{D}'(\mathbb{R}^3), \quad (3)$$

where δ_p is the Dirac-delta centered at $p \in \mathbb{R}^3$ and $|\Omega_L|$ is the volume of the Wigner-Seitz cell, also referred to as the covolume of the lattice L . The value of K_L determines the Coulombic energy $K_L e^2 / R_{\text{WS}}$ of the Wigner crystal electrons in Gaussian units per single charge e and does not change upon rescaling of L . Hence without loss of generality we may fix the scale by choosing $|\Omega_L| = 1$, which we will do from now on. Note that to within the normalization, K_L coincides with the renormalized energy of the Coulomb gas introduced in [33] (see also [35]). Wigner's conjecture would then state that the BCC lattice minimizes the Madelung constant K_L or, equivalently, the renormalized Coulombic energy, among all Bravais lattices L of covolume one in three space dimensions.

To get a basic idea of the magnitude of the optimal Madelung constant, one can make a simple approximation [38] that replaces the Wigner-Seitz cell Ω_L of a tightly packed lattice with a ball $B_{R_{\text{WS}}}$ of the same volume, with Neumann boundary condition on $\partial B_{R_{\text{WS}}}$. A simple

calculation then yields the spherical approximation value to the Madelung constant:

$$K_{\text{WS}} = -0.9. \quad (4)$$

This value turns out to be surprisingly close to the exact values of the Madelung constants for the BCC and FCC lattices computed numerically [10, 25] (for certified numerical values, see the following sections):

$$K_{\text{BCC}} \approx -0.895929255682, \quad K_{\text{FCC}} \approx -0.895873615195. \quad (5)$$

By inspection, K_{BCC} is the smallest among several lattice types (see, e.g., the zero screening values in [24]), making the conjecture among all Bravais lattices quite plausible. Nevertheless, the chief difficulty in proving such a result is a very small relative energy gap of 6.2×10^{-5} between the two lattices, which necessitates a very accurate evaluation of the Coulombic energy.

It is well known that on a formal level the electrostatic potential v solving (3) may be thought of as the superposition of the Coulombic potentials of point charges on the lattice minus that of the neutralizing background. However, such sums are notoriously ill-behaved [8], so a suitable regularization is necessary to make sense of such statements. Following the original definition of Born [6], for a covolume-one lattice L define its Coulombic energy as

$$E(L) := \lim_{\kappa \rightarrow 0^+} \left(\sum_{p \in L \setminus \{0\}} \frac{e^{-\kappa|p|}}{|p|} - \frac{4\pi}{\kappa^2} \right) \sim \sum_{p \in L \setminus \{0\}} \frac{1}{|p|}, \quad (6)$$

where the sum under the limit is an absolutely convergent series for every $\kappa > 0$, representing the sum of the *screened* Coulomb potentials of the charges on the lattice outside the origin that formally corresponds to the (suitably renormalized) sum of the electrostatic contributions of all the other charges. In fact, it is easy to see that the limit in (6) is well defined, and by Lemma A1 we have

$$K_L = \frac{R_{\text{WS}}}{2} E(L). \quad (7)$$

Alternatively, as is commonly done in the literature [7, 8, 26], the function $E(L)$ may be obtained via an analytic continuation of the Epstein zeta function [15, 16] (written in the convention of [28]):

$$E(L, s) := \sum_{p \in L \setminus \{0\}} \frac{1}{|p|^{2s}}, \quad \text{Re } s > \frac{3}{2}, \quad (8)$$

to $0 < s < \frac{3}{2}$, which is known to be a meromorphic function of s with only a simple pole at $s = \frac{3}{2}$ [15, 16, 34], by noting that [7, 27]

$$E(L) = E(L, \tfrac{1}{2}). \quad (9)$$

Define the covolume-one FCC and BCC lattices [28]:

$$L_{\text{F}} := 2^{-1/3} \{m \in \mathbb{Z}^3 : \sum_i m_i \equiv 0 \pmod{2}\}, \quad L_{\text{B}} := 2^{-2/3} \{m \in \mathbb{Z}^3 : m_1 \equiv m_2 \equiv m_3 \pmod{2}\}. \quad (10)$$

Our main result of this paper is the following theorem.

Theorem 1. *For every Bravais lattice $L \subset \mathbb{R}^3$ of covolume one we have*

$$E(L) \geq E(L_B),$$

with equality if and only if L is equal to L_B , up to an orthogonal transformation.

As we already noted, with $E(L_B) \approx -2.888461503$ the margin to be established is

$$E(L_F) - E(L_B) \approx 1.7938403 \times 10^{-4}, \quad (11)$$

which makes the problem rather delicate.

Below we provide the description of our computer-assisted proof of Theorem 1, with the code that can be found in the depositary [30]. The code has been built and executed, using AI (Claude Opus 5), and was then cross-validated by AI (ChatGPT-6 Astra). The authors also manually verified all the arguments and codes, and redid the verifying runs.

Our proof essentially follows that of Sarnak and Strömbergsson in their proof that the FCC lattice uniquely minimizes the height function of flat 3-tori, equivalently, minimizing the regular part of the Epstein zeta function $E(L, s)$ at its pole $s = \frac{3}{2}$ in three space dimensions [34]. We also use several analytic tools from the work of Luo and Wei, who extended the conclusion of Sarnak and Strömbergsson to the three-dimensional Epstein zeta function $E(L, s)$ for all $s > \frac{3}{2}$ in a recent preprint [28]. More precisely, as in [34] we set up the minimization problem by using the Iwasawa coordinates to represent all the Bravais lattices in $\mathbb{R}^3$ as a 5-parameter family and then minimize their Coulombic energy. We represent the latter, using Ewald summation [17], which gives the energy, up to an additive constant, in the form of two rapidly convergent series of positive terms:

$$E(L) = -3 + \sum_{p \in L \setminus \{0\}} \frac{\operatorname{erfc}(\sqrt{\pi}|p|)}{|p|} + \frac{1}{\pi} \sum_{q \in L^* \setminus \{0\}} \frac{e^{-\pi|q|^2}}{|q|^2}, \quad (12)$$

for any covolume-one lattice L , whose dual is L^* (see the next section for details). Note that the minimization problem can be equivalently posed in terms of the dual lattice L^* instead, which is what we actually do. Using just two terms in the Ewald sum, we produce a short lattice vector cutoff that restricts the minimization problem to a compact rectangular domain in $\mathbb{R}^5$. The proof then obtains quantitative Hessian estimates in the neighborhood of the FCC dual lattice, where we quantify the local minimality result of Ennola for the FCC lattice with respect to $E(L, 1)$ [14]. We then evaluate the energy on a finite partition of the remaining parameter space, using interval arithmetic and rigorous bounds on the summands. Some care is required to ensure a sufficiently high certified accuracy of these calculations that are carried out by a computer.

