“Magic” numbers in Smale’s 7th problem

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Abstract

Smale’s 7th problem concerns \( N \)-point configurations on the sphere \( S^2 \) which minimize the logarithmic pair-energy \( V_0(r) = \ln \frac{1}{r} \) averaged over the \( \binom{N}{2} \) pairs in a configuration; here, \( r \) is the chordal distance between the points forming a pair. More generally, \( V_0(r) \) may be replaced by the standardized Riesz pair-energy \( V_s(r) = s^{-1}(r^{-s} - 1), s \neq 0 \), which becomes \( -\ln r \) in the limit \( s \to 0 \), and \( S^2 \) may be replaced by other compact manifolds. This paper inquires into the concavity of the map \( N \mapsto v_s(N) \) from the integers \( N \geq 2 \) into the minimal average standardized Riesz pair-energies \( v_s(N) \) of the \( N \)-point configurations on \( S^2 \) for various \( s \in \mathbb{R} \). It is known that \( N \mapsto v_s(N) \) is strictly increasing for each \( s \in \mathbb{R} \), and for \( s < 2 \) also bounded above, hence “overall concave.” It is (easily) proved that \( N \mapsto v_{-2}(N) \) is even locally strictly concave, and that so is the map \( 2n \mapsto v_s(2n) \) for \( s < -2 \). By analyzing computer-experimental data of putatively minimal average Riesz pair-energies \( v_s(N) \) for \( s \in \{-1, 0, 1, 2, 3\} \) and \( N \in \{2, ..., 200\} \), it is found that the map \( N \mapsto v_{-1}(N) \) is locally strictly concave, while \( N \mapsto v_1(N) \) is not always locally strictly concave for \( s \in \{0, 1, 2, 3\} \): concavity defects occur whenever \( N \in \mathcal{C}_s^x(s) \) (an \( s \)-specific empirical set of integers). It is found that the empirical map \( s \mapsto \mathcal{C}_s^x(s) \), \( s \in \{-2, -1, 0, 1, 2, 3\} \), is set-theoretically increasing; moreover, the percentage of odd numbers in \( \mathcal{C}_s^x(s) \), \( s \in \{0, 1, 2, 3\} \), is found to increase with \( s \). The integers in \( \mathcal{C}_0^x(0) \) are few and far between, forming a curious sequence of numbers, reminiscent of the “magic numbers” in nuclear physics. It is conjectured that the “magic numbers” in Smale’s 7th problem are associated with optimally symmetric optimal-energy configurations.

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1 Introduction

1.1 Optimal configurations on $S^2$: a brief survey

In various fields of science, ranging from biology over chemistry and physics to computer science, one encounters $N$-point optimization problems of which the following one is archetypical. Consider $N \geq 2$ distinct points on the standard two-sphere $S^2$. Any such $N$-point configuration will be denoted by $\omega_N \subset S^2$. The positions of the $N$ points are conveniently given by $N$ vectors $q_k \in \mathbb{R}^3$ of Euclidean length $|q_k| = 1$, $k = 1, \ldots, N$, and the distance between the two points in the pair $(i, j)$ is taken to be the chordal distance $|q_i - q_j|$. Any pair $(i, j)$ is now assigned a standardized Riesz pair-energy $V_s(|q_i - q_j|)$, with

$$V_s(r) \equiv s^{-1} (r^{-s} - 1), \quad s \in \mathbb{R}, \quad s \neq 0;$$

$$V_0(r) \equiv - \ln r \quad \left(= \lim_{s \to 0} V_s(r) \right).$$

The average standardized Riesz pair-energy of a configuration is given by

$$\langle V_s \rangle(\omega_N) \equiv \frac{2}{N(N-1)} \sum_{1 \leq i < j \leq N} V_s(|q_i - q_j|),$$

and the minimal average standardized Riesz pair-energy by

$$v_s(N) \equiv \inf_{\omega_N \subset S^2} \langle V_s \rangle(\omega_N).$$

The problem is to determine $v_s(N)$ together with the minimizing configuration(s) $\omega_N^*$ (also known as $N$-tuple of $s$-Fekete points) whenever such exist. In general this is a challengingly hard but also intriguingly beautiful and rich mathematical problem. Only for one distinguished value of $s$ has it been solved for all $N$, and only for a few $N$-values has it been conquered for all $s$.

1 Traditionally the Riesz pair-energy is defined as $\tilde{V}_s(r) = r^{-s}$ for $s \neq 0$, and $\tilde{V}_0(r) = - \ln r$ for $s = 0$. This has the disadvantages that $\tilde{V}_0(r) \neq \lim_{s \to 0} \tilde{V}_s(r)$, and that one has to seek energy-minimizing configurations for $s \geq 0$ yet energy-maximizing ones for $s < 0$.

2 Our $v_s(N) = 2 \varepsilon_s(N)$, where $\varepsilon_s(N)$ denotes the so-called “pair-specific ground state energy” in physics (cf. [EvSp93, Kie09a, Kie09b]). While $\varepsilon_s(N)$ is indeed a physically meaningful quantity, its attribute “pair-specific” is a misnomer — it should actually refer to the statistically meaningful $v_s(N)$, for the number of different pairs is $N(N-1)/2$.

3 Originally, M. Fekete (cf. [Fek23]) studied points from an infinite compact set in the complex plane that maximize the product of all mutual distances, which is equivalent to minimizing the average standardized Riesz pair-energy for $s \to 0$.

4 By the lower semi-continuity of the standardized Riesz pair-energy and the compactness of the sphere, there always exist $N$ labeled points (not necessarily pairwise different if $s \leq -2$) whose average pair-energy equals $v_s(N)$. A minimizing set of $N$ labeled points is not a proper minimizing $N$-point configuration unless all points are pairwise different.
The distinguished special value for which this problem has been completely solved for all \( N \) by explicit calculation is \( s = -2 \), which yields the energy law for the completely integrable Newtonian \( N \)-body problem with repulsive harmonic forces. Any \( N \)-point configuration satisfying \( \sum_{i=1}^{N} q_i = 0 \) is a minimizing configuration of \( \langle V_s \rangle(\omega_N) \), and only such are. The minimal energy reads

\[
\nu_{-2}(N) = -\frac{1}{2} \frac{N+1}{N-1}.
\] (5)

The (presumably) next-simplest parameter regime is \( s < -2 \). Here one is confronted with the possibly startling observation that for large \( N \) the \( N \)-tuple Fekete points accumulate around two opposite points, and the localization sharpens as \( N \) is getting larger; this is a consequence of Theorem 7 in \[Bjo56]. In particular, it follows right away from Theorem 7 in \[Bjo56] that for even \( N \) the infimum \( \nu_s(N) \), \( s < -2 \), is achieved if and only if half of the particles each are placed at two antipodal points, yielding

\[
\nu_s(N) = -\frac{1}{|s|} \frac{\left(2^{|s|}-1\right)N+1}{N-1}, \quad s < -2, \quad N = 2n,
\] (6)

which converges to \( \nu_{-2}(N) \) when taking the limit \( s \uparrow -2 \) of (6). When \( N \) is odd the situation is already more tricky, and more interesting! For instance, for the smallest allowed odd \( N = 3 \) it is suggestive to conjecture that the minimizing configuration consists of the corners of an equilateral triangle in an arbitrary equatorial plane; yet comparison with an antipodal “configuration” (arrangement) with two labeled points in the North and one in the South Pole reveals that the equilateral configuration yields a lower average standardized Riesz pair-energy only for \( s_3 < s < -2 \), where \( s_3 \equiv \ln(4/9)/\ln(4/3) \), while for \( s < s_3 \) the antipodal arrangement yields the lower average standardized Riesz pair-energy; in this case one can easily show rigorously that the antipodal arrangement is in fact optimal: namely, the equilateral triangle and the antipodal arrangement are the only equilibrium arrangements of 3 labeled points. When comparing the average standardized Riesz pair-energy for antipodal and equilateral arrangements for other odd \( N \), this changeover happens only if \( N \) is a multiple of 3. The critical \( s_{3(2n-1)} \) tends monotonically to \( -2 \) as \( N = 3(2n-1) \to \infty \). Of course, this does not prove that either arrangement is optimal in the respective range of \( s \). To the best of our knowledge, the optimal arrangement of odd-\( N \) points as a function of \( s < -2 \) is far from being settled.

The concentration of the minimizing “\( N \)-point configuration” for \( s < -2 \) at a few distinct points indicates that the optimization problem is incorrectly posed in the set of proper \( N \)-point configurations. (The deeper reason is that

\[\text{By Theorem 7 of [Bjo56], the infimum is not achieved by a proper } N \text{-point configuration.} \]
\[\text{This was already noted by Rachmanov, Saff, and Zhou [RSZ94].} \]
the Riesz pair-energy ceases to be positive definite in the sense of Schoenberg [Sch38] for $s < -2$.) Interestingly, the sum of distance problem for $s < -2$ plays a central role in the theory of Quasi-Monte Carlo integration schemes for functions in smooth enough function spaces over $\mathbb{S}^2$; we refer the interested reader to [BSSW12, BrDi12b, BrDi13] and papers cited therein.

When $s > -2$ the problem becomes drastically more complicated. One needs to distinguish the cases $-2 < s < 2$, $s = 2$, $s > 2$, and the limit $s \to \infty$.

The interval $-2 < s < 2$ is known as the potential-theoretical regime, since concepts and methods of potential theory can be applied to study both the discrete and the continuous (i.e. $N \to \infty$) optimization problems. Within this regime the integer values $s = -1$, $s = 0$, and $s = 1$ are of particular interest. When $s = -1$ the minimal average standardized Riesz pair-energy problem is equivalent to the maximal average pairwise chordal distance problem; see [FejT56, Sto75, Bec84]. In [BrDi13] it is shown that maximum-sum-of-distance configurations are ideal integration nodes for a certain optimal-order Quasi-Monte Carlo integration scheme on $\mathbb{S}^2$; we will come back to this in Appendix B. The case $s = 0$, i.e. the limit $s \to 0$, which yields the logarithmic pair-energy (2) (also known as the Coulomb energy for a pair of “two-dimensional unit point charges” on $\mathbb{S}^2$, respectively the Kirchhoff energy of a pair of unit point vortices on $\mathbb{S}^2$), occurs in a stunning variety of problems (on $\mathbb{S}^2$ and other manifolds) in the sciences and mathematics; see, e.g. [FJM92, ShiSm93, ChKi94, SaTe97, BCNT02, Ketal04, NeCh09, For10, KiWa12]. Originally Smale’s 7th problem for the 21st century [Sma98] was formulated for the logarithmic energy, see below. Lastly, the value $s = 1$ yields the Coulomb pair-energy of “three-dimensional unit point charges” associated with the so-called Thomson problem (see [Tho04, Why52, ErHo97, Acta97, Petal97, BCM]).

Amongst the values $s \geq 2$, the borderline value $s = 2$ is special in the sense that the finite-$N$ behavior is qualitatively different from both, the regime $-2 < s < 2$, and the regime $s > 2$. Yet it can be understood by considering a certain limit process $s \to 2$; cf. [CaHa09] for the limit process $s \to d$ in analogous optimization problems formulated on $d$-dimensional manifolds. The Riesz pair interaction for $s = 2$, in physics considered as correction term to Newton’s gravity [Man25], is also special in the sense that it yields a Newtonian $N$-body problem in $\mathbb{R}^3$ with additional isolating integrals of motion [BoIb89, LyBe99, CaLe13], besides those associated with Galilei invariance. Restricted to $\mathbb{R}$ the motion is even completely integrable for all $N$ [Cal71, Mos75].

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7The potential function $q \mapsto V_s(|q|)$ is strictly superharmonic (i.e. $\Delta V_s(|q|) < 0$ in $\mathbb{R}^3$) for $s \in (-2, 1)$, harmonic ($\Delta V_s(|q|) = 0$) for $s = 1$, and strictly subharmonic ($\Delta V_s(|q|) > 0$) for $s \in (1, 2)$; here, $\Delta$ is the Laplacian in the ambient space $\mathbb{R}^3$, and $\mathbb{R}^3$ is $\mathbb{R}^3$ with its origin removed. One consequence is that $N$-point configurations with minimal average standardized Riesz pair-energy in the closed unit ball in $\mathbb{R}^3$ live on its boundary $\mathbb{S}^2$ in the superharmonic case, but extend “into the solid” in the subharmonic case as some points need to move into the volume to lower the energy (“charge injection”) (cf. [Lan72, Ber86]).
The large-\(s\) behavior of \(\langle V_s \rangle(\omega_N)\) (\(N\) fixed) is intimately connected with the classical Tamme’s problem (\cite{Tam30}) or hard sphere (best-packing) problem (cf. \cite{CoSl99}); that is, to find a configuration of \(N\) points on the sphere with the minimal pairwise (chordal) distance between the points being as large as possible.\(^8\) It is not too difficult to see (cf. Appendix A) that for any \(N\)-point configuration \(\omega_N = \{q_1, \ldots, q_N\} \subset S^2\) the following limit relation holds:

\[
\lim_{s \to \infty} \left[ \langle V_s \rangle(\omega_N) + \frac{1}{s} \right]^{-1/s} = \min_{1 \leq i < j \leq N} |q_i - q_j| \equiv \rho(\omega_N).
\]

(7)

Moreover, whenever a family of minimizing configurations \(\omega_N^s\) converges to a limit configuration \(\omega_N^\infty\), one has the relation (cf. Appendix A)

\[
\lim_{s \to \infty} \left[ v_s(\omega_N) + \frac{1}{s} \right]^{-1/s} = \rho(\omega_N^\infty) \equiv \rho(N),
\]

(8)

where \(\rho(N)\) is the best-packing (chordal) distance, which maximizes the least distance \(\rho(\omega_N)\) among all \(N\)-point configurations on \(S^2\), and \(\omega_N^\infty\) is the best-packing configuration.\(^8\) The best-packing distance \(\rho(N)\) is only known for \(N = 2, 3, \ldots, 12\) and 24 (cf. \cite{FejT43, SchW51, Rob61, Bor83, Da86}).\(^9\)

Another way of obtaining a nontrivial limit problem is to let \(s \to \infty\) in \(V_s(\omega_N)\), which gives

\[
V_\infty(r) \equiv \lim_{s \to \infty} V_s(r) = \begin{cases} 
\infty & \text{if } r < 1, \\
0 & \text{if } r \geq 1.
\end{cases}
\]

(9)

In that case \(v_\infty(\omega_N) = 0\) for \(N \leq N_\ast\), while \(v_\infty(\omega_N) = \infty\) for \(N > N_\ast\), viz. \(N_\ast\) is the maximum number of non-overlapping calottes with spherical radius \(\pi/6\) which can be placed on the unit sphere. By picking any ball, \(B\), from a hexagonal close packing (hcp) of \(\mathbb{R}^3\) with unit balls, then projecting its 12 nearest neighbors (unit balls) radially onto the surface of the central ball \(B\), one sees that \(N_\ast \geq 12\). And dividing the surface area of the unit sphere, \(4\pi\), by the area of a calotte, \(\pi(2 - \sqrt{3})\), yields \(\approx 14.92820323\), giving the upper bound \(N_\ast < 15\). But how large is \(N_\ast\), exactly?