Our paper is organized as follows. In Sec. 2, we present the setup of the optimization problem by defining the energy with the help of Iwasawa coordinates on the modified Grenier domain. In Sec. 3, we calculate the certified reference value of the energy and reduce the minimization to a compact reduced domain. In Sec. 4, we carry out a quantitative minimality study in a sufficiently small neighborhood of the reference lattice. In Sec. 5, we reduce the problem of minimization outside the neighborhood of the reference lattice characterized in Sec. 4 to estimating the energy on a union of boxes with almost disjoint interior. Finally, in Sec. 6 we construct a finite cover of the minimization domain that allows us to certify the reference lattice as the unique global energy minimizer, concluding the proof of Theorem 1. We also briefly discuss several possible directions of related future research in Sec. 7.

2 Setup

Throughout the paper, all vectors $p \in \mathbb{R}^3$ are assumed to be column vectors, $|p|$ denotes their Euclidean norm and $|p|_\infty$ their infinity norm. For $g \in GL(3, \mathbb{R})$ with $\det g = 1$ put $Y = g^\top g$ to be the Gram matrix of the columns of g , and for $m \in \mathbb{Z}^3$ define $Y[m] = m^\top Y m = |gm|^2$. Then Y belongs to

$$\mathcal{P}_3^\circ = \{Y \in \mathbb{R}^{3 \times 3} : Y = Y^\top > 0, \det Y = 1\}, \quad (13)$$

while the vectors gm run over the covolume-one lattice L formed by the columns of g as m runs over $\mathbb{Z}^3$, see (1). Moreover, every $Y \in \mathcal{P}_3^\circ$ arises this way, L is uniquely determined by Y up to rotations, and Y is determined by L up to arithmetic congruence $Y \sim \gamma^\top Y \gamma$ for $\gamma \in GL(3, \mathbb{Z})$. The dual lattice has Gram matrix Y^{-1} . We write Y_F, Y_B for Gram matrices of (10).

We next define the representation of the energy in terms of Ewald sums. As these formulas are not specific to the Coulomb kernel, we introduce a general expression for the Epstein zeta function of a lattice defined by its Gram matrix $Y \in \mathcal{P}_3^\circ$ via the function (see [34, Sec. 4]):

$$\mathcal{H}_s(Y) := \sum_{m \in \mathbb{Z}^3 \setminus \{0\}} \left[G(s, \pi Y[m]) + G\left(\frac{3}{2} - s, \pi Y^{-1}[m]\right) \right], \quad (14)$$

where for every $a \in \mathbb{R}$ and $x > 0$ the positive kernel $G(a, x)$ is defined as

$$G(a, x) := \int_1^\infty e^{-xt} t^{a-1} dt. \quad (15)$$

Then the following identity holds [34, Eq. (23)]:

$$\pi^{-s} \Gamma(s) E(Y, s) = \frac{1}{s - 3/2} - \frac{1}{s} + \mathcal{H}_s(Y), \quad (16)$$

where $\Gamma(s)$ is the gamma function, which, in particular, yields

$$E(L) = \mathcal{H}_{1/2}(Y_L) - 3, \quad (17)$$

where Y_L is the Gram matrix of the covolume-one lattice L . Thus, minimizing $E(L)$ among all such L is equivalent to minimizing $\mathcal{H}_{1/2}(Y)$ among all $Y \in \mathcal{P}_3^\circ$. Also, from the duality relation [34, Eq. (2)]

$$\mathcal{H}_s(Y) = \mathcal{H}_{3/2-s}(Y^{-1}) \quad (18)$$

for every $Y \in \mathcal{P}_3^\circ$ follows that minimizing $E(L)$ in L is equivalent to minimizing $\mathcal{H}_1(Y)$ among all $Y \in \mathcal{P}_3^\circ$, and the statement of Theorem 1 that $E(L)$ attains its minimum exactly at $L = L_B$ is equivalent to

$$\mathcal{H}_1(Y) \geq \mathcal{H}_1(Y_F) \quad \text{for all } Y \in \mathcal{P}_3^\circ, \text{ with equality only if } Y \text{ is congruent to } Y_F. \quad (19)$$

From now, we refer to $\mathcal{H}_1(Y)$ as the energy to be minimized among all $Y \in \mathcal{P}_3^\circ$. Notice that

$$G\left(\frac{1}{2}, x\right) = \frac{\sqrt{\pi} \operatorname{erfc}(\sqrt{x})}{\sqrt{x}}, \quad G(1, x) = \frac{e^{-x}}{x}, \quad (20)$$

so together with (14) and (17) this gives (12).

We now introduce the parametrization of the matrices in $\mathcal{P}_3^\circ$ by the Iwasawa coordinates $\xi = (y_1, y_2, a, b, c)$, which form a five-dimensional parameter space [34, Sec. 4]:

$$Y = N^T D N, \quad N = \begin{pmatrix} 1 & a & b \\ 0 & 1 & c \\ 0 & 0 & 1 \end{pmatrix}, \quad D = \text{diag}(d_1, d_2, d_3), \quad (21)$$

$$d_1 = (y_1^2 y_2)^{1/3}, \quad d_2 = (y_2 / y_1)^{1/3}, \quad d_3 = (y_1 y_2^2)^{-1/3}, \quad (22)$$

so that $\det Y = 1$ identically. This defines a diffeomorphism from $\mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R} \times \mathbb{R}$ onto $\mathcal{P}_3^\circ$. We then use the modified Grenier fundamental domain [21] that is specified by $0 \leq a \leq \frac{1}{2}$, $0 \leq b \leq 1$, $0 \leq c \leq \frac{1}{2}$ together with

$$\begin{aligned} 1 &\leq (1 + a - b)^2 + y_1^{-1}((1 - c)^2 + y_2^{-1}), & 1 &\leq (a - b)^2 + y_1^{-1}((1 - c)^2 + y_2^{-1}), \\ 1 &\leq a^2 + y_1^{-1}, & 1 &\leq b^2 + y_1^{-1}(c^2 + y_2^{-1}), \\ 1 &\leq (b - 1)^2 + y_1^{-1}(c^2 + y_2^{-1}), & 1 &\leq c^2 + y_2^{-1}. \end{aligned} \quad (23)$$

We call ξ , or the corresponding Y_ξ , reduced if it satisfies the coordinate constraints on a, b, c together with (23). By [34, Sec. 4] every $Y \in \mathcal{P}_3^\circ$ is $GL(3, \mathbb{Z})$ -congruent to at least one reduced Y_ξ , and $\mathcal{H}_1$ is invariant under such congruences, so it suffices to minimize over reduced representatives. Note that

$$Y[(1, 0, 0)] = d_1. \quad (24)$$

Also note that in this domain the FCC lattice has a unique representative [34]

$$\xi_F = \left(\frac{4}{3}, \frac{9}{8}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3} \right), \quad (25)$$

for which

$$Y_F = 2^{-2/3} \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}. \quad (26)$$

Lastly, for $m = (i, j, k) \in \mathbb{Z}^3$ the Iwasawa form (21) and direct inversion give

$$Y[m] = d_1(i + aj + bk)^2 + d_2(j + ck)^2 + d_3k^2, \quad (27)$$

$$Y^{-1}[m] = \frac{i^2}{d_1} + \frac{(j - ai)^2}{d_2} + \frac{(k - cj + (ac - b)i)^2}{d_3}, \quad (28)$$

both weighted sums of squares and, hence, enclosable tightly in the interval arithmetic to obtain outward-rounded intervals of IEEE-754 binary64 numbers. The computation of $Y[m]$ and $Y^{-1}[m]$ involves extraction of cube roots in (22), which is done by first using library seeds and then proving them in interval arithmetics by cubing the result with directed rounding. The same seed-and-prove procedure is used for the square roots appearing in the reduced-domain enclosure and in the Frobenius norms of the Hessian tail estimates. In computing the Hessian, derivatives are obtained throughout by second-order forward automatic differentiation: the value, gradient and Hessian are propagated together through each arithmetic operation, with the derivatives of x^{-1} , $x^{1/3}$ and $G(a, \cdot)$ supplied in closed form, so that no gradient or Hessian of (27) or (28) is ever transcribed.

3 Reduction to a compact rectangle

We now proceed to the proof of (19). We start by observing that the modified Grenier domain defined above is not compact, since one can choose, for example, $a = b = c = 0$ and $y_1 = y_2 = d \rightarrow 0^+$, with the limit not in the domain. This, however, produces $d_1 = d \rightarrow 0$, and (24) then implies that the corresponding lattice degenerates, causing the energy to explode. Such a behavior, however, may be excluded by an energy comparison.

First, we need a tight bound on the energy of Y_F .

Lemma 2. *We have*

$$\mathcal{H}_1(Y_F) \in [0.1115384969460437, 0.11153849694607266]. \quad (29)$$

Proof. To obtain a precise bracketing of the value of $\mathcal{H}_1(Y_F)$, we use the fact that the Ewald sum (14) is a sum of positive terms and, therefore, a lower bound follows by truncating the sum to a finite number of shells around the origin. An upper bound is then obtained by estimating the rapidly converging tail of the series in (14) outside those shells. To achieve the desired accuracy, it is sufficient to consider the shells satisfying $|m|_\infty \leq 8$ and combine every pair $\pm m$ into a single summand. The formula is built from the exponential function in the definition of $G(1, \pi Y[m])$, which is evaluated by repeated halving of the argument (which carries no error in binary arithmetic) to reduce it to the interval $[0, \frac{1}{2}]$ with a geometric tail bound and subsequent repeated squaring. On the other hand, as in [28] the function $G(\frac{1}{2}, \pi Y^{-1}[m])$ can be bracketed [36, Ch. III] between the two consecutive convergents of the Stieltjes continued fraction representation [12, Eq. (12.6.15b)] of

$$G\left(\frac{1}{2}, x\right) = \frac{e^{-x}}{x + \frac{1/2}{1 + \frac{1}{x + \frac{3/2}{1 + \frac{2}{x + \frac{5/2}{1 + \ddots}}}}}}, \quad x > 0, \quad (30)$$

at orders 39 and 40. Numerically at order 39/40 the bracket is already tight: for $Y = Y_F$ we have $x = \pi Y^{-1}[m] > 3.7$, where the bracket is below 10^{-14} . All the algebra is done in outward-rounding interval arithmetic.