Interestingly, the sharp value for \(N_\ast\) is found by studying the related Tammes problem. For \(2 \leq N \leq 12\) one has \(13\) \(\rho(\omega_N) > 1\). L. Fejes Tóth’s

\(^8\)From \cite{BoHS07} it readily follows that a certain limit of the leading coefficient in the asymptotic expansion of \(v_s(N)\) for large \(N\) (and the \(d\)-sphere) is closely related to the largest sphere packing density in \(\mathbb{R}^d\). Only the densities for \(d = 1, 2\) and 3 are known, and only quite recently Hales \cite{Ha05} could settle the last case by proving the famous Kepler Conjecture, which states that no packing of congruent balls in Euclidean space has density greater than the density of the face-centered cubic packing (which is identical to the density of the hexagonal close packing).

\(^9\)See \cite{ClKe86, Meetal77} for tables of \(\omega_N^\infty\) and numerical values of \(\rho(\omega_N)\).

\(^{10}\)Very recently, a proof for \(N = 13\) has been proposed in \cite{MuTa12}.

\(^{11}\)In particular, \(\rho(12) \approx 1.051462225\) implies that the 12 calotte arrangement \(\omega_{\text{hcp}}\) obtained from the hexagonal close packing of \(\mathbb{R}^3\), which has \(\rho(\omega_{\text{hcp}}) = 1\), is not the optimizer of the Tammes problem with \(N = 12\), which is \(\omega_{12}^\infty\): the regular icosahedron.
famous inequality \((\text{FejT43})\),
\[
[\rho(N)]^2 \leq 4 - \left[\csc\left(\frac{\pi}{6} \frac{N}{N-2}\right)\right]^2,
\]
where equality holds only for \(N = 3, 4, 6\) and 12, gives \(\rho(N) < 1\) for \(N \geq 14\). From \([\text{BaVa08}]\) follows \(\rho(13) < 1\). Hence, \(N_* = 12\).

To our best knowledge, the following point sets are the only ones for which one can rigorously prove that they have minimal average standardized Riesz pair-energy for all \(s > -2\). One can easily characterize the minimizing configuration explicitly only when \(N = 2\) or 3 (as the antipodal and equilateral configuration, respectively). The minimizing configuration has been characterized explicitly also for \(N = 4, 6,\) and 12 as the vertices of Platonic solids\(^{12}\) (tetrahedron, octahedron, and icosahedron), which are known to be universally optimal (see \([\text{CoKu07}]\)); such configurations minimize the potential energy of completely monotonic pair-energy functions. The standardized Riesz pair-energies for \(s > -2\) (including the logarithmic pair-energy at \(s = 0\)) fall into this category. The listed configurations for \(N = 2, 3, 4, 6,\) and 12 exhaust the possibilities for universally optimal configurations on \(S^2\); cf. \([\text{Le57}, \text{CoKu07}]\).

The surprisingly difficult task of finding a proof of minimality can, perhaps, be best illustrated with the only partly resolved five point problem on \(S^2\). It is clear from \([\text{CoKu07}, \text{Prop. 14}]\) that there is no universally optimal 5-point configuration on \(S^2\). Indeed, computational optimization reveals that the minimal-energy arrangement of five labeled points on \(S^2\) changes many times as \(s\) varies over the real line\(^{13}\). Thus, for \(-2.368335... \leq s \leq -2\) the antipodal arrangement with two labeled points in the South, and three in the North Pole (say) is the optimizer; at \(s = -2.368335...\) a crossover takes place, and for \(-2.368335... \leq s \leq -2\) the energy-minimizing arrangement of five labeled points is an isosceles triangle on a great circle, with one point in the North Pole and two labeled points each in the other two corners, with (numerically) optimized height. At \(s = -2\) the isosceles arrangement bifurcates off of a continuous family of rectangular pyramids with height \(h = 5/4\), all of which have the same energy \(-3/4\) at \(s = -2\), and of which the isosceles arrangement is the degenerate limit. At \(s = -2\) also another crossover happens, and for \(-2 \leq s < 15.048077392...\) the regular triangular bi-pyramid is the putative energy-minimizing configuration. At \(s = 15.048077392...\), yet another crossover happens, at which the triangular bi-pyramid and a square pyramid with height \(h \approx 1.1385\) have the same average (standardized)

\(^{12}\)Surprisingly, perhaps, the vertices of the Platonic cube \((N = 8)\) have a higher average pair-energy than the square-antiprism derived from the cube by twisting (angle of 45 degrees) and squeezing together two opposite faces of the cube. Similarly, the dodecahedron \((N = 20)\) is not a minimizing configuration either, for any \(s > -2\).

\(^{13}\)The numerical study for \(s \leq -2\) is our own. For \(1 \leq s \leq 400,\) and \(s \to \infty,\) cf. \([\text{Meetal77}]\).
Riesz pair-energy. A square pyramid with (numerically) optimized height
as function of $s$ appears to have lower (standardized) Riesz pair-energy for
$s \in [15.04807..., \infty)$. Lastly, it is well-known that the triangular bi-pyramid
and the square pyramid with height 1 both are particular best-packing config-
urations, with $\theta(\omega^\infty_s) = \sqrt{2}$, so that “at $s = \infty$” an “asymptotic crossover, or
degenerate bifurcation,” happens.

How much of this has been proved rigorously? By traditional method
(see [DLT02], it can be shown that the triangular bi-pyramid consisting of
two antipodal points at, say, the North and the South Pole, and three equally
spaced points on the Equator, is the unique (up to orthogonal transfor-
mation) minimizer of the logarithmic average pair-energy. The proof that the
same configuration maximizes the sum of distances (that is: assumes $v_{-1}(5)$)
is computer-aided, exploiting interval methods and related techniques (see
[HoSh11]). In [Schw10] a computer-aided approach is proposed to show optim-
mality of the triangular bi-pyramid for $s = 1$ and $s = 2$. The optimality of
both the triangular bi-pyramid and the family of rectangular pyramids with
height $5/4$ at $s = -2$ can be shown with elementary techniques. The rest of
the $s$-parameter regime still awaits its rigorous treatment.

Numerical results in [Meetal77], carried out with varying $s \in [1, 400]$ for
$N \in \{2, ..., 16\}$ fixed, suggest that also for other values of $N \notin \{2, 3, 4, 6, 12\}$
the minimizing configuration $\omega^s_N$ may generally change as $s$ passes through
critical values, and their number seem to depend on $N$. In particular, for $N = 7$
there seem to be three(!) critical $s$-values in $[1, 6]$ at which the minimizing
configuration changes, and presumably a few more when $s < 1$, cf. [BeHa77]
for $s = -1$. The general dependence on $s$ of the optimal $N$-point configurations
$\omega^s_N$ is one of the intriguing features of this minimization problem. All the
same, it makes it plain why the rigorous determination of the optimizers is a
highly nontrivial task even for moderate $N$-values other than the special ones
2, 3, 4, 6, 12, becoming hopelessly complicated when $N$ increases.

Yet, the large-$N$ asymptotics of the minimal average standardized Riesz
pair-energy $v_s(N)$ can be determined without seeking the exact Fekete points,
see [RSZ94]. In particular, $\lim_{N \to \infty} v_s(N)$ is for all $s$ determined by the vari-
ational principle\textsuperscript{16} (see [Sze24], [Bjo56], [Lan72], [KiSp99])

$$\lim_{N \to \infty} v_s(N) = \inf_{\mu \in \mathcal{P}(S^2)} \int_{S^2 \times S^2} V_s(|p-q|) \mu(dp)\mu(dq); \quad (10)$$

here, $\mathcal{P}(S^2)$ is the set of all Borel probability measures supported on $S^2$. For

\textsuperscript{14}Curiously, for $-2 \leq s \leq 0$ the optimal height of the square-pyramidal configuration is
constant, equal to $5/4$. Only for $s > 0$ does the optimized height depend on $s$.

\textsuperscript{15}The five point problem on the sphere can be also studied as (unconstrained) external
field problem in the plane (J.B., manuscript in preparation).

\textsuperscript{16}Our usage here of both $p$ and $q$ as points in space (i.e., on $S^2$) should not be confused
with the usage in Hamiltonian dynamics of $(p, q)$ as a pair of canonical variables.
s \leq -2$ the minimizer is not unique, but all minimizers are known; in particular, for $s < -2$ the minimizer, after factoring out $SO(3)$, is a symmetric measure which is concentrated on two antipodal points, see [Bjo56]. From classical potential theory (cf. [Lan72] for $s \in [0, 2)$ and [Bjo56] for $s \in (-2, 0)$) it is well-known that the uniform normalized (Lebesgue) surface area measure on $S^2$, denoted by $\sigma$, uniquely minimizes the right-hand side in (10) for $-2 < s < 2$. For $s \geq 2$ the l.h.s. and r.h.s. of (10) are both $\infty$; in this case the rate of divergence of $v_s(N)$ can be determined. It “suffices” to know that for large $N$ the Voronoi cells around the charges are mostly hexagons of a certain size; see [SaKu97] for an enlightening discussion. The picture one should have in mind, when $N$ is large, is a vast sea of hexagonal Voronoi cells around most of the points. Thus, the dual structure of the Voronoi cell decomposition, the Delaunay triangulation, is a network of mostly six-fold coordinated sites. The reason for the qualification “mostly” lies in the topology of the sphere, which gives rise to geometric frustration (see [SaMo99] for a thorough exposition of this notion). Certain points “pick up” a topological charge that measures the departure from the ideal coordination number, 6, of the planar triangular lattice. The celebrated Euler theorem of topology yields that the total topological charge on $S^2$ is always 12. This accounts, for example, for the appearance of 12 (isolated) pentagons in the common soccer ball design. For large $N$ one observes “scars” emerging from these isolated centres that attract pentagon-heptagon pairs (having total topological charge 0). Scars and other topology-induced defects of the hexagonal lattice become important when pushing the asymptotic analysis to higher order, and are not well understood. For instance, to the best of our knowledge it is an unresolved question if there are $n$-gon Voronoi cells with $n \geq 8$ in a minimizing configuration. See [BoGi09] for an approach using elastic continuum formalism.

The truly hard regime is the vast intermediate range of $N$ which are generically too large to allow for an explicit determination of the minimizing configuration, but not large enough for the asymptotic formulas to yield sufficiently accurate results. Empirical insight can be gained from computer experiments (e.g. [RSZ94], [RSZ95], [Aetal97], [Petal97], [ErHo97], [BCNT02], [BCNT06], [Betal07]), which help finding candidates for the minimizing configuration, and in any event yield empirical upper bounds $v_s^*(N)$ on the minimal average standardized Riesz pair-energy $v_s(N)$. Up to $N \approx 100$ one can pretty much trust the computational results: several different computational routines all have yielded the same putatively minimizing configurations. For larger $N$, fewer independent computer experiments have been carried out, and since the number

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17 The investigation of the “energy integral” $\int_{S^2 \times S^2} |p - q|^\lambda \mu(dp)\mu(dq)$, $\lambda$ real, can be traced back to [PoSz31].

18 This also works for $s < 2$; cf. [Ber86], where a “semi-continuous approach” is used to model the large-$N$ behavior.
of local minimum energy configurations which are not global seems to grow exponentially with $N$ \cite{ErHo97}, it becomes quite likely that a computer-assisted (random) search finds only one of these non-global minima when $N$ is too large. Since it is so difficult to find the optimizing configurations, one may need to settle for less. Smale’s 7th problem is formulated in this spirit:

*Find an algorithm which, upon input $N$, in polynomial time returns a configuration $\omega_N$ on $\mathbb{S}^2$ whose average standardized Riesz pair-energy does not deviate from the optimal value obtained with $\omega_s^*$ by more than a certain conjectured $s$-specific function of $N$."

**Remark 1.** Smale’s problem was originally posed for $s = 0$, viz. $V_0(r) = -\ln r$, and then not for the average logarithmic pair-energy but for the total logarithmic energy of the $N$-point configurations, i.e. for $\left(\frac{N}{2}\right)v_0(N)$. The “$s$-specific function of $N$” in this original formulation is the fourth term of the partially proved, partially conjectured large-$N$ asymptotic expansion of the optimal logarithmic energy of $N$-point configurations on $\mathbb{S}^2$ \cite{RSZ94, RSZ95},

\[
\left(\frac{N}{2}\right)v_0(N) = aN^2 + bN \ln N + cN + d \ln N + O(1),
\]  

(11)

with $a = \frac{1}{4} \ln \frac{e}{4}$ and $b = -\frac{1}{4}$ rigorously known, and with rigorous upper and lower bounds on $c$\(^{20}\) and numerical estimates for $d$, given in \cite{RSZ94} (for an update, see \cite{BHS12}). The coefficient “$d$” in Smale’s problem is unspecified and allowed to be bigger than any asymptotically determined \(^{21}\) “$d$.”

Subsequently Smale extended his problem to other values of $s \in (0,2)$; and he remarked that analogous problems can be formulated for higher-dimensional spheres $\mathbb{S}^d$, $d = 3, 4, ...$ \cite{Sma98}.\(^\dagger\)

This concludes our brief introduction into this fascinating field. Further information can be found in the survey articles \cite{ErHo97, SaKu97, HaSa04}, and on the websites [BCM] and [Wom09]. See also the delightful article \cite{AtSu03} where, based on numerical evidence, the first dozen minimizers are discussed mostly for Thomson’s problem ($s = 1$).

We next explain what we are up to in this paper.

\(^{19}\)The growth rate should have a significance similar to “the complexity of the energy landscape.” Studies about the $s$-Riesz energy landscape for $N$-point configurations on $\mathbb{S}^2$ have only begun recently, see \cite{Cetal13} and references therein. For background information on energy landscapes and their complexity, see \cite{Wal04}.

\(^{20}\)In \cite{BHS12} it is conjectured that $c = \ln \left(\frac{2(2/3)^{1/4} \pi^{3/4}}{\Gamma(1/3)^{3/2}}\right)$. Recently, a rigorous determination of $c$ for weighted logarithmic Fekete problems in $\mathbb{R}^2$, to which the logarithmic Fekete problem on $\mathbb{S}^2$ is related by stereographic projection, was proposed in \cite{SaSa13}; unfortunately, the conditions on the weights imposed in \cite{SaSa13} just barely miss the particular weight obtained by stereographic projection.

\(^{21}\)Currently only numerical evidence is available for the fourth term in the putative asymptotic expansion, and it is also conceivable that this term is actually not truly asymptotic.
1.2 The second discrete derivative of \( N \mapsto v_s(N) \)

Our point of departure is the observation that the strict monotonic increase of the sequence \( N \mapsto v_s(N) \) (see [Lan72] for a proof\(^{22}\) and its boundedness above for \( s < 2 \) (a simple variational estimate using \( \| \mathbf{t} \| = \| \mathbf{t} \|_2 \) together imply that the overall shape of the graph \( \{(N, v_s(N)) : N = 2, 3, \ldots \} \) must be “concave in the large” for each \( s < 2 \). This raises the question whether this graph is perhaps even locally, at each \( N > 2 \), strictly concave when \( s < 2 \). Explicitly, the question is whether the discrete second derivative of \( v_s(N) \), given by

\[
\ddot{v}_s(N) = v_s(N - 1) - 2v_s(N) + v_s(N + 1), \quad N > 2,
\]

is perhaps strictly negative for all \( N > 2 \) when \( s < 2 \).

Moreover, although \( v_s(N) \) is not bounded above for \( s \geq 2 \), since the leading-order terms of the asymptotic large-\( N \) expansion of \( v_s(N) \), namely \( v_2(N) \propto \ln N \) [KuSa98] and \( v_s(N) \propto N^{(s - 2) / 2} \) for \( s > 2 \) [HaSa05], are strictly locally concave for \( 2 \leq s < 4 \), it is even conceivable that so is \( N \mapsto v_s(N) \).

An affirmative answer is readily obtained for the special value \( s = -2 \) simply by differentiating the expression (5) for \( v_{-2}(N) \) twice. Furthermore, twofold discrete differentiation of \( v_s(2n) \) when \( s < -2 \) (see (6)) shows that also \( 2n \mapsto v_s(2n) \) is strictly locally concave for \( s < -2 \); of course, this does not prove that \( N \mapsto v_s(N) \) is strictly concave for all \( N > 2 \) when \( s < -2 \).

In the absence of any closed form representation of \( v_s(N) \) for \( s > -2 \) we turned to the empirical data published in [ErHo97] [HSS94] [RSZ95] [Ca09], and to those publicly available at the website [Cec] (some of which we generated ourselves), to gather some experimental input. All the experimental data \( \mathcal{E}_s^x(N) \) reported in [ErHo97] [HSS94] [RSZ95] [Ca09] [Cec] have been computed with the conventional expression for the Riesz \( s \)-energy; if optimal, these Riesz \( s \)-energies are related to our minimal average standardized Riesz pair-energies by \( \mathcal{E}_s(N) = \frac{N(N-1)}{2} (sv_s(N) + 1) \) for \( s \in \{-1, 1, 2, 3\} \). We converted the computer-experimental data \( \mathcal{E}_s^x(N) \) into putatively minimal (empirical) average standardized Riesz pair-energies \( v_s^x(N) \) for \( s \in \{-1, 0, 1, 2, 3\} \) and inspected these as functions of \( N \). A first impression was gained by plotting \( \ddot{v}_s(N) \) computed from the first 200 or so empirical data \( v_s^x(N) \) versus \( N \), for the five chosen \( s \)-values. The following empirical picture emerged.

Fig. 1 shows the graph \( (N, v_s^x(N)) \) in the range \( N \in \{2, 3, \ldots, 200\} \) computed with consecutive data for \( \mathcal{E}_s^x(N) \) from [RSZ95].

\(^{22}\)The monotonicity proof was recently rediscovered [Kie09a] [Kie09b], with the remark ([Kie09b], p. 276) that the “monotonic increase of \( N \mapsto v_s(N) \)” and its proof are quite elementary and presumably known, yet after a serious search in the pertinent literature I came up empty-handed...”. (cf. also [Kie09a], p. 1188). Subsequently Ed Saff pointed out to M.K. that the monotonicity result and its proof were already given in [Lan72]. Happily, the applications of the monotonicity presented in [Kie09a] and [Kie09b] were novel.
Figure 1: Putatively minimal average standardized Riesz pair-energy $v_{-1}(N)$ vs. $N$.

To the human eye the empirical map $N \mapsto v_{-1}(N)$ appears to be strictly locally concave. This impression is re-enforced by the graph $(N, \dot{v}_{-1}(N))$ for $N \in \{3, ..., 199\}$, shown in Fig. 2, which appears to remain below the $N$ axis.

Figure 2: $\dot{v}_{-1}(N)$ as a function of $N$. The solid line is drawn to guide the eyes.

However, since the human eye can only distinguish so much, we confirmed the optical impression of the strict local concavity of the function $N \mapsto v_{-1}(N)$ with a detailed data analysis; see Section 2.

$^{23}$In addition, the limited resolution of the plotting programs can yield deceptive plots.
Also for $s \in \{0, 1\}$ the plots of $N \mapsto v^s_\epsilon(N)$ do look pretty much strictly concave everywhere, see our Fig. 3 and Fig. 4, where we show the graphs $(N, v^0_\epsilon(N))$ and $(N, v^1_\epsilon(N))$, respectively, in the range $N \in \{2, 3, \ldots, 200\}$, both computed with consecutive data for $\mathcal{E}_\epsilon(N)$ pooled from [RSZ95, Ca09].

**Figure 3:** Putatively minimal average Riesz pair-energy $v^0_\epsilon(N)$ as a function of $N$.

**Figure 4:** Putatively minimal average standardized Riesz pair-energy $v^1_\epsilon(N)$ vs. $N$.

However, the graphs of $N \mapsto \tilde{v}^s_\epsilon(N)$ for $s = 0$ and $s = 1$, shown in Fig. 5.

---

\(^{24}\)See also Fig.s 1 and 2 in [Kie09b] for $s = 0$ and $s = 1$, respectively.
and Fig. 6 for \( N \in \{3, \ldots, 199\} \), reveal that the graphs of \( N \mapsto v^x_s(N) \) for \( s \in \{0, 1\} \), are not locally strictly concave!

![Figure 5: \( \ddot{v}_0^x(N) \) as a function of \( N \). The solid line is drawn to guide the eyes.](image1)

Despite the strictly concave optical appearance of \( N \mapsto v_s^x(N) \) for \( s = 0 \) and \( s = 1 \), tiny violations of concavity occur every now and then, in fact already when \( N \) is less than a dozen.

![Figure 6: \( \ddot{v}_1^x(N) \) as a function of \( N \). The solid line is drawn to guide the eyes.](image2)
In Fig. 7 and Fig. 8 we show the graphs \((N, v_2^x(N))\) and \((N, v_3^x(N))\) in the range \(N \in \{2, 3, \ldots, 200\}\), both computed with consecutive data for \(\mathcal{E}_s^x(N)\), \(s \in \{2, 3\}\), pooled from [Ca09] and [Cec].

Upon closer inspection one realizes that neither the graph of \(N \mapsto v_2^x(N)\) nor...
Fig. 7 nor of $N \mapsto v_{N}^{x}(N)$ (Fig. 8) appears locally strictly concave, not even to the human eye. Indeed, the graphs $(N, \ddot{v}_{s}^{x}(N))$ for $N \in \{3, \ldots, 199\}$ and $s \in \{2, 3\}$ clearly cross the $\ddot{v}_{s}^{x}(N) = 0$ axis many times; see Fig. 9 and Fig. 10.

![Figure 9](image)

**Figure 9:** $\ddot{v}_{2}^{x}(N)$ as a function of $N$. The solid line is drawn to guide the eyes.

![Figure 10](image)

**Figure 10:** $\ddot{v}_{3}^{x}(N)$ as a function of $N$. The solid line is drawn to guide the eyes.

Since the minimizing configurations for $N$ less than a dozen or so have been determined numerically with a high degree of confidence, the empirical
violations of strict local concavity for \( s \in \{0, 1, 2, 3\} \) at the smaller \( N \) values do not seem to be due to incorrect computations of the minimal average pair-energies. The strict local concavity of \( N \mapsto v^x_{-1}(N) \), on the other hand, can only be taken as an empirical support for the conjecture that \( N \mapsto v_{-1}(N) \) is strictly local concave.

We summarize our findings so far: First, the map \( N \mapsto v_{-2}(N) \) is strictly locally concave. Second, based on our empirical data analysis, we conjecture that the map \( N \mapsto v_s(N) \) is strictly locally concave also for \( s = -1 \), while its strict local concavity is occasionally violated when \( s \in \{0, 1, 2, 3\} \).

1.2.1 “Magic” numbers: “Optimally optimal” configurations?

Although not clearly discernable in our Figures above, the \( N \)-values at which \( \ddot{v}_x(N) \geq 0 \) seem to become more frequent, and apparently more random, the larger \( s \) is. Interestingly, for the smallest \( s \)-value for which we found empirical violations of strict local \( N \)-concavity, namely \( s = 0 \), i.e. for the logarithmic pair interaction invoked in the original formulation of Smale’s 7th problem, the violations of strict local concavity were few and far between. They occurred at the following experimental sequence of integers:

\[
C^x_+(0) = \{6, 12, 24, 32, 48, 60, 67, 72, 80, 104, 108, 122, 132, 137, \ldots \}. \quad (13)
\]

Curiously, the majority of the numbers in the sequence (13) are multiples of 6 (underlined), or almost multiples (like 67 and 137) — coincidence?

We note that the logarithmic-energy minimizers for the first two “integers of convexity,” i.e. \( N = 6 \) and \( N = 12 \), are two “optimally symmetric” configurations, namely Platonic polyhedra: the octahedron \( (N = 6) \) and icosahedron \( (N = 12) \); also the (putative) minimizers for \( N \in \{24, 48, 60\} \) are highly symmetric configurations; in particular, the one for \( N = 24 \) is an Archimedean polyhedron (also for \( N \in \{48, 60\} \) there are Archimedean polyhedra, but these are NOT log-energy optimizers). To be sure, there is an integer inbetween which is not divisible by 6, namely \( N = 32 \) (the highly symmetric optimizer is a Catalan polyhedron), and also the “odd-balls” \( N = 67 \) and (of all integers!) \( N = 137 \) show up.

Yet it is an intriguing thought that the \( N \)-values in \( C^x_+(0) \) may correspond to log-energy-optimizing configurations which are “optimally symmetric” in the following sense. Most of the log-energy-optimizing configurations associated with \( C^x_+(0) \) are separated by longer \( N \)-intervals in which \( N \mapsto v_0^x(N) \) is strictly concave. This suggests that, perhaps, the configurations in an interval of concavity form a family of more-and-more symmetric optimizers which better-and-better approximate a highly symmetric endpoint configuration. Once an endpoint configuration is reached, the addition of the next point inevitably will destroy a high amount of symmetry, for which an extra large amount of energy may be required.
These “concave families” would thus be vaguely analogous to the “periods” in the so-called periodic table of the chemical atoms. The endpoints of the periods are the chemically very inert noble gases which are associated with highly symmetric “electronic configurations” about the nuclei with charge number \( Z \in \{2, 10, 18, \ldots\} \). Incidentally, also the atomic nuclei seem to form something akin to “periods,” in the sense that the set of nucleon numbers \( \{2, 8, 20, 28, 50, 82, 126, \ldots\} \) is associated with nuclei that have a particular high binding energy per nucleon. This set of nucleon numbers is known as the Magic Numbers of nuclear physics. By analogy, we call the set \( \mathcal{C}_x^+ (0) \) the “Magic Numbers of Smale’s 7th problem.”

### 1.2.2 A catalog of interesting new questions

The upshot of all these findings is a list of interesting new mathematical questions. To pose these sharply, we define several new quantities.

First of all, for each \( s \) we partition the integer subset \( \{N > 2\} \) into three mutually disjoint subsets: the set of strict local concavity \( \mathcal{C}_-(s) \), the set of strict local convexity \( \mathcal{C}_+(s) \), and the set of local linearity \( \mathcal{C}_0(s) \), defined as

\[
\begin{align*}
\mathcal{C}_-(s) & \equiv \{N > 2|\ddot{v}_s(N) < 0\}, \\
\mathcal{C}_+(s) & \equiv \{N > 2|\ddot{v}_s(N) > 0\}, \\
\mathcal{C}_0(s) & \equiv \{N > 2|\ddot{v}_s(N) = 0\},
\end{align*}
\]

respectively. We note that \( \{N > 2\} = \mathcal{C}_-(s) \cup \mathcal{C}_0(s) \cup \mathcal{C}_+(s) \).

Next, we define \( s_* \) as follows,

\[
s_* \equiv \sup\{s'|\mathcal{C}_0(s) \cup \mathcal{C}_+(s) = \emptyset \ \forall \ s \leq s'\}. \quad (17)
\]

Note that the “sup” cannot be a “max” because for any fixed configuration \( \omega_N \) the map \( s \mapsto \langle V_s \rangle (\omega_N) \) is a \( C^\infty \) function, which implies that the map \( s \mapsto v_s(N) \) is a \( C^0 \) function. (The \( C^\infty \) regularity should still hold almost everywhere also for \( s \mapsto v_s(N) \), but for each \( N > 2 \) the minimizing configuration may be changing discontinuously at some specific \( s \)-value(s), at which only \( C^0 \) regularity can be guaranteed.) Note also that alternatively, \( s_* \) is defined as

\[
s_* \equiv \inf\{s|\ddot{v}_s(N) \geq 0 \ \text{for at least one} \ N > 2\}, \quad (18)
\]

and “inf = min” if and only if \( s_* > -\infty \). In the absence of a complete control of all the odd-\( N \) cases for \( s < -2 \) we cannot rule out that \( s_* = -\infty \).