Finally, to estimate the tail we note that shell $|m|_\infty = n \in \mathbb{N}$ has $24n^2 + 2 \leq 26n^2$ vectors and $Y[m] \geq \mu n^2$, where $\mu := 1/\text{tr}(Y^{-1})$ is a lower bound for the smallest eigenvalue of Y , while $Y^{-1}[m] \geq \mu^* n^2$, where $\mu^* := 1/\text{tr}(Y)$ is a lower bound for the smallest eigenvalue of Y^{-1} , respectively. Since $G(a, x)$ is increasing in a and decreasing in x for all $a \in \mathbb{R}$ and $x > 0$, we can estimate the contribution S_n of that shell by

$$\begin{aligned} S_n &= \sum_{|m|_\infty=n} [G(1, \pi Y[m]) + G(\tfrac{1}{2}, \pi Y^{-1}[m])] \leq 26n^2 [G(1, \pi \mu n^2) + G(1, \pi \mu^* n^2)] \\ &\leq \frac{26r_N^{n-N} e^{-\pi \mu N^2}}{\pi \mu} + \frac{26r_N^{n-N} e^{-\pi \mu^* N^2}}{\pi \mu^*}, \quad r_N = e^{-\pi(2N+1)\min(\mu, \mu^*)}, \end{aligned} \quad (31)$$

for all $n \geq N \in \mathbb{N}$. Therefore, the contribution of all the shells for $|m|_\infty > 8$ is bounded above by

$$\sum_{n=N}^{\infty} S_n \leq \frac{26e^{-\pi\mu N^2}}{\pi(1-r_N)\mu} + \frac{26e^{-\pi\mu^* N^2}}{\pi(1-r_N)\mu^*}, \quad N = 9. \quad (32)$$

For $Y = Y_F$ we have, computing the traces of Y_F and Y_F^{-1} from (27) and (28) in interval arithmetic, $\mu \geq 0.27998245553219342$ and $\mu^* \geq 0.26456684199469938$, yielding an 1.85×10^{-28} upper bound on the tail. The final interval is the result of combining this estimate with the evaluation of the finite sum in interval arithmetic by the code. $\square$

Note that the same procedure for the BCC lattice, whose unique representative in the reduced domain is $\xi_B = (\frac{9}{8}, \frac{4}{3}, \frac{1}{3}, \frac{2}{3}, \frac{1}{2})$, gives $\mathcal{H}_1(Y_B) \in [0.11171788097966455, 0.11171788097968673]$, which is disjoint and above the interval in Lemma 2.

The next lemma provides a lower bound for d_1 for all $Y \in \mathcal{P}_3^\circ$ whose energy does not exceed that of Y_F . Note that by (24) it rules out the presence of a short lattice vector.

Lemma 3. *If $Y \in \mathcal{P}_3^\circ$ and $d_1 < \frac{2}{3}$, where d_1 is as in Section 2, then $\mathcal{H}_1(Y) > \mathcal{H}_1(Y_F)$, with the margin of at least 6.056×10^{-3} .*

Proof. By positivity of the summands in (14) and with the help of (20) and (24), we have $\mathcal{H}_1(Y) \geq 2G(1, \pi Y[(1, 0, 0)]) = 2e^{-\pi d_1}/(\pi d_1)$, which is strictly decreasing in d_1 and is hence bounded below by its value at $d_1 = 2/3$ for all $d_1 \leq 2/3$. By direct computation of the exponential function as in Lemma 2 we obtain

$$2G(1, 2\pi/3) \geq 0.1175945368946040. \quad (33)$$

Comparing this with the bound in Lemma 2 yields the claim, with a certified separation of at least 6.0560399×10^{-3} . $\square$

Lemma 3 restricts attention in the minimization of $\mathcal{H}_1$ to $d_1 \geq 2/3$. The third and sixth inequalities of (23), together with the upper bounds on a and c give $y_1, y_2 \leq 4/3$. Combining this with $d_1^3 = y_1^2 y_2 \geq \frac{8}{27}$ then yields $y_1 \geq \frac{\sqrt{2}}{3}$ and $y_2 \geq \frac{1}{6}$. Hence every remaining reduced representative of $Y \in \mathcal{P}_3^\circ$ whose energy does not exceed that of Y_F lies in the compact rectangle

$$\mathcal{K} = \left[\frac{\sqrt{2}}{3}, \frac{4}{3}\right] \times \left[\frac{1}{6}, \frac{4}{3}\right] \times \left[0, \frac{1}{2}\right] \times [0, 1] \times \left[0, \frac{1}{2}\right]. \quad (34)$$

Since $\mathcal{K}$ is compact and $\mathcal{H}_1$ is continuous in the Iwasawa coordinates, the global minimum is attained; it remains to locate it.

On $\mathcal{K}$ one has $\frac{1}{3} \leq d_1 \leq \frac{4}{3}$, $\frac{1}{2} \leq d_2 \leq \sqrt{2}$ and $\frac{3}{4} \leq d_3 \leq 3\sqrt{2}$. Consequently, for every nonzero $m \in \mathbb{Z}^3$,

$$Y[m] \geq \frac{1}{3}, \quad Y^{-1}[m] \geq \frac{\sqrt{2}}{6} \quad (Y \in \mathcal{K}). \quad (35)$$

These bounds guarantee that no kernel is ever evaluated near its singularity.

4 Local analysis at the reference lattice

We now discuss the behavior of the energy around the reference FCC lattice. As was shown by Ennola [14], FCC lattice is a strict local minimizer of $\mathcal{H}_1$ (for criticality, see also [2]). However, Ennola's result does not quantify the region of strict local minimality around FCC, which is what we need to exclude a finite neighborhood of Y_F in our exhaustive search of the minimizer of $\mathcal{H}_1(Y)$. The latter is the contents of the following proposition.

Proposition 4. *Let $\delta_0 = 2 \times 10^{-4}$ and let $R_0 := \prod_{j=1}^5 [\xi_{F,j} - \delta_0, \xi_{F,j} + \delta_0] \subset \mathbb{R}^5$, where ξ_F is defined in (25), be a rectangle of Iwasawa coordinates. Then the Hessian of $\mathcal{H}_1$ is positive definite for every Y_ξ such that $\xi \in R_0$ and, as a consequence, $\mathcal{H}_1(Y_\xi) \geq \mathcal{H}_1(Y_F)$ for all $\xi \in R_0$, with equality only at ξ_F .*

Proof. Write $\mathcal{H}_1(Y_\xi) = P(\xi) + T(\xi)$, where

$$P(\xi) := \sum_{0 < |m|_\infty \leq 2} \left[G(1, \pi Y_\xi[m]) + G\left(\frac{1}{2}, \pi Y_\xi^{-1}[m]\right) \right], \quad T(\xi) := \mathcal{H}_1(Y_\xi) - P(\xi). \quad (36)$$

By the local uniform convergence of (14) and of its derivatives of any fixed order on compact subsets of $\mathcal{P}_3^\circ$, both P and T are C^2 on a neighborhood of R_0 and may be differentiated termwise.