We are now ready to raise our first pair of mathematical questions:

**Q 1:** Is \( s_* > -\infty \)?

**Q 2:** If \( s_* > -\infty \), then what is the value of \( s_* \)?

---

25 Actually, what is symmetric is the structure of the wave function of the electrons.

26 Since there are protons and neutrons in the nucleus, some nuclei are “doubly magic.”
Because of the strict local concavity of the map $2n \mapsto v_s(2n)$ for $s < -2$, and of the map $N \mapsto v_{-2}(N)$, we not only conjecture that $s_* > -\infty$, but that $s_* \geq -2$, at least. In fact, the strict local concavity of the empirical map $N \mapsto \bar{v}_x(N)$ even suggests that $s_* \geq -1$.

If $s_* > -\infty$, then $\mathcal{C}_+(s) = \emptyset$ for $s \leq s_*$, and $\mathcal{C}_0(s) = \emptyset$ for $s < s_*$ but not for $s = s_*$. This leads us to now define the critical set of local linearity,

$$\mathcal{L}_* \equiv \mathcal{C}_0(s_*) \text{ (if } s_* > -\infty).$$

(19)

Under the assumption that $s_* > -\infty$, we now expand our list of mathematical questions, thus:

Q 3: *Is the set $\mathcal{L}_*$ finite or infinite?*

Q 4: *Can one explicitly compute the set $\mathcal{L}_*$?*

Q 5: *Which optimal configurations correspond to the set $\mathcal{L}_*$?*

Again supposing that $s_* > -\infty$, there are then also interesting questions to ask about the regime $s > s_*$. In particular, since $\mathbb{N}$ is countable while $\mathbb{R}$ is not, the continuity of $s \mapsto \bar{v}_s(N)$ suggests that $\mathcal{C}_0(s)$ is empty almost everywhere (w.r.t. Lebesgue measure). Thus it is natural to ask:

Q 6: *Is the set of $s$-values for which $\mathcal{C}_0(s) \neq \emptyset$ finite or infinite?*

Q 7: *Can one compute the set of $s$-values at which $\mathcal{C}_0(s) \neq \emptyset$?*

As with $\mathcal{L}_*$, one can raise similar questions for all non-empty $\mathcal{C}_0(s)$, thus

Q 8: *For each non-empty $\mathcal{C}_0(s)$: is it finite or infinite?*

Q 9: *For each non-empty $\mathcal{C}_0(s)$: can one compute it?*

Q10: *For each non-empty $\mathcal{C}_0(s)$: which configurations does it represent?*

Empirically we found that $\mathcal{C}_x^+(0) \subset \mathcal{C}_x^+(1) \subset \mathcal{C}_x^+(2) \subset \mathcal{C}_x^+(3)$. Thus we ask:

Q11: *Is $s \mapsto \mathcal{C}_+(s)$ monotonic non-decreasing, defined in the sense of set-theoretic inclusion?*

If the answer to Q11 is positive, then $\lim_{s \to \infty} \mathcal{C}_+(s) \equiv \mathcal{C}_+(\infty)$ exists. Thus, under the hypothesis that Q11 is answered affirmatively, we also ask:

Q12: *Can one explicitly characterize $\mathcal{C}_+(\infty)$?*

Q13: *Does there exist an $s^* < \infty$ such that $\mathcal{C}_+(s) = \mathcal{C}_+(\infty)$ for all $s > s^*$?*

Q14: *If yes, can one compute $s^* < \infty$?*
All these questions are presumably quite difficult to answer. In any event, we expect valuable insights even from some partial answers. Also possible applications may follow. For instance, knowledge of any \( s \)-values for which the map \( N \mapsto \ddot{v}_s(N) \) is strictly negative will yield a necessary criterion for minimality of energy-minimizing configurations that can be fielded as a test for lists of empirical data of putatively minimal energies; cf. the tests based on the monotonicity of \( N \mapsto v_s(N) \) carried out successfully in [Kie09b]. In this vein, some partial answers are reported in this paper — after the presentation of our data analysis. The data lists are given in a supplementary section after the bibliography.

The remainder of this paper is structured as follows.

- In Section 2 we present the details of our analysis of the data of [HSS94, RSZ95, Ca09, Cec], which induced us to formulate questions Q1 – Q14.
- In Section 3 we obtain some rigorous and some quasi-rigorous upper bounds on \( s^* \). More to the point, with the help of the exactly computable \( s \mapsto \ddot{v}_s(3) \) we show rigorously that \( C_+(s) \) is nonempty whenever \( s \geq 10 > s_* \). We also show quasi-rigorously that \( C_+(s) \) is nonempty whenever \( s > \hat{s}_* \geq s_* \) with \( \hat{s}_* < 0 \). For this we explicitly compute the (putative) expressions for \( s \mapsto \ddot{v}_s(N) \) for \( N \in \{3, 4, 5, 6\} \) when \( s \) runs through certain intervals in which these functions are elementary, easily discussed, and readily evaluated with MAPLE, MATHEMATICA, or MATLAB.
- In Section 4 we prove various rigorous upper and lower bounds on \( \ddot{v}_s(N) \) which go to zero like a power of \( N \) when \( N \to \infty \) and \( s < 0 \). For \( N \in \{4, 6\} \) we rigorously prove negativity of \( \ddot{v}_s(N) \) for some regime of negative \( s \)-values by taking advantage of the explicitly known optimizers for these \( N \)-values (and for \( N = 2 \)); yet, for general \( N \) such rigorous knowledge is not available, and our best rigorous bounds are not strong enough to prove negativity of \( \ddot{v}_s(N) \) in general for any \( s \), save \( s = -2 \).
- In Section 5 we present an asymptotic analysis of \( N \mapsto \ddot{v}_s(N) \) for the large-\( N \) regime and produce several well-motivated conjectures that relate the concavity of \( N \mapsto v_s(N) \) to the large-\( N \) asymptotics. The character of the asymptotics depends on whether \( s \) is in the potential regime \( s \in (-2, 2) \), in the hypersingular regime \( s > 2 \), or exactly inbetween — at the singular \( s = 2 \). A discussion of the “degeneracy regime” \( s \leq -2 \) will be left for some future work.
- In Section 6 we summarize our findings and suggest future inquiries.
- In Appendix A we prove relations (7) and (8).
- In Appendix B we include a brief study of data of spherical digital nets.
2 Data analysis

2.1 Putative $s$-Fekete points on $S^2$ for $s \in \{-1, 0, 1, 2, 3\}$

There are many studies of putatively minimal (standardized) Riesz $s$-energies, but only a few feature data lists for consecutive $N$-values which are sufficiently long for our purposes. In [ErHo97] the first 110 consecutive data for the Thomson problem ($s = 1$) are reported; similarly on the website [HSS94] the first 130 consecutive data for $s = 1$ are listed$^{27}$ and they are never worse than those of [ErHo97]. In [RSZ95] one finds the first 200 consecutive data for $s \in \{-1, 0, 1\}$, and these authors remark that their data for $s = 1$ agree with those of [HSS94] for the same $N$-values. M. Calef in his thesis [Ca09] lists 180 consecutive data for minimizing configurations, starting at $N = 20$, covering the cases $s \in \{0, 1, 2, 3\}$; he also identified the number of “stable” configurations observed during many trials. In 16 cases the obtained results for $s = 0$ and 1 differed by more than $10^{-6}$ compared to results in [RSZ95] ($s = 0$ and 1) and [Moetal96] ($s = 1$), some lower and some higher than those of these other two works. On the interactive website [Cec] putatively minimal Riesz energies are reported for $s \in \{0, 1, \ldots, 12\}$, yet for variously many consecutive $N$-values. Although on the website [Cec] one finds consecutive data for $s = 0$ and $s = 1$ up to $N$ in the thousands, data become less and less trustworthy with increasing $N$; yet whenever a user happens across a lower-energy configuration than previously observed, this new record holder is substituted for the old one.

For our analysis we chose to work with about 200 numerical data each for $s \in \{-1, 0, 1, 2, 3\}$. In each case, we selected the lowest-energy data available from any of the mentioned lists. Thus, for $s \in \{-1, 0, 1\}$ we worked with the data from [RSZ95], except that for $s = 0$ and 1 we replaced a few data points by lower-energy data from [Ca09]. For $s \in \{2, 3\}$ and $N \in \{20, \ldots, 200\}$, we used the data from [Ca09], supplemented by data from [Cec] for $s \in \{2, 3\}$ and$^{28} N \in \{3, \ldots, 19\}$; however, for $s = 3$ consecutive data were available at [Cec] only for $N \in \{3, \ldots, 12\}$, together with data for $N \in \{16, 18, 19\}$. We therefore used the applet [Cec] to create our own experimental $s = 3$ data for $N \in \{13, 14, 15, 17\}$. Moreover, we also used the applet [Cec] to create our own experimental $s = 2$ and $s = 3$ data for $N = 177$ and $N = 197$, improving over those reported in [Ca09]; see below.

All the experimental data $E^x_s(N)$ reported in [RSZ95] [Ca09] [Cec] (and in the other above-named publications, too) have been computed with the conventional expression for the Riesz $s$-energy. Therefore our first task was to convert all these data into putatively minimal average standardized Riesz pair-energies, using the formula $v^s(N) = \frac{1}{s} \left( \frac{2}{N(N-1)} E^x_s(N) - 1 \right)$ for $s \in \{-1, 1, 2, 3\}$;

---

$^{27}$Save the exactly computable data for $N = 2$ and $N = 3$.

$^{28}$We have completed all lists by computing $v_s(2) = (1/s)(2^{-s} - 1)$ whenever necessary.
when \( s = 0 \) only multiplication by \( 2/N(N - 1) \) was required to obtain \( v_0^+(N) \).

Since the forward derivative \( \dot{v}_s^+(N) \equiv v_s(N + 1) - v_s(N) \) is a strictly increasing function of \( N \), for each \( s \in \{-1, 0, 1, 2, 3\} \) we first checked whether \( v_s(N + 1) > v_s(N - n) \) for all \( 0 \leq n \leq N - 2 \). All the data that we have pooled together for each \( s \)-value passed the test \(^{29}\).

We then inspected the second discrete derivative \( \ddot{v}_s^+(N) \equiv \dot{v}_s^+(N) - \dot{v}_s(N) \) (where \( \dot{v}_s(N) \equiv v_s(N) - v_s(N - 1) \) is the first backward derivative) for \( N \in \{3, \ldots, 199\} \) and \( s \in \{-1, 0, 1, 2, 3\} \). For each of these \( s \)-values we have collected the \( N \)-values at which \( \ddot{v}_s^+(N) > 0 \) \(^{29}\) into the empirical set \( C_s^+(s) \); see next.

2.1.1 The sets \( C_s^+(s) \)

Empirically, we have found the following experimental sets of convexity:

\[
C_s^+(1) = \emptyset, \tag{20}
\]

\[
C_s^+(0) = \{6, 12, 24, 32, 48, 60, 67, 72, 80, 104, 108, 122, 132, 137, 146, 150, 153, 168, 182, 187, 192, 195, \ldots ? \ldots \}, \tag{21}
\]

\[
C_s^+(1) = \{4, 6, 12, 18, 20, 22, 24, 27, 32, 44, 48, 50, 60, 62, 67, 72, 75, 77, 78, 80, 88, 94, 100, 104, 108, 111, 112, 117, 122, 127, 132, 135, 137, 141, 144, 146, 150, 153, 155, 159, 160, 162, 168, 170, 174, 180, 182, 184, 187, 192, 195, 197, \ldots ? \ldots \}, \tag{22}
\]

\[
C_s^+(2) = \{4, 6, 10, 12, 18, 20, 22, 24, 27, 28, 30, 32, 34, 40, 44, 45, 48, 50, 51, 54, 56, 60, 62, 67, 70, 72, 75, 77, 78, 80, 83, 88, 90, 92, 94, 96, 100, 104, 106, 108, 111, 112, 115, 117, 122, 127, 130, 132, 135, 137, 141, 144, 146, 148, 150, 153, 155, 157, 159, 160, 162, 168, 170, 171, 174, 175, 177, 180, 182, 184, 187, 192, 195, 197, \ldots ? \ldots \}, \tag{23}
\]

\[
C_s^+(3) = \{4, 6, 8, 9, 10, 12, 14, 18, 20, 22, 24, 27, 28, 30, 32, 34, 36, 40, 42, 44, 45, 48, 50, 51, 54, 56, 60, 62, 63, 67, 70, 72, 75, 77, 78, 80, 83, 88, 90, 92, 94, 96, 100, 104, 106, 108, 111, 112, 115, 117, 122, 124, 127, 130, 132, 135, 137, 141, 143, 144, 146, 148, 150, 153, 155, 157, 159, 160, 162, 165, 168, 170, 171, 174, 175, 177, 178, 180, 182, 184, 187, 192, 195, 197, \ldots ? \ldots \}. \tag{24}
\]

\(^{29}\)We remark that for sufficiently large \( N \)-values (not included here) failures of monotonicity have been spotted in some data lists at \( C \).\(^{e}\)\(^{c}\)\(^{e}\), cf. [Kie09b].

\(^{30}\)We note that it is futile to look for \( N \)-values for which \( \ddot{v}_s^+(N) = 0 \) in the empirical data.
Here, the numbers $N = 177$, marked **bold** in $\mathcal{C}_{+}^{x}(3)$, and $N = 197$, marked **bold** in $\mathcal{C}_{+}^{x}(s)$ for $s \in \{2, 3\}$, were absent when we used the data of [Ca09], but appeared after we replaced the corresponding energy data from [Ca09] with lower energy data discovered ourselves by using the applet [Cec]. The reason for why we became suspicious of those data in [Ca09] is explained next.

Namely, inspection of the empirical sets $s \mapsto \mathcal{C}_{+}^{x}(s)$ reveals a quite interesting property: the map $s \mapsto \mathcal{C}_{+}^{x}(s)$ increases, set-theoretically! More precisely, before replacing the data of [Ca09] for $N = 177$ when $s = 3$, and for $N = 197$ when $s \in \{2, 3\}$, with lower-energy data obtained with the help of the applet [Cec], we had noticed that the map $s \mapsto \mathcal{C}_{+}^{x}(s)$ seemed to be “mostly increasing,” set-theoretically, with the exception of exactly those three data points. Thus we found that $\mathcal{C}_{+}^{x}(0) \setminus \mathcal{C}_{+}^{x}(1) = \emptyset$, whereas

$$\mathcal{C}_{+}^{x}(1) \setminus \mathcal{C}_{+}^{x}(0) = \{4, 18, 20, 22, 27, 44, 50, 62, 75, 77, 78, 88, 94, 96, 98, 100, 111, 112, 117, 127, 135, 141, 144, 155, 159, 160, 162, 170, 174, 180, 184, 197\};$$

and without the **bold** data we found $\mathcal{C}_{+}^{x}(1) \setminus \mathcal{C}_{+}^{x}(2) = \{197\}$, whereas

$$\mathcal{C}_{+}^{x}(2) \setminus \mathcal{C}_{+}^{x}(1) = \{10, 28, 30, 34, 40, 45, 51, 54, 56, 70, 83, 90, 92, 106, 115, 130, 148, 157, 171, 175, 177\};$$

and finally, without the **bold** data we found $\mathcal{C}_{+}^{x}(2) \setminus \mathcal{C}_{+}^{x}(3) = \{177\}$, whereas

$$\mathcal{C}_{+}^{x}(3) \setminus \mathcal{C}_{+}^{x}(2) = \{8, 9, 14, 36, 42, 63, 124, 143, 165, 178\}.$$  \hfill (27)

So, restricted to $N \leq 176$, and to $s \in \{-2, -1, 0, 1, 2, 3\}$, the map $s \mapsto \mathcal{C}_{+}^{x}(s)$ increased set-theoretically. Also $\mathcal{C}_{+}^{x}(s) \cap \{178, \ldots, 196\}$ increased set-theoretically. Curiously, $N = 177 \in \mathcal{C}_{+}^{x}(2)$ but $177 \not\in \mathcal{C}_{+}^{x}(3)$ without the **bold** data; even more curious was the fact that $N = 197 \in \mathcal{C}_{+}^{x}(1)$ but $197 \not\in \mathcal{C}_{+}^{x}(2)$ and $197 \not\in \mathcal{C}_{+}^{x}(3)$ without the **bold** data. Since these non-monotonic outliers occurred for quite large $N$-values, it was tempting to conjecture that $s \mapsto \mathcal{C}_{+}(s)$ may actually increase set-theoretically. To test this hypothesis we tried to beat Calef’s $N = 177$ data for $s = 3$ and $N = 197$ data for $s = 2$ and $s = 3$; cf. [Ca09]. We achieved this goal by loading the (presumably optimal) $s = 1$ configurations for $N = 177$, respectively $N = 197$, and evaluated their Riesz $s$-energies for $s = 2$ and $s = 3$. These new data are now available at [Cec]. With these new **bold** data in place for those of [Ca09], the set-theoretical differences became $\mathcal{C}_{+}^{x}(1) \setminus \mathcal{C}_{+}^{x}(2) = \emptyset$, as well as $\mathcal{C}_{+}^{x}(2) \setminus \mathcal{C}_{+}^{x}(3) = \emptyset$, while the set-theoretical differences $\mathcal{C}_{+}^{x}(2) \setminus \mathcal{C}_{+}^{x}(1)$ and $\mathcal{C}_{+}^{x}(3) \setminus \mathcal{C}_{+}^{x}(2)$ remained as shown in (26) and (27).

We summarize: with the best available data in place, the empirical map $s \mapsto \mathcal{C}_{+}^{x}(s), s \in \{-1, 0, 1, 2, 3\}$, increases strictly, set-theoretically. **Thus we conjecture that the actual map $s \mapsto \mathcal{C}_{+}(s), s \in \mathbb{R}$, increases set-theoretically.**

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The increase of the map $s \mapsto \mathcal{C}_+^x(s)$ becomes easier discernable by collecting the sets $\mathcal{C}_+^x(s) \subset \{3, \ldots, 199\}$ for $s \in \{-1, 0, 1, 2, 3\}$ into the following table.

Table 1: The sets $\mathcal{C}_+^x(s)$ for $s \in \{-1, 0, 1, 2, 3\}$ and $2 < N < 200$.

| $\mathcal{C}_+^x(-1)$ | $\mathcal{C}_+^x(0)$ | $\mathcal{C}_+^x(1)$ | $\mathcal{C}_+^x(2)$ | $\mathcal{C}_+^x(3)$ |
|------------------------|-----------------------|-----------------------|-----------------------|-----------------------|
|                        |                       | 4                     | 4                     | 4                     |
|                        |                       | 6                     | 6                     | 6                     | 8                     |
|                        |                       |                       |                       |                       | 9                     |
|                        |                       |                       |                       |                       | 10                    |
|                        |                       | 12                    | 12                    | 12                    | 14                    |
|                        |                       | 18                    | 18                    | 18                    |
|                        |                       | 20                    | 20                    | 20                    |
|                        |                       | 22                    | 22                    | 22                    |
|                        |                       | 24                    | 24                    | 24                    | 24                    |
|                        |                       | 27                    | 27                    | 27                    |
|                        |                       | 28                    | 28                    |
|                        |                       | 30                    | 30                    |
|                        |                       | 32                    | 32                    | 32                    |
|                        |                       |                       |                       |                       | 34                    |
|                        |                       |                       |                       |                       | 36                    |

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Table 1 – continued from previous page

| $c^x_+(-1)$ | $c^x_+(0)$ | $c^x_+(1)$ | $c^x_+(2)$ | $c^x_+(3)$ |
|------------|------------|------------|------------|------------|
|            |            |            |            |            |
| 40         | 40         |            |            |            |
|            |            |            |            |            |
| 42         |            |            |            |            |
| 44         | 44         | 44         |            |            |
| 45         | 45         |            |            |            |
| 48         | 48         | 48         | 48         |            |
| 50         | 50         | 50         |            |            |
| 51         | 51         |            |            |            |
| 54         | 54         |            |            |            |
| 56         | 56         |            |            |            |
| 60         | 60         | 60         | 60         |            |
| 62         | 62         | 62         |            |            |
| 63         |            |            |            |            |
| 67         | 67         | 67         | 67         |            |
|            |            |            |            |            |
| 70         | 70         |            |            |            |
| 72         | 72         | 72         | 72         |            |

Continued on next page
Table 1 – continued from previous page

| $C_x^e(-1)$ | $C_x^e(0)$ | $C_x^e(1)$ | $C_x^e(2)$ | $C_x^e(3)$ |
|-------------|------------|------------|------------|------------|
| 75          | 75         | 75         | 75         |            |
| 75          | 75         | 75         |            |            |
| 77          | 77         | 77         |            |            |
| 78          | 78         | 78         |            |            |
| 80          | 80         | 80         | 80         |            |
|             |            |            |            | 83         |
|             |            |            |            | 83         |
| 88          | 88         | 88         |            |            |
|             |            |            |            | 90         |
|             |            |            |            | 90         |
|             |            |            |            | 92         |
|             |            |            |            | 92         |
| 94          | 94         | 94         |            |            |
| 96          | 96         | 96         |            |            |
| 98          | 98         | 98         |            |            |
| 100         | 100        | 100        |            |            |
| 104         | 104        | 104        | 104        |            |
|             |            |            |            | 106        |
|             |            |            |            | 106        |
| 108         | 108        | 108        | 108        |            |
| 111         | 111        | 111        |            |            |
| 112         | 112        | 112        |            |            |

Continued on next page
| $C_x^x(-1)$ | $C_x^x(0)$ | $C_x^x(1)$ | $C_x^x(2)$ | $C_x^x(3)$ |
|------------|------------|------------|------------|------------|
|            |            |            | 115        | 115        |
|            |            |            | 117        | 117        |
|            |            | 122        | 122        | 122        |
|            |            |            |            | 124        |
|            |            |            | 127        | 127        |
|            |            |            |            | 130        |
|            |            | 132        | 132        | 132        |
|            |            |            | 135        | 135        |
|            |            |            | 137        | 137        |
|            |            |            |            | 141        |
|            |            |            |            | 143        |
|            |            |            |            | 144        |
|            |            |            |            | 146        |
|            |            |            |            | 148        |
|            |            |            |            | 150        |

Continued on next page
Table 1 – continued from previous page

| $C_x^+(-1)$ | $C_x^+(0)$ | $C_x^+(1)$ | $C_x^+(2)$ | $C_x^+(3)$ |
|------------|-----------|-----------|-----------|-----------|
| 153        | 153       | 153       | 153       |           |
| 155        | 155       | 155       |           |           |
|            | 157       | 157       |           |           |
| 159        | 159       | 159       |           |           |
| 160        | 160       | 160       |           |           |
|            | 162       | 162       | 162       |           |
|            |           |           |           | 165       |
| 168        | 168       | 168       | 168       |           |
| 170        | 170       | 170       |           |           |
|            | 171       | 171       |           |           |
|            | 174       | 174       | 174       |           |
|            |           |           |           | 175       |
|            | 177       | 177       |           |           |
|            |           |           |           | 178       |
| 180        | 180       | 180       |           |           |
| 182        | 182       | 182       | 182       |           |
|            | 184       | 184       | 184       |           |
| 187        | 187       | 187       | 187       |           |

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Table 1 – continued from previous page

| $C^x_+(-1)$ | $C^x_+(0)$ | $C^x_+(1)$ | $C^x_+(2)$ | $C^x_+(3)$ |
|------------|------------|------------|------------|------------|
| 192        | 192        | 192        | 192        |
| 195        | 195        | 195        | 195        |
|            | 197        | 197        | 197        |

It is also of interest to supplement the qualitative statement, that $s \mapsto C^x_+(s); s \in \{-1, 0, 1, 2, 3\}$ increases monotonically, by some quantitative pieces of information about bulk properties of these increasing sets $C^x_+(s)$ as $s$ varies through $\{-1, 0, 1, 2, 3\}$. Thus, the percentage of integers in $\{3, ..., 199\}$ belonging to $C^x_+(s)$ increases with $s$ as follows:

- $C^x_+(-1)$ contains 0% of the integers from $\{3, ..., 199\}$;
- $C^x_+(0)$ contains 11% of the integers from $\{3, ..., 199\}$;
- $C^x_+(1)$ contains 27% of the integers from $\{3, ..., 199\}$;
- $C^x_+(2)$ contains 38% of the integers from $\{3, ..., 199\}$;
- $C^x_+(3)$ contains 43% of the integers from $\{3, ..., 199\}$.

These percentages suggest that more and more integers are contained in $C^x_+(s)$ when $s$ increases continuously, but they of course do not reveal that $C^x_+(s)$ increases monotonically with $s$.

Similarly, it is readily seen that:

- 5 out of 22 integers in $C^x_+(0)$ are odd, or 23%;
- 16 out of 54 integers in $C^x_+(1)$ are odd, or 30%;
- 24 out of 75 integers in $C^x_+(2)$ are odd, or 32%;
- 28 out of 85 integers in $C^x_+(3)$ are odd, or 33%.

This second table of percentages reveals yet another monotonicity: the percentage of odd integers in $C^x_+(s)$ increases monotonically with $s$. This raises the question whether such a monotonicity is perhaps a property of the theoretical map $s \mapsto C_+(s)$ for $s \in \mathbb{R}$. If the percentage of odd numbers in $C_+(s)$ is indeed increasing, then — since it cannot increase beyond 100% — it will converge to some limit when $s$ increases (provided the percentage remains meaningful, i.e. as long as $C_+(s)$ is not empty), and also when $s \downarrow s_* < 0$, if such a $s_*$ exists. In particular, it makes one wonder whether only even integers will remain in $C_+(s_*)$. 

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To further aid the visualization of the set-theoretical differences for \( s_1 < s_2 \), we defined “signed indicator functions” \( \Delta_{s_1}{}^{s_2}(N) \equiv I_{C_+^x(s_2)}(N) - I_{C_+^x(s_1)}(N) \), where \( I_{C_+^x(s)}(N) = 1 \) if \( N \in C_+^x(s) \), and \( I_{C_+^x(s)}(N) = 0 \) if \( N \not\in C_+^x(s) \). Thus,

\[
\Delta_{s_1}{}^{s_2}(N) = \begin{cases} 
1 & \text{if } N \not\in C_+^x(s_1) \text{ and } N \in C_+^x(s_2), \\
0 & \text{if } N \in C_+^x(s_1) \cap C_+^x(s_2) \text{ or } N \not\in C_+^x(s_1) \cup C_+^x(s_2), \\
-1 & \text{if } N \in C_+^x(s_1) \text{ and } N \not\in C_+^x(s_2). 
\end{cases}
\] (28)

In words, whenever a convexity point \( N' \) is lost by passing from \( s_1 \) to \( s_2 \), the signed indicator function \( N \mapsto \Delta_{s_1}{}^{s_2}(N) \) will take the value \(-1\) at \( N = N' \); otherwise \( N \mapsto \Delta_{s_1}{}^{s_2}(N) \) is non-negative. This affords a convenient way of checking for set-theoretical monotonicity, compared to the painstaking sifting through numerical tables.