Step 0: recurrence and an elementary kernel bound. Integration by parts in (15) gives, for every $a \in \mathbb{R}$ and $x > 0$,

$$G(a+1, x) = \frac{e^{-x} + aG(a, x)}{x}, \quad (37)$$

so the orders $a+1$ and $a+2$ required in (40) below are obtained from $G(1, x) = \frac{e^{-x}}{x}$ and $G(\frac{1}{2}, x)$ by up to two applications of (37). In particular, we have $G(3, x) = \frac{e^{-x}}{x} \left(1 + \frac{2}{x} + \frac{2}{x^2}\right)$. Since $G(a, x)$ is increasing in a , for every $a \leq 3$ and $x \geq 1$ there holds

$$G(a, x) \leq \frac{5e^{-x}}{x}. \quad (38)$$

Step 1: the omitted shells. Set

$$\tau := \max_{1 \leq j, k \leq 5} \sup_{\xi \in R_0} \sum_{|m|_\infty > 2} \left| \partial_{jk}^2 \left[G(1, \pi Y_\xi[m]) + G\left(\frac{1}{2}, \pi Y_\xi^{-1}[m]\right) \right] \right|. \quad (39)$$

Differentiating twice and using $\partial_x G(a, x) = -G(a+1, x)$, we get the terms of the type

$$\partial_{jk}^2 G(a, \pi Q) = \pi^2 G(a+2, \pi Q) \partial_j Q \partial_k Q - \pi G(a+1, \pi Q) \partial_{jk}^2 Q \quad (40)$$

in (39), for $Q = Y_\xi[m]$ when $a = 1$ and for $Q = Y_\xi^{-1}[m]$ when $a = \frac{1}{2}$. Note that only the orders $a \leq 3$ of $G(a, \pi Q)$ occur. The shells $3 \leq |m|_\infty \leq 8$ are bounded by evaluating the same second-order jets over R_0 and accumulating the absolute values entrywise in interval arithmetic. For $|m|_\infty = n > 8$ put $\mu := 1/\text{tr}(Y_\xi^{-1})$ and $\mu^* := 1/\text{tr}(Y_\xi)$, lower bounds for the smallest eigenvalues of Y_ξ and Y_ξ^{-1} , respectively. An evaluation over R_0 yields $\mu \in [0.279890149, 0.280074769]$. Hence $Y_\xi[m] \geq \mu n^2 \geq 1$ on R_0 , and with $K_1 \leq 2.360$ and $K_2 \leq 2.521$ denoting Frobenius bounds for

$\partial_j Y_\xi$ and $\partial_{jk}^2 Y_\xi$ on R_0 obtained by automatic differentiation of (27) and evaluating the bounds over R_0 in interval arithmetic, we have

$$|\partial_j Q| \leq K_1 \|m\|_2^2 \leq 3K_1 n^2, \quad |\partial_{jk}^2 Q| \leq 3K_2 n^2, \quad (41)$$

since $\|m\|_2^2 \leq 3n^2$ on the shell. Combining (38), (40) and (41) with $\#\{|m|_\infty = n\} \leq 26n^2$, the shell contributes at most

$$S_n \leq \frac{26 e^{-\pi \mu n^2}}{\mu} (45\pi K_1^2 n^4 + 15K_2 n^2). \quad (42)$$

Analogously, we compute $\mu^* \in [0.264483750, 0.264649949]$, and with $K_1^* \leq 2.102$ and $K_2^* \leq 2.978$ the respective Frobenius bounds for $\partial_j Y_\xi^{-1}$ and $\partial_{jk}^2 Y_\xi^{-1}$, for $Q = Y^{-1}[m] \geq \mu^* n^2 \geq 1$ on R_0 each summand has the form $Cn^p e^{-cn^2}$ with $p \leq 4$, so consecutive ratios of those terms are $(1 + n^{-1})^p e^{-c(2n+1)}$. These ratios are decreasing in n , hence their value at $n = 9$ and $p = 4$ majorizes all later ones and the series is summed by comparison with a geometric one as in the proof of Lemma 2. The resulting far-field contribution is below 10^{-20} , whence from the dominant contribution of the $n = 3$ shell we get

$$\tau \leq 7.977613 \times 10^{-9}, \quad (43)$$

and $|\partial_{jk}^2 T(\xi)| \leq \tau$ for all $\xi \in R_0$ and all j, k .

Step 2: an enclosure of the Hessian. Evaluating the second-order jets of P over R_0 in interval arithmetic — that is, with each Iwasawa coordinate replaced by the interval $[\xi_{F,j} - \delta_0, \xi_{F,j} + \delta_0]$ — yields intervals $[p_{jk}, \bar{p}_{jk}]$ containing $\partial_{jk}^2 P(\xi)$ simultaneously for every $\xi \in R_0$. Widening each entry by the bound (43) of Step 1,

$$A_{jk} := [p_{jk} - \tau, \bar{p}_{jk} + \tau], \quad 1 \leq j, k \leq 5, \quad (44)$$

and recalling $\mathcal{H}_1(Y_\xi) = P(\xi) + T(\xi)$, we obtain $\partial_{jk}^2 \mathcal{H}_1(\xi) \in A_{jk}$ for every $\xi \in R_0$. Thus the symmetric matrix $\nabla^2 \mathcal{H}_1(\xi)$ belongs to the interval matrix A at each point of R_0 .