Fig.s 11, 12, and 13 show, respectively, \( \Delta_0^1(N) \), \( \Delta_1^2(N) \), and \( \Delta_2^3(N) \), as function of \( N \in \{3, ..., 199\} \). Since \( C_+^x(0) \subset C_+^x(1) \subset C_+^x(2) \subset C_+^x(3) \), our diagnostic functions take only the values 0 and 1.
This concludes our section on the data analysis. We next present our theoretical results.
3 (Quasi-)rigorous upper bounds on $s_*$

While it may not be so easy to obtain a rigorous lower bound on $s_*$, it is relatively easy to find a rigorous upper bound on $s_*$ by studying the $s$-dependence of $\bar{v}_s(3)$; and with the help of computer evaluations of $\bar{v}_s(N)$ for $N \in \{3, 4, 5, 6\}$ we easily obtained better, though only “quasi-rigorous,” upper bounds on $s_*$. To study the $s$-dependence of $\bar{v}_s(N)$ for $N \in \{3, 4, 5, 6\}$ when $s > -2$, one needs to know the minimizing $N$-point configurations for $N \in \{2, 3, 4, 5, 6, 7\}$ and $-2 \leq s < \infty$. We begin by summarizing what we know about these.

3.1 $\omega^s_N$ for $N \in \{2, 3, 4, 5, 6, 7\}$ and $s \in (-2, \infty)$

Below we list the four rigorously known optimizers $\omega^s_N$, $N \in \{2, 3, 4, 6\}$, together with the partly rigorously known but mostly computer-generated putative optimizer $\omega^s_5$ and $\omega^s_7$ for $s \in (-2, \infty)$. Note that for $N \in \{2, 3, 4, 6\}$ each optimizer $\omega^s_N$ is independent of $s \in (-2, \infty)$, while the (putative) optimizers $\omega^s_5$ and $\omega^s_7$ display a non-trivial dependence on $s \in (-2, \infty)$:

$$\omega^s_2 : \text{two antipodal points} \quad s \in (-2, \infty);$$
$$\omega^s_3 : \text{equatorial equilateral triangle} \quad s \in (-2, \infty);$$
$$\omega^s_4 : \begin{cases} \text{triangular bi-pyramid} & s \in (-2, 15.04807\ldots], \\ \text{square pyramid (} f = 1 \text{)} & s \in [15.04807\ldots, \infty); \end{cases}$$
$$\omega^s_5 : \text{regular octahedron} \quad s \in (-2, \infty);$$
$$\omega^s_6 : \begin{cases} C_2(1^{12^3})(f = 5) & s \in (-2, 0], \\ \text{pentagonal bi-pyramid} & s \in [0, 2], \\ C_2(1^{14}\ldots^2)(f = 5) & s \in [2, 5], \\ C_2(1^{14}\ldots^2)(f = 3) & s \in [5, 5.5979\ldots], \\ C_3(1^{13^2})(f = 2) & s \in [5.5979\ldots, \infty). \end{cases}$$

In the above we use the Schönflies point group notation; $f$ is the number of degrees of freedom of the configuration; e.g., for the square pyramid at $N = 5$ the height varies with $s$. The configurations for $N \in \{5, 7\}$ are taken from Meetal77 for $s \geq 1$, and from BeHa77 for $s = -1$. As to the $C_2$-symmetric $N = 7$ configuration at $s = -1$, we quote from BeHa77: “It consists of two points almost antipodal and the remaining five points sprinkled around an equatorial band.” This suggested to us that this configuration belongs to

\[31\] Since the $s$-range has not been — and cannot be — covered exhaustively with a computer, our list of 5-point and 7-point optimizers should be seen as preliminary.

\[32\] Recall that $\omega^s_5$ depends on $s \in (-\infty, -2]$ when $N$ is odd; recall also that at $s = -2$ the minimizer is not unique even after factoring out $SO(3)$, except when $N = 2$. 

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a family which bifurcates off of the pentagonal bi-pyramid, which we then computed numerically ourselves to happen at $s = 0$. Moreover, by the nearly complete degeneracy of the $s = -2$ problem, this family of configurations will have another bifurcation point at $s = -2$. Intriguingly, geometrically this is the “same” $C_2$ family of configurations which was discovered by [Meetal77] to bifurcate off of the pentagonal bi-pyramid at $s = 2$ and to merge with the $C_{2v}$ configuration at $s = 5$ (note, though, that [Meetal77] did not carry out a complete bifurcation analysis); yet, presumably the five degrees of freedom in the family will be differently optimized in each family, in the sense that for most (if not all) $s \in (-2, 0)$ there is no $s \in (2, 5)$ with the same configuration.

3.2 Explicit maps $s \mapsto v_s(N)$ for $N \in \{2, 3, 4, 5, 6, 7\}$

Based on the table shown in Subsection 3.1 we computed explicit expressions for $v_s(N)$ in all situations where we did not have to numerically optimize any of the degrees of freedom. Thus, for $N \in \{2, 3, 4, 6\}$ and $s \in (-2, \infty)$ one has

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

$$v_s(3) = \frac{1}{s} \left( \left( \frac{1}{3} \right)^{\frac{s}{2}} - 1 \right),$$

$$v_s(4) = \frac{1}{s} \left( \left( \frac{2}{3} \right)^{\frac{s}{2}} - 1 \right),$$

and

$$v_s(6) = \frac{1}{s} \left( \left( \frac{1}{5} \right)^s + \frac{4}{5} \left( \frac{1}{2} \right)^{\frac{s}{2}} - 1 \right),$$

while for $v_s(5)$ an explicit expression is available for $s \in (-2, 15.04807...)$, viz.

$$v_s(5) = \frac{1}{s} \left( \frac{1}{10} \left( \frac{1}{2} \right)^s + \frac{3}{10} \left( \frac{1}{3} \right)^{\frac{s}{2}} + \frac{3}{5} \left( \frac{1}{2} \right)^{\frac{s}{2}} - 1 \right),$$

and for $v_s(7)$ the following expression is valid for $s \in (0, 2)$:

$$v_s(7) = \frac{1}{s} \left( \frac{1}{21} \left( \frac{1}{2} \right)^s + \frac{5}{21} \left( 2 \sin \frac{2\pi}{5} \right)^{-s} + \left( 2 \sin \frac{2\pi}{5} \right)^{-s} \right) + \frac{10}{21} \left( \frac{1}{2} \right)^{\frac{s}{2}} - 1.$$

3.3 Bounds on $s_*$ from $s \mapsto \dot{v}_s(3)$ for $s \in (-2, \infty)$

Only for $N = 3$ can we compute $\ddot{v}_s(N)$ for all $s > -2$, viz.

$$\ddot{v}_s(3) = \frac{1}{s} \left( \left( \frac{1}{2} \right)^s + \left( \frac{3}{5} \right)^{\frac{s}{2}} - 2 \left( \frac{1}{3} \right)^{\frac{s}{2}} \right).$$

The elementary function $s \mapsto \ddot{v}_s(3)$ is sufficiently simple to allow a thoroughly rigorous discussion. Thus, inserting $s = -2$ we obtain $\ddot{v}_{-2}(3) = -1/3$, but
we already knew that any function \( s \mapsto \ddot{v}_s(N) \) had to be strictly negative at \( s = -2 \). On the other hand, rewriting \( \ddot{v}_s(3) \) as

\[
\ddot{v}_s(3) = \frac{1}{s} \left( \frac{3}{8} \right)^{\frac{s}{2}} \left( 1 - \left( \frac{8}{9} \right)^{\frac{s}{2}} \left( 1 - \left( \frac{3}{4} \right)^{\frac{s}{2}} \right) \right),
\]

(42)

we can right away extract the large-\( s \) asymptotic behavior \( \ddot{v}_s(3) \simeq \frac{1}{s} \left( \frac{3}{8} \right)^{\frac{s}{2}} > 0 \). As a continuous function, \( \ddot{v}_s(3) \) therefore has to have an odd number of zeros in \((-2, \infty)\). Let \( \dot{s}_1^{(3)} \) denote the smallest zero of \( \ddot{v}_s(3) \) in \((-2, \infty)\). Then \( \dot{s}_1^{(3)} \) is a rigorous upper bound on \( s_\ast \), viz. \( s_\ast \leq \dot{s}_1^{(3)} \).

Of course, the bound \( s_\ast \leq \dot{s}_1^{(3)} \) is not explicit. An explicit upper bound is obtained by inserting \( s = 10 \) into (41), or (42), which yields the strictly positive (tiny) value \( \ddot{v}_{10}(3) = 1289/79626240 \). Thus we have rigorously proved:

**Proposition 1.** The critical \( s_\ast \) satisfies the upper bound \( s_\ast \leq \dot{s}_1^{(3)} < 10 \).

With a little extra effort one can show that \( \ddot{v}_s(3) \) has exactly one zero in \((-2, \infty)\). Namely, starting at \( s = -2 \) with a strictly negative value, \( \ddot{v}_s(3) \) then increases monotonically to a single — strictly positive — maximum, after which it decays monotonically to zero as \( s \to \infty \). We illustrate this behavior with a MATHEMATICA plot of \( s \mapsto \ddot{v}_s(3) \), see Fig. 14.

![Figure 14: Behavior of \( \ddot{v}_s(3) \) as a function of \( s \).](image)

Numerically we get \( \dot{s}_1^{(3)} \approx 9.4 \), so that our explicit upper bound on \( s_\ast \) is not much worse than this numerically computed bound on \( s_\ast \).

The bound stated in Proposition 1 is the only upper bound on \( s_\ast \) which we were able to establish with complete rigor. Quantitatively this bound is lousy. In the ensuing subsections we will obtain several (much) better upper bounds, alas aided by a computer. Some of these will be stated as a (conditional) propositions.
3.4 \( s_* \)-bounds via \( s \mapsto \bar{v}_s(N) \), \( N \in \{4, 5\} \), \(-2 < s < 15.048\ldots\)

For \( N \in \{4, 5\} \) we can explicitly compute \( \bar{v}_s(N) \) when \(-2 < s < 15.04807\ldots\):

\[
\bar{v}_s(4) = \frac{1}{s} \left( \frac{1}{10} \right)^s + \frac{13}{10} \left( \frac{1}{2} \right)^{\frac{s}{2}} + \frac{3}{5} \left( \frac{1}{2} \right)^{\frac{s}{2}} - 2 \left( \frac{3}{5} \right)^{\frac{s}{2}} ,
\]

\( s = 4 \)

\[
\bar{v}_s(5) = \frac{1}{s} \left( \frac{3}{8} \right)^{\frac{s}{2}} - \frac{2}{5} \left( \frac{1}{2} \right)^{\frac{s}{2}} - \frac{3}{5} \left( \frac{1}{3} \right)^{\frac{s}{2}} .
\]

The \( s \)-dependence of these elementary functions is also simple enough to allow a thoroughly rigorous discussion, which reveals the following. Both \( \bar{v}_{-2}(4) \) and \( \bar{v}_{-2}(5) \) are strictly negative, again as we know already they must. Also the large-\( s \) asymptotics of r.h.s.(43) and r.h.s.(44) can be worked out immediately.

r.h.s.(43)\( \propto \frac{1}{2} \left( \frac{1}{2} \right)^{\frac{3}{2}} > 0 \) and r.h.s.(44)\( \propto -\frac{1}{2} \left( \frac{1}{2} \right)^{\frac{3}{2}} < 0 \), yielding the information that r.h.s.(43) has an odd number of zeros in \((-2, \infty)\) while r.h.s.(44) has an even number of zeros in \((-2, \infty)\) — possibly none. However, since the validity of the expressions (43) and (44) is restricted to \( s \in (-2, 15.04807\ldots) \), these asymptotic results do not yield relevant information which — in concert with the strict negativity of \( \bar{v}_{-2}(4) \) and \( \bar{v}_{-2}(5) \) — would allow us to draw any conclusions about \( s \mapsto \bar{v}_s(4) \) or \( s \mapsto \bar{v}_s(5) \) in \( s \in (-2, 15.04807\ldots) \). Instead we need to take a closer look.

Beginning with \( s \mapsto \bar{v}_s(4) \), inserting \( s = 2 \) we easily find \( \bar{v}_2(4) = \frac{41}{120} > 0 \). As a continuous function, \( \bar{v}_s(4) \) therefore has to have an odd number of zeros in \((-2, 2)\). Let \( s_1^{(4)} \) denote the smallest zero of \( \bar{v}_s(4) \) in \((-2, 2)\). Then \( s_1^{(4)} \) is a (quasi-)rigorous upper bound on \( s_* \). Also the bound \( s_* \leq s_1^{(4)} \) is not explicit, but \( s_1^{(4)} < 2 \) gives the explicit (quasi-)rigorous upper bound \( s_* < 2 \) which improves over \( s_* < 10 \).

Also, with the aid of MAPLE (or such) the explicit quasi-rigorous upper bound can be improved to \( s_* < 1 \), for numerically \( \bar{v}_1(4) = 0.0000745467\ldots > 0 \) (in remarkable agreement with the numerical data extracted from the computer experiments), so that \( s_1^{(4)} < 1 \). In fact, this can also be made quasi-rigorous.

**Proposition 2.** The critical \( s_* \) satisfies the upper bound \( s_* < 1 \) as

\[
\bar{v}_1(4) = \frac{1}{20} + \frac{12}{10} \left( \frac{1}{3} \right)^{\frac{1}{2}} + \frac{2}{5} \left( \frac{1}{2} \right)^{\frac{1}{2}} - \left( \frac{3}{2} \right)^{\frac{1}{2}} > 0 .
\]

**Proof.** First, we derive a sufficiently tight lower bound of \((1 - x)^{1/2}\) in terms of a polynomial that gives a rational number if \( x \) is rational. (The usual Taylor polynomial with Lagrange remainder term does not provide good enough

\[33\]The reason for the prefix “quasi” is the absence of a rigorous proof that the triagonal bi-pyramid is the \( N = 5 \) optimizer for \( s \in (-2, 2 + \epsilon) \). For such a small \( N \)-values it is reasonable, though, to take the numerically found optimizers for granted.

34
Using the binomial formula, Pochhammer symbols, and Gauss hypergeometric functions, we get for every positive integer \( K \)

\[
(1 - x)^{1/2} = \sum_{k=0}^{\infty} \left( \frac{1/2}{k} \right) (-x)^k = \sum_{k=0}^{K-1} \frac{(-1/2)_k}{k!} x^k + \sum_{k=K}^{\infty} \frac{(-1/2)_k}{k!} x^k
\]

\[
= \sum_{k=0}^{K-1} \frac{(-1/2)_k}{k!} x^k + \frac{(-1/2)_K x^K}{K!} \, _2F_1\left( K - 1/2, 1; x \right).
\]

As \((-1/2)_K = \Gamma(K - 1/2)/\Gamma(-1/2) < 0\) and the Gauss hypergeometric function is strictly increasing in \( x \) on \([0, 1]\) assuming the value \( 2K \) at \( x = 1 \) (cf. DLMF Eq. 15.4.20), we arrive at

\[
(1 - x)^{1/2} > \sum_{k=0}^{K-1} \frac{(-1/2)_k}{k!} x^k - \frac{(1/2)_{K-1}}{(K-1)!} x^K
\]

for \( 0 < x < 1 \).

Thus, we estimate

\[
\left( \frac{1}{3} \right)^{1/2} = \left( 1 - \frac{2}{3} \right)^{1/2} > \sum_{k=0}^{K-1} \frac{(-1/2)_k}{k!} \left( \frac{2}{3} \right)^k - \frac{(1/2)_{K-1}}{(K-1)!} \left( \frac{2}{3} \right)^K
\]

\[
\left( \frac{1}{2} \right)^{1/2} = \left( 1 - \frac{1}{2} \right)^{1/2} > \sum_{k=0}^{K-1} \frac{(-1/2)_k}{k!} \left( \frac{1}{2} \right)^k - \frac{(1/2)_{K-1}}{(K-1)!} \left( \frac{1}{2} \right)^K
\]

for any positive integer \( K \), whereas for even positive integers \( K \)

\[
\left( \frac{3}{2} \right)^{1/2} = \left( 1 + \frac{1}{2} \right)^{1/2} < 1 + \sum_{k=1}^{K-1} \frac{(-1/2)_k}{k!} (-1)^k \left( \frac{1}{2} \right)^k
\]

because the binomial expansion of \( (1 + x)^{1/2} - 1 \) is an alternating series.

Let \( K = 20 \). Combining everything, we get

\[
\hat{v}_1(4) = \frac{1}{20} + \frac{13}{10} \left( \frac{1}{3} \right)^{1/2} + \frac{3}{5} \left( \frac{1}{2} \right)^{1/2} - \left( \frac{3}{2} \right)^{1/2}
\]

\[
> \frac{5764409437417341241721}{209374412387531441339105280} > 0.
\]

For the computation of the rational bounds one can use, e.g., MATHEMATICA. Hence, by the definition of \( s_s \), we obtain the desired result.

With some extra energy one should be able to make the above bounds totally rigorous, but this would require to prove that the triagonal bi-pyramid is the \( N = 5 \) optimizer for \( s \in [0, 2] \), at least, say.

\[34\text{Digital Library of Mathematical Functions.}\ http://dlmf.nist.gov/15.4.E20\]
For the sake of completeness, in Fig. 15 we display a numerical plot of \( s \mapsto \ddot{v}_s(4) \) for \( s \in (-2, 15.04807...) \).

![Figure 15: Behavior of \( \ddot{v}_s(4) \) as a function of \( s \) for \( s \in (-2, 15.04807...) \).](image1)

Coming to the map \( s \mapsto \ddot{v}_s(5) \), numerical evaluation of r.h.s. (44) reveals that it remains strictly negative for all \( s \in (-2, 15.04807...) \); see Fig. 16.

![Figure 16: Behavior of \( \ddot{v}_s(5) \) as a function of \( s \) for \( s \in (-2, 15.08407...) \).](image2)

Moreover, combined with the asymptotics mentioned above, the numerics shows that r.h.s. (44) remains strictly negative for \( s \in (-2, \infty) \). Unfortunately, r.h.s. (44) is not the correct formula for \( \ddot{v}_s(5) \) when \( s \in (15.04807..., \infty) \).

In fact, since both \( \omega_s^4 \) and \( \omega_s^6 \) do not depend on \( s \) when \( s \in (-2, \infty) \), whereas \( \omega_s^5 \) does, it follows that:

**Proposition 3.** R.h.s. (44) is a rigorous lower bound on \( \ddot{v}_s(5) \) for \( s \in (-2, \infty) \).

Therefore we cannot rule out that \( \ddot{v}_s(5) \) becomes positive for some \( s \in (15.04807..., \infty) \).
3.5 Bounds on $s_*$ from $s \mapsto \ddot{v}_s(6)$ for $0 < s < 2$

Lastly, for $0 < s < 2$ we find

$$
\ddot{v}_s(6) = \frac{1}{\pi} \left( \frac{5}{21} \left( \left( 2 \sin \frac{2\pi}{5} \right)^{-s} + \left( 2 \sin \frac{\pi}{5} \right)^{-s} \right) + \frac{3}{10} \left( \frac{1}{3} \right)^{\frac{s}{2}} - \frac{11}{21} \left( \frac{1}{2} \right)^{\frac{s}{2}} - \frac{53}{210} \left( \frac{1}{7} \right)^{s} \right). \tag{46}
$$

The $s$-dependence of this elementary function is less simple. Moreover, the bifurcation at $s = 0$ is known to us only through our numerical bifurcation analysis, so that it seems prudent for now to be satisfied with a computer-assisted evaluation. Fig. 17 shows a numerical rendering of r.h.s.$(46)$.

![Graph of $\ddot{v}_s(6)$ for $s \in (0, 2)$](image)

Figure 17: Graph of $\ddot{v}_s(6)$ for $s \in (0, 2)$.

Numerically, $\lim_{s \to 0} \ddot{v}_s(6) = 0.000084098... > 0$, and since $\ddot{v}_{-2}(6) < 0$, we conclude that the continuous map $s \mapsto \ddot{v}_s(6)$ has an odd number of zeros in $(-2, 0)$. Let $s_1^{(6)}$ be the smallest one. Then $s_* \leq s_1^{(6)} < 0$.

**Proposition 4.** Under the assumption that the configurations for $N \in \{5, 7\}$ listed in Subsection 3.1 are optimal in the indicated range of $s$-values, one has

$$
\text{Proposition 4.} \ \text{Under the assumption that the configurations for } N \in \{5, 7\} \text{ listed in Subsection 3.1 are optimal in the indicated range of } s\text{-values, one has }
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$$

3.6 Remarks on $s \mapsto \ddot{v}_s(12)$ for $-2 < s < 2$

Fig.s 5 and 6 suggest that the $N = 6$ peak increases more rapidly with $s$ than the $N = 12$ peak when $s$ runs from 0 to 1. Since the $N = 12$ peak appears to be the highest peak for $s = 0$ while the $N = 6$ peak is barely above zero then, we suspect that by lowering $s$ below 0 the $N = 12$ peak will vanish at a lower $s$-value than the $N = 6$ peak, so that the first zero of $s \mapsto \ddot{v}_s(12)$ will yield a better upper bound on $s_*$ than the one we have found with $N = 6$.

Unfortunately, to evaluate $s \mapsto \ddot{v}_s(12)$ one needs to know the optimal configurations for $N \in \{11, 13\}$. We are planning a computer-assisted evaluation of $s \mapsto \ddot{v}_s(12)$, which seems to be the best one can do right now.
4 Rigorous bounds on $\ddot{v}_s(N)$

4.1 Generic $O(N^{-2})$ upper bounds on $\ddot{v}_s(N)$ for $s < 0$

We now derive the following positive $O(N^{-2})$ upper bound on $\ddot{v}_s(N)$ for $s < 0$.

**Proposition 5.** For $s < 0$ the second derivative of $v_s(N)$ is bounded above by

$$\ddot{v}_s(N) \leq -\frac{2}{(N + 1)N} \left(v_s(N - 1) + \frac{1}{s}\right). \quad (47)$$

**Proof.** We rewrite

$$2v_s(N) = (1 + \delta)v_s(N) + (1 - \delta)v_s(N), \quad (48)$$

where $\delta = 2/(N + 1)$. Next, since

$$v_s(N) = \langle V_s \rangle (\omega^*_s),$$

using (3) we now rewrite (48) further as

$$2v_s(N) = (1 + \delta) \frac{2}{N(N - 1)} \sum_{1 \leq i < j \leq N-1} V_s(|q^*_i - q^*_j|)$$

$$+ (1 + \delta) \frac{2}{N(N - 1)} \sum_{1 \leq i \leq N-1} V_s(|q^*_i - q^*_N|)$$

$$+ (1 - \delta) \frac{2}{N(N - 1)} \sum_{1 \leq i < j \leq N} V_s(|q^*_i - q^*_j|),$$

and so, using that $\delta = 2/(N + 1)$,

$$2v_s(N) = \frac{2(N + 3)}{(N + 1)N(N - 1)} \sum_{1 \leq i < j \leq N-1} V_s(|q^*_i - q^*_j|)$$

$$+ \frac{2(N + 3)}{(N + 1)N(N - 1)} \sum_{1 \leq i \leq N-1} V_s(|q^*_i - q^*_N|)$$

$$+ \frac{2}{(N + 1)N} \sum_{1 \leq i < j \leq N} V_s(|q^*_i - q^*_j|). \quad (49)$$

For the term in the second line we use that $N + 3 = (N - 1) + 4$ and rewrite

$$\frac{2(N + 3)}{(N + 1)N(N - 1)} = \frac{2}{(N + 1)N} + \frac{8}{(N + 1)N(N - 1)}. \quad (50)$$
In the single sum receiving the factor $2/(N + 1)N$ we now rename the point $q_N^s$ into $q_{N+1}^s$ and pool this single sum together with the double sum in the last line in (49), obtaining

$$
\sum_{1 \leq i \leq N-1} V_s(|q_i^s - q_{N+1}^s|) + \sum_{1 \leq i < j \leq N} V_s(|q_i^s - q_j^s|) = \frac{1}{s} + \sum_{1 \leq i < j \leq N+1} V_s(|q_i^s - q_j^s|),
$$

(51)

where $q_k = q_k^s$ for $1 \leq k \leq N$ and $q_{N+1}^s = q_N^s$, and where we used that $V_s(0) = -\frac{1}{s}$ for $s < 0$; now multiplying by $2/(N + 1)N$ and recalling (3) yields

$$
\frac{2}{(N + 1)N} \left( \sum_{1 \leq i \leq N-1} V_s(|q_i^s - q_{N+1}^s|) + \sum_{1 \leq i < j \leq N} V_s(|q_i^s - q_j^s|) \right) = \frac{2}{(N + 1)N} \frac{1}{s} + \langle V_s \rangle(\omega'_{N+1}),
$$

(52)

where $\omega'_{N+1} = \{q_1^s, \ldots, q_{N+1}^s\}$.

For the remaining single sum, with factor $8/(N + 1)N(N - 1)$, we note that without loss of generality we may assume that

$$
\sum_{1 \leq i \leq N-1} V_s(|q_i^s - q_N^s|) \geq \sum_{1 \leq i \leq N, \ i \neq j} V_s(|q_i^s - q_j^s|), \quad \forall j = 1, \ldots, N.
$$

But then

$$
\frac{1}{N - 1} \sum_{1 \leq i \leq N-1} V_s(|q_i^s - q_N^s|) \geq \frac{2}{N(N - 1)} \sum_{1 \leq i < j \leq N} V_s(|q_i^s - q_j^s|)
$$

and therefore also

$$
\frac{1}{N - 1} \sum_{1 \leq i \leq N-1} V_s(|q_i^s - q_N^s|) \geq \frac{2}{(N - 1)(N - 2)} \sum_{1 \leq i < j \leq N-1} V_s(|q_i^s - q_j^s|).
$$

(53)

This estimate of the single sum from the middle line of (49) in terms of the double sum in the first line of (49) gives us

$$
\frac{2(N + 3)}{(N + 1)N(N - 1)} \sum_{1 \leq i < j \leq N-1} V_s(|q_i^s - q_j^s|)
$$

$$
+ \frac{8}{(N + 1)N(N - 1)} \sum_{1 \leq i \leq N-1} V_s(|q_i^s - q_N^s|)
$$

$$
\geq \frac{(N + 3)(N - 2) + 8}{(N + 1)N} \frac{2}{(N - 1)(N - 2)} \sum_{1 \leq i < j \leq N-1} V_s(|q_i^s - q_j^s|)
$$

$$
= \left( 1 + \frac{2}{(N + 1)N} \right) \langle V_s \rangle(\omega_N^s \{q_N^s\}).
$$
In total we therefore have the estimate

$$2v_s(N) \geq \frac{2}{(N+1)N} \left( \frac{1}{s} + \langle V_s \rangle(\omega_{N+1}) + \left( 1 + \frac{2}{(N+1)N} \right) \langle V_s \rangle(\omega_N^s \backslash q_N^s) \right),$$ (54)

which can be estimated again with the help of (11) to get

$$2v_s(N) \geq \frac{2}{(N+1)N} \left( \frac{1}{s} + v_s(N+1) + \left( 1 + \frac{2}{(N+1)N} \right) v_s(N-1) \right).$$ (55)

Lastly we regroup terms in (55) to get

$$v_s(N - 1) - 2v_s(N) + v_s(N + 1) \leq - \frac{2}{(N+1)N} \left( \frac{1}{s} + v_s(N-1) \right).$$ (56)

The proof is complete. □

**Remark 2.** Step (51) requires $V_s(0) < \infty$, which is true only for $s < 0$.

**Remark 3.** For $s < 0$ we have $\frac{1}{s} + v_s(N-1) < 0$ so that r.h.s. (56) $> 0$.

**Remark 4.** For the special value $s = -2$ we have the exact result (5) and a direct computation shows that $\bar{v}_{-2}(N) = -2/(N-1)^3 < 0$. Therefore, at least for $s = -2$, the upper estimate is not optimal.

Also, for $s < -2$ and even $N$, we have the exact result (6) which converges to $v_{-2}(N)$ when taking the limit $s \uparrow -2$ of (5). Again, a simple computation shows that $\bar{v}_s(N) < 0$ for $s < -2$ and $N$ even. Modulo confirming that the situation doesn't change when $N$ is odd, the upper bound on $\bar{v}_s(N)$ for $s < 0$ would be non-optimal for all $s \leq -2$.