Step 3: positive definiteness. If A were a fixed symmetric positive definite matrix, we could determine its positivity by carrying out the square-root-free Cholesky factorization $A = LDL^\top$, where L is the unit lower triangular matrix and D is a diagonal matrix [20, Sec. 4.1.2]. However, our A is an interval matrix, hence to determine the bounds on the respective pivots we apply the $LDL^\top$ recursion:

$$d_j = A_{jj} - \sum_{k < j} L_{jk}^2 d_k, \quad L_{ij} = \frac{1}{d_j} \left(A_{ij} - \sum_{k < j} L_{ik} L_{jk} d_k \right) \quad (i > j), \quad (45)$$

in interval arithmetic. The computation returns

$$\begin{aligned} d_1 &\in [0.084881, 0.088247], & d_2 &\in [0.095808, 0.114909], \\ d_3 &\in [0.367913, 0.379133], & d_4 &\in [0.232841, 0.264387], \\ d_5 &\in [0.076444, 0.157416], \end{aligned} \quad (46)$$

so every pivot is bounded away from zero, with τ smaller by a factor of 10^7 . In particular, no division in (45) is by an interval containing 0, and inclusion monotonicity of the interval operations gives, by induction on j , that for *every* symmetric $H \in A$ the exact recursion is

well defined and its quantities lie in the computed intervals. Each exact pivot therefore satisfies $d_j \geq \min_j \underline{d}_j \geq 0.0764$, so $H = LDL^\top$ with L unit lower triangular and D diagonal with positive entries, whence for $x \neq 0$

$$x^\top Hx = y^\top Dy = \sum_{j=1}^5 d_j y_j^2 > 0, \quad y := L^\top x \neq 0, \quad (47)$$

since $L^\top$ is invertible. By Step 2 this applies to $H = \nabla^2 \mathcal{H}_1(\xi)$ for every $\xi \in R_0$, which proves the first assertion.

Step 4: the comparison. The rectangle R_0 is convex and contains ξ_F . Fix $\xi \in R_0$ and put $v := \xi - \xi_F$, so that $\xi_F + tv \in R_0$ for all $t \in [0, 1]$. Taylor's formula with integral remainder, together with the stationarity $\nabla \mathcal{H}_1(Y_F) = 0$, gives

$$\mathcal{H}_1(Y_\xi) - \mathcal{H}_1(Y_F) = \int_0^1 (1-t) v^\top \nabla^2 \mathcal{H}_1(\xi_F + tv) v dt. \quad (48)$$

By Step 3 the integrand is nonnegative on $[0, 1]$, and strictly positive for $v \neq 0$ and all $t \in (0, 1)$. Hence $\mathcal{H}_1(Y_\xi) \geq \mathcal{H}_1(Y_F)$ throughout R_0 , with equality only at $\xi = \xi_F$. $\square$

5 The exterior comparison

Let $\mathcal{V}$ contain one representative of each pair $\{m, -m\}$ in $([-2, 2]^3 \cap \mathbb{Z}^3) \setminus \{0\}$, so $|\mathcal{V}| = 62$, and

$$P(\xi) = 2 \sum_{m \in \mathcal{V}} [G(1, \pi Y_\xi[m]) + G(\tfrac{1}{2}, \pi Y_\xi^{-1}[m])] \quad (49)$$

be as in the proof of Proposition 4. Positivity of the summands gives $\mathcal{H}_1(Y_\xi) \geq P(\xi)$ for every $\xi \in \mathbb{R}_+^2 \times \mathbb{R}^3$, with no correction term: the omitted part may simply be discarded. Being a finite sum of smooth functions of ξ , P is C^2 on $\mathbb{R}_+^2 \times \mathbb{R}^3$.

Proposition 5. *Let $B = \prod_{j=1}^5 [c_j - r_j, c_j + r_j] \subset \mathbb{R}_+^2 \times \mathbb{R}^3$ be a box of Iwasawa coordinates with center $c \in \mathbb{R}_+^2 \times \mathbb{R}^3$ and coordinate radii $r \in \mathbb{R}_+^5$, and let H be an interval enclosure of the Hessian of P over B , with $\underline{H}_{ii}$ and $\overline{H}_{ij}$ denoting the corresponding bounds. Put*

$$\kappa_i := \underline{H}_{ii} - \sum_{j \neq i} \overline{H}_{ij} \frac{r_j}{r_i}, \quad i = 1, \dots, 5. \quad (50)$$

Then

$$\inf_B P \geq P(c) - \sum_{j=1}^5 r_j |\partial_j P(c)| + \tfrac{1}{2} \sum_{i=1}^5 \min(0, \kappa_i) r_i^2. \quad (51)$$

Proof. Every point of B is $c + v$ with $|v_j| \leq r_j$. By Taylor's theorem with Lagrange remainder there is a w on the segment from c to $c + v$ with

$$P(c + v) = P(c) + \nabla P(c) \cdot v + \tfrac{1}{2} v^\top \nabla^2 P(w) v. \quad (52)$$

The gradient is evaluated at the single point c , whereas w is unknown and the Hessian must therefore be estimated through its enclosure H over all of B . The linear term is bounded directly from $|v_j| \leq r_j$:

$$\nabla P(c) \cdot v \geq - \sum_{j=1}^5 r_j |\partial_j P(c)|. \quad (53)$$

For the quadratic term, separating the diagonal from the off-diagonal entries and using $\nabla^2 P(w) \in H$ gives

$$v^\top \nabla^2 P(w) v \geq \sum_{i=1}^5 \underline{H_{ii}} v_i^2 - \sum_{i \neq j} \overline{|H_{ij}|} |v_i| |v_j|. \quad (54)$$