**Remark 5.** The $1/s$ at r.h.s. (56) is a consequence of our definition of $V_s(r)$. By working with $\bar{V}_s(r) = r^{-s}/s$ instead, the $1/s$ term will not show up in (51) and (52) and hence be absent in (56), which would read

$$\bar{v}_s(N - 1) - 2\bar{v}_s(N) + \bar{v}_s(N + 1) \leq - \frac{2}{(N+1)N} \bar{v}_s(N - 1).$$ (57)

Note that indeed, the $1/s$ at r.h.s. (56) cancels against the $-1/s$ implicit in $v_s(N-1)$, and the l.h.s. of (55) is invariant under the change $V_s(r) \rightarrow \bar{V}_s(r)$ so that our (56) is quantitatively identical to (57).

**Remark 6.** If one could improve the factor 2 at r.h.s. (53) into a 3/2, this would prove concavity. However, the inequality (53) turns out to be sometimes an equality (e.g. when $s = -1$ and $N = 3$ or $N = 4$). Also (54), rewritten as

$$v_s(N - 1) - 2v_s(N) + v_s(N + 1) \leq v_s(N+1) - \langle V_s \rangle(\omega_{N+1}) + v_s(N - 1) - \langle V_s \rangle(\omega_N^s \backslash q_N^s)$$

$$\quad - \frac{2}{(N+1)N} \left( \frac{1}{s} + \langle V_s \rangle(\omega_N^s \backslash q_N^s) \right),$$ (58)
is still sometimes an equality! For instance, take \( s = -1 \), then \( v_{-1}(2) = 1 - 2 \) and \( v_{-1}(3) = 1 - \sqrt{3} \) and \( v_{-1}(4) = 1 - 2\sqrt{2}/3 \), so for \( N = 3 \) then \( v_{-1}(3) = v_{-1}(2) - 2v_s(3) + v_s(4) = 2(-1 + \sqrt{3} - \sqrt{2}/3) = -0.168891546... \), and the exact evaluation of r.h.s. \( (58) \) yields the same answer.

Remark 7. The only true inequality is in the step from \( (54) \) to \( (55) \). Thus, to prove concavity at least for some \( s \)-values one has to improve this estimate.

We have checked that for \( s = -1 \) and \( N = 3 \) the sum of the second line at r.h.s. \( (58) \) alone does not dominate the term in the third line; namely the sum of these two terms is \((7/6)\sqrt{3} - 2 > 0\). Also, the term in the first line at r.h.s. \( (58) \) alone does not dominate the one in the third line in this case; namely, their sum equals \( \sqrt{3}(1 - 2\sqrt{2}/3) > 0 \), too. Therefore, to prove concavity (for some negative \( s \)-values, say \( s \leq -1 \)), one will need to prove that the first two lines at the r.h.s. \( (58) \) together are more negative than the last line is positive, at least for a certain range of negative \( s \)-values.

4.2 Point-energies: better \( \Theta(N^{-2}) \) bounds on \( \ddot{v}_s(N) \), \( s < 0 \)

So far our analysis has only used the concept of an “energy of a configuration of \( N \) points,” which is based on the interpretation of \( V_s(|q - q'|) \) as a pair-energy. We now bring in the well-known concept of an “energy of an individual point,” or point-energy for short, which is based on the interpretation of \( V_s(|q - q'|) \) as the (potential) energy of a particle located at \( q \) in the potential field of a particle at \( q' \), a notion which is clearly reflexive.

We recall that every (unlabeled) \( N \)-point configuration \( \omega_N \) on \( S^2 \) can be assigned a unique compatible family of normalized, so-called empirical \( n \)-point measures, \( 1 \leq n \leq N \), and vice versa. For instance, with the help of any labeling, the first two of these can be written as

\[
\Delta_{\omega_N}^{(1)}(dq) = \frac{1}{N} \sum_{1 \leq j \leq N} \delta_{q_j}(dq),
\]

\[
\Delta_{\omega_N}^{(2)}(dq dq') = \frac{2}{N(N-1)} \sum_{1 \leq j < k \leq N} \delta_{q_j}(dq) \delta_{q_k}(dq'),
\]

and analogously one writes the empirical measures of higher order \( n = 3, ..., N \); here, with a mild abuse of notation, \( \delta_{q_j}(dq) \) denotes the Dirac measure on \( S^2 \) concentrated at \( q_j \), i.e. for any Borel subset \( \Lambda \) of \( S^2 \) we have \( \int_{\Lambda} \delta_{q_j}(dq) = 0 \) if \( q_j \notin \Lambda \), and \( \int_{\Lambda} \delta_{q_j}(dq) = 1 \) if \( q_j \in \Lambda \). With the help of \( \Delta_{\omega_N}^{(2)} \) we can rewrite

\[\text{35Note that the expressions at the r.h.s. are invariant under the permutation group } S_N, \text{ which is why the mapping } \omega_N \leftrightarrow \{\Delta_{\omega_N}^{(n)}\}_{n=1}^N \text{ is one-to-one only for unlabeled configurations.}\]
the average standardized Riesz pair-energy of an \( N \)-point configuration \( \omega_N \) as

\[
(V_s)(\omega_N) = \int_{\mathbb{S}^2 \times \mathbb{S}^2} V_s(|q - q'|) \Delta^{(2)}_{\omega_N}(dqdq').
\]  

(61)

Moreover, with the help of \( \Delta^{(1)}_{\omega_N} \) we can now associate with each \( N \)-point configuration \( \omega_N \) a standardized Riesz \( s \)-potential function on \( \mathbb{S}^2 \), given by

\[
(V_s \ast \Delta^{(1)}_{\omega_N})(q) \equiv \int_{\mathbb{S}^2} V_s(|q - q'|) \Delta^{(1)}_{\omega_N}(dq'), \quad q \in \mathbb{S}^2, \quad s < 0.
\]

(62)

Remark 8. Since \( s < 0 \), the potential function \( (62) \) is well-defined and finite on all of \( \mathbb{S}^2 \) because \( V_s : \mathbb{R}_+ \rightarrow \mathbb{R} \) is continuous for \( s < 0 \). Of course, provided one restricts \( q \) to \( \mathbb{S}^2 \setminus \omega_N \), one can also extend \( (62) \) continuously to the regime \( s \geq 0 \). Moreover, when \( s \in [0, 2) \) the function \( q' \mapsto V_s(|q - q'|) \) is weakly lower semi-continuous (i.e. \( V_s \) is the pointwise limit of an increasing sequence of continuous functions), and therefore the potential function \( (62) \) is well-defined (in the sense that it may be positive infinite for certain \( q \)) also for \( N \rightarrow \infty \), whenever \( \Delta^{(1)}_{\omega_N}(dq') \rightharpoonup \mu(dq') \) in the weak* sense, where \( \mu(dq') \) is some regular Borel measure on \( \mathbb{S}^2 \). Note that \( (V_s \ast \mu)(q) \leq \liminf (V_s \ast \Delta^{(1)}_{\omega_N})(q) \).

Of special interest to us are the standardized Riesz \( s \)-potentials of \( N \)-point configurations \( \omega_N \) on \( \mathbb{S}^2 \) obtained from \((N + 1)\)-point configurations by removing any particular point — or rather: their analogues with \( \omega_{N-1} \) replaced by \( \omega_{N-1} \). Every \( \omega_N \) defines a set of \( N \) such \((N - 1)\)-point configurations. After introducing any convenient labeling of the points in \( \omega_N \), this set of \((N - 1)\)-point configurations reads \( \{\omega_N\setminus\{q_\ell\}\}_{\ell=1}^N \). For every \((N - 1)\)-point configuration there is a standardized Riesz \( s \)-potential function on \( \mathbb{S}^2 \), given by \( (V_s \ast \Delta^{(1)}_{\omega_N\setminus\{q_\ell\}})(q) \).

For every point \( q_\ell \in \omega_N \), \( \ell \in \{1, \ldots, N\} \), its average standardized Riesz point-energy w.r.t. the reduced \((N - 1)\)-point configuration \( \omega_N\setminus\{q_\ell\} \) is simply the standardized Riesz \( s \)-potential of \( \omega_N\setminus\{q_\ell\} \) evaluated at \( q = q_\ell \), viz.

\[
\frac{1}{N - 1} \sum_{1 \leq j \leq N, \quad j \neq \ell} V_s(|q_j - q_\ell|) = (V_s \ast \Delta^{(1)}_{\omega_N\setminus\{q_\ell\}})(q_\ell), \quad \ell = 1, \ldots, N.
\]

(63)

Thus every \( \omega_N \) defines a set of \( N \) point-energies \( \{ (V_s \ast \Delta^{(1)}_{\omega_N\setminus\{q_\ell\}})(q_\ell) \}_{\ell=1}^N \). The average standardized Riesz pair-energy of \( \omega_N \) is the mean of these:

\[
(V_s)(\omega_N) = \frac{1}{N} \sum_{1 \leq \ell \leq N} (V_s \ast \Delta^{(1)}_{\omega_N\setminus\{q_\ell\}})(q_\ell).
\]

(64)

Remark 9. Given a minimizing configuration \( \omega_N^s \), it can easily be seen that

\[
(V_s \ast \Delta^{(1)}_{\omega_N^s\setminus\{q_\ell\}})(q) \geq (V_s \ast \Delta^{(1)}_{\omega_N^s\setminus\{q_\ell\}})(q_\ell^s) \quad \text{for all} \ q \in \mathbb{S}^2,
\]

(65)
which simply says that each (generalized) unit point charge in a minimal-energy configuration occupies a point of minimal potential energy in the potential field generated by the remaining (generalized) unit point charges.

With the help of the so-defined potential functions and point energies, we are ready to prove our next result, which improves the upper bound in Proposition 5 and also supplies a lower bound of the same type.

**Proposition 6.** For $s < 0$ the second discrete derivative of $v_s(N)$ is bounded above and below like

$$\frac{2}{(N+1)(N-2)} \left( v_s(N) + \frac{1}{s} \right) \leq \ddot{v}_s(N) \leq -\frac{2}{(N+1)N} \left( v_s(N) + \frac{1}{s} \right).$$

**Proof.** Using the definitions (3) and (63), for each $\ell = 1, \ldots, N$ we have

$$\langle V_s(\omega_N) \rangle = \frac{N - 2}{N} \langle V_s(\omega_N \setminus \{q_\ell\}) \rangle + \frac{2}{N} \langle V_s * \Delta_\omega'(\omega_N \setminus \{q_\ell\}) \rangle(q_\ell).$$

This will be our “master identity.”

First, averaging (66) over all $q_\ell$, $\ell = 1, \ldots, N$, and recalling (64), gives

$$\langle V_s(\omega_N) \rangle = \frac{1}{N} \sum_{1 \leq \ell \leq N} \langle V_s(\omega_N \setminus \{q_\ell\}) \rangle.$$  (67)

Now replacing $\omega_N$ by $\omega_N^s = \{q_1^s, \ldots, q_N^s\}$, a minimizing $N$-point configuration, and using (4) for $(N-1)$-point configurations at the r.h.s., we recover the monotonicity relation

$$v_s(N) \geq v_s(N-1), \quad \text{for all integers } N > 2; \quad (68)$$

cf. [Lan72, Kie09a, Kie09b].

Second, replacing $\omega_N$ in (66) with $\omega_N \cup \{q\}$, $q \in S^2$, and $q_\ell$ by $q$, yields

$$\langle V_s(\omega_N \cup \{q\}) \rangle = \frac{N - 1}{N + 1} \langle V_s(\omega_N) \rangle + \frac{2}{N + 1} \langle V_s * \Delta_\omega'(\omega_N) \rangle(q),$$

or, equivalently,

$$\langle V_s(\omega_N) \rangle = \frac{N + 1}{N - 1} \langle V_s(\omega_N \cup \{q\}) \rangle - \frac{2}{N - 1} \langle V_s * \Delta_\omega'(\omega_N) \rangle(q).$$  (69)

Now setting $q = q_\ell \in \omega_N$ and averaging (69) over all $q_\ell$, $\ell = 1, \ldots, N$, and recalling (63) and (64), gives

$$\langle V_s(\omega_N) \rangle = \frac{N}{N + 2} \frac{N + 1}{N - 1} \left\{ \frac{1}{N} \sum_{1 \leq \ell \leq N} \langle V_s(\omega_N \cup \{q_\ell\}) \rangle - \frac{2V_s(0)}{(N+1)N} \right\}.$$
Once again replacing \( \omega_N \) by \( \omega^s_N \), then using (4) with \( N \) replaced by \( N + 1 \) at the r.h.s., we find an estimate in the opposite direction to (68),

\[
v_s(N) \geq \frac{(N + 1)N}{(N + 2)(N - 1)} v_s(N + 1) - \frac{2v_s(0)}{(N + 2)(N - 1)}, \quad N > 2; \quad (70)
\]

note that \( V_s(0) = -1/s \) for \( s < 0 \).

Next, inserting a minimizing \( N \)-point configuration \( \omega^s_N = \{ q^s_1, \ldots, q^s_N \} \) directly into (66), and also into (69) with \( q = q^s_\ell \), then using (4), yields

\[
v_s(N) \geq \frac{N - 2}{N} v_s(N - 1) + \frac{2}{N}(V_s * \Delta^{(1)}_{\omega_N \setminus \{ q^s_\ell \}})(q^s_\ell), \quad (71)
\]

\[
v_s(N) \geq \frac{N + 1}{N - 1} v_s(N + 1) - \frac{2}{N}(V_s * \Delta^{(1)}_{\omega_N \setminus \{ q^s_\ell \}})(q^s_\ell) - \frac{2V_s(0)}{N(N - 1)}, \quad (72)
\]

for each \( \ell = 1, \ldots, N \). Recalling definition (12) of \( \ddot{v}_s(N) \), we split \( 2v_s(N) \) in (12) into \( (1 - \delta)v_s(N) + (1 + \delta)v_s(N) \), then use inequality (71) to estimate \((1 - \delta)v_s(N)\) and inequality (72) to estimate \((1 + \delta)v_s(N)\), arriving (after simplifications) at

\[
\ddot{v}_s(N) \leq \frac{2 + (N - 2)\delta}{N} v_s(N - 1) - \frac{2 + (N + 1)\delta}{N - 1} v_s(N + 1)
\]

\[
+ \frac{4\delta}{N} \left( V_s * \Delta^{(1)}_{\omega_N \setminus \{ q^s_\ell \}} \right)(q^s_\ell) - \frac{2(1 + \delta)}{s} \frac{1}{N(N - 1)}. \