We now apply Young's inequality with the weights r_j/r_i supplied by the box itself,

$$|v_i| |v_j| \leq \frac{1}{2} \left(\frac{r_j}{r_i} v_i^2 + \frac{r_i}{r_j} v_j^2 \right), \quad (55)$$

to each cross term; this is where $r_i > 0$ is used. Summing over $i \neq j$ and using the symmetry $H_{ij} = H_{ji}$, the two halves of (55) coincide after relabelling $i \leftrightarrow j$, so the cross terms contribute $\sum_i v_i^2 \sum_{j \neq i} \overline{|H_{ij}|} r_j / r_i$ and, by (50),

$$v^\top \nabla^2 P(w) v \geq \sum_{i=1}^5 \kappa_i v_i^2. \quad (56)$$

A term with $\kappa_i \geq 0$ is nonnegative and may be discarded, while a term with $\kappa_i < 0$ satisfies $\kappa_i v_i^2 \geq \kappa_i r_i^2$; in both cases $\kappa_i v_i^2 \geq \min(0, \kappa_i) r_i^2$. Combining this with (52) and (53), the right-hand side of (51) bounds $P(c + v)$ from below for every admissible v , and taking the infimum over v proves the claim. $\square$

In the implementation, the center c is a floating-point vector chosen inside the original box B , and the radii are rounded upward so that $|\xi_j - c_j| \leq r_j$ for every $\xi \in B$. The Hessian enclosure is evaluated on B . The preceding proof applies with these possibly enlarged radii, since the segment joining c to any ξ in B remains in B ; an exact midpoint and an equality $B = \prod_{j=1}^5 [c_j - r_j, c_j + r_j]$ are not required.

6 Proof of Theorem 1

We now describe the sequential subdivision of the compact set $\mathcal{K} \subset \mathbb{R}_+^2 \times \mathbb{R}^3$ into a finite set of rectangles by bisecting the parent at the midpoint of its widest coordinate, with both closed box children retained, so their union is the parent. The endpoints of (34) are rounded outward to binary64 numbers; the resulting rectangle contains (34), so covering it suffices. A box $B \subseteq \mathcal{K}$ is terminal if one of the following is verified, in this order:

- (R) one of the six inequalities (23) has upper endpoint below 1 throughout B , so B contains no reduced representative;
- (C) $d_1 < \frac{2}{3}$ throughout B , so Lemma 3 applies;

(B) $B \subseteq R_0$ from Proposition 4;

(E) the right-hand side of (51) exceeds the upper endpoint of the certified enclosure of $\mathcal{H}_1(Y_F)$ in Lemma 2.

By induction the terminal boxes cover $\mathcal{K}$. Each of (R), (C), (B), (E) is decidable in interval arithmetic, and the process is run until no box remains unresolved. That it does so after finitely many subdivisions, and with how many boxes, is the computational content of the proof, as summarized in the following proposition.

Proposition 6. *The bisection described above terminates. It produces a covering of the rectangle (34) by 46 414 closed boxes, on each of which one of (R), (C), (B), (E) is verified, with no unresolved box:*

<i>terminal boxes</i>	46 414
<i>(R) reduction-empty</i>	6 967
<i>(C) short lattice vector</i>	2 444
<i>(B) small FCC neighborhood</i>	45
<i>(E) second-order comparison</i>	36 958
<i>unresolved</i>	0
<i>smallest margin</i>	5.10236×10^{-12}

Building the cover takes under 5 minutes, and the certification run takes about two minutes on one core of a current laptop computer. The subdivision is recorded as a sequence of split instructions, each naming the coordinate that was bisected and the midpoint used. The certifying program takes this record as untrusted input: it constructs the root rectangle itself, and for every instruction checks that the midpoint lies strictly inside the current box before forming both children, so that the union of the boxes it builds is the root at every stage. It then re-tests each terminal box against (R), (C), (B), (E) in interval arithmetic, and verifies that the record is exhausted with no box left open and that the number of terminal boxes exceeds the number of splits by exactly one. A corrupted record is therefore rejected rather than believed; in particular the covering of Proposition 6 does not depend on the program that produced it.

Proof of Theorem 1. Let $\xi \in \mathcal{K}$ be a reduced representative. By Proposition 6, ξ lies in some terminal box B . If B is of type (R) then B contains no reduced representative, contradicting the fact that ξ is reduced. If B is of type (C) then Lemma 3 gives $\mathcal{H}_1(Y_\xi) > \mathcal{H}_1(Y_F)$. If B is of type (B) then $B \subseteq R_0$, and Proposition 4 gives $\mathcal{H}_1(Y_\xi) \geq \mathcal{H}_1(Y_F)$, with equality only at $\xi = \xi_F$. Finally, if B is of type (E) then, by positivity of the summands and Proposition 5,

$$\mathcal{H}_1(Y_\xi) \geq P(\xi) \geq \inf_B P > \mathcal{H}_1(Y_F).$$

Hence $\mathcal{H}_1(Y_\xi) \geq \mathcal{H}_1(Y_F)$ for every reduced $\xi \in \mathcal{K}$, with equality only at ξ_F ; by the passage from the reduced domain established in Lemma 3 and (34) this is a global minimum over $\mathcal{P}_3^\circ$. The theorem now follows by the passage to the dual lattice. $\square$

7 Further directions

We finish by discussing several possible directions to extend our work.

Other Riesz exponents. An immediate extension is to minimize the analytically continued Epstein zeta function $E(L, s)$ for exponents other than the Coulomb value $s = 1/2$ in three space dimensions. In the present convention, where the interaction is $|x|^{-2s}$, the expected phase diagram among covolume-one Bravais lattices is [34, Eq. (44)]

$$\begin{cases} \text{BCC}, & 0 < s < 3/4, \\ \text{BCC and FCC}, & s = 3/4, \\ \text{FCC}, & 3/4 < s < 3/2, \end{cases} \quad (57)$$

with uniqueness up to isometries away from the transition. The crossing at $s = 3/4$ follows from duality; global optimality there remains conjectural. Sarnak and Strömbergsson established the FCC comparison for the height of flat three-tori at the pole $s = 3/2$ [34], and Luo and Wei proved FCC optimality for $s > 3/2$ [28]. Thus the interval $0 < s < 3/2$, apart from the dual pair $s = 1/2$ and $s = 1$ settled here, remains a natural target.

More general periodic crystals. Another extension of Theorem 1 is to periodic sets $\bigcup_{j=1}^m (L + a_j)$ with $m \geq 2$ identical particles per period cell. This includes hexagonal close packing (HCP) lattice, which is not a Bravais lattice but has a two-point basis over a hexagonal lattice. Already for $m = 2$, an unrestricted configuration has five lattice-shape parameters and three relative-position parameters, rather than the five parameters considered here. Numerical Madelung energies favor BCC over HCP [25]. Proving the corresponding comparison uniformly for two-point, and eventually larger finite bases would be an important intermediate step towards relaxing the overall periodicity assumption imposed by lattice L . Ultimately, the question is whether BCC minimizes the renormalized Coulomb energy among configurations without any periodicity assumption. This is a substantially harder three-dimensional crystallization problem; see [5, 26, 33].

Ionic crystals. Yet another natural generalization would be to consider lattices with several *distinct* charges of the same sign per lattice period that model, for example, mixtures of different atomic nuclei in a uniform neutralizing electron background at ultra-high densities of nuclear matter. Here BCC lattices with the larger charge in the center of each elementary cubic cell are natural candidates as minimizers for two charge types when the charge contrast is not too high. At the same time, at strong contrast one would expect the high charges themselves to form a BCC lattice. Notice that from the point of view of the macroscopic ground states one would also need to consider *phase separated* configurations consisting of each charge type organizing into its own BCC lattice. A further question concerns charges of *different signs*, whose classical application is the crystalline structure of ionic crystals. Here, however, the original model would fail to produce energy minimizers, as the energy would go to minus infinity when the opposite charges approach one another. Therefore, one needs to introduce an additional short-range repulsion between all the charges, such as, for example, a repulsive Riesz potential with high exponent (e.g. the standard soft core potential with $s = 6$ in our exponent convention). The volume of the unit cell now also needs to be determined, considering the energy minimality against lattice dilations. This problem goes back to the classical works [6, 29] and would provide a rich playground for further applications of our methodology (for some recent studies, see [3, 4]).

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A The zero screening limit

Lemma A1. *Let L be a lattice of covolume one and let v be the zero-mean L -periodic solution of (3). Then the limit in (6) exists, equals $\lim_{x \rightarrow 0}(v(x) - |x|^{-1})$, and (7) holds. Moreover*

$$\sum_{p \in L \setminus \{0\}} \frac{e^{-\kappa|p|}}{|p|} - \frac{4\pi}{\kappa^2} - \kappa = \lim_{x \rightarrow 0} \left(v(x) - \frac{1}{|x|} \right) + O(\kappa^2) \quad \text{as } \kappa \rightarrow 0^+. \quad (58)$$

Proof. Since $e^{-\kappa r}/r$ is the Green's function of $-\Delta + \kappa^2$ with the 4π normalization, the function

$$v_\kappa(x) := \sum_{p \in L} \frac{e^{-\kappa|x-p|}}{|x-p|} - \frac{4\pi}{\kappa^2} \quad (59)$$

solves

$$(-\Delta + \kappa^2)v_\kappa = 4\pi \left(\sum_{p \in L} \delta_p - 1 \right). \quad (60)$$

The series in (59) converges absolutely and locally uniformly off L for every $\kappa > 0$. Because Ω_L tiles $\mathbb{R}^3$ and has unit volume,

$$\int_{\Omega_L} \sum_{p \in L} \frac{e^{-\kappa|x-p|}}{|x-p|} dx = \int_{\mathbb{R}^3} \frac{e^{-\kappa|y|}}{|y|} dy = 4\pi \int_0^\infty r e^{-\kappa r} dr = \frac{4\pi}{\kappa^2}, \quad (61)$$

so v_κ has mean zero over Ω_L , the same normalization as v .

For an L -periodic locally integrable function $f : \mathbb{R}^3 \rightarrow \mathbb{R}$, we now introduce the Fourier representation [11]

$$f(x) = \sum_{q \in L^*} e^{2\pi i q \cdot x} \widehat{f}(q), \quad \widehat{f}(q) = \int_{\Omega_L} e^{-2\pi i q \cdot x} f(x) dx, \quad (62)$$

where L^* is the dual lattice to L . With this convention, for every nonzero $q \in L^*$ we have

$$\widehat{v}(q) = \frac{1}{\pi|q|^2}, \quad \widehat{v}_\kappa(q) = \frac{4\pi}{4\pi^2|q|^2 + \kappa^2}, \quad (63)$$

while $\widehat{v}(0) = \widehat{v}_\kappa(0) = 0$. Hence

$$|\widehat{v}(q) - \widehat{v}_\kappa(q)| = \frac{\kappa^2}{\pi|q|^2(4\pi^2|q|^2 + \kappa^2)} \leq \frac{\kappa^2}{4\pi^3|q|^4}. \quad (64)$$

Since $\sum_{q \in L^* \setminus \{0\}} |q|^{-4} < \infty$ in dimension three, the Fourier series of $v - v_\kappa$ converges absolutely; therefore, $v - v_\kappa$ is continuous, may be evaluated at the origin, and

$$\|v - v_\kappa\|_\infty \leq \frac{\kappa^2}{4\pi^3} \sum_{q \in L^* \setminus \{0\}} \frac{1}{|q|^4} = O(\kappa^2). \quad (65)$$

In particular the singular parts of v and v_κ at the origin agree and cancel.

Finally, isolating the term $p = 0$ in (59) and using

$$\lim_{x \rightarrow 0} \left(\frac{e^{-\kappa|x|}}{|x|} - \frac{1}{|x|} \right) = -\kappa, \quad (66)$$

we obtain

$$\lim_{x \rightarrow 0} \left(v_\kappa(x) - \frac{1}{|x|} \right) = \sum_{p \in L \setminus \{0\}} \frac{e^{-\kappa|p|}}{|p|} - \frac{4\pi}{\kappa^2} - \kappa. \quad (67)$$

Letting $\kappa \rightarrow 0^+$ and using $\|v - v_\kappa\|_\infty = O(\kappa^2)$ shows that the limit in (6) exists and equals $\lim_{x \rightarrow 0} (v(x) - |x|^{-1})$. Comparing with (2) gives (7). $\square$

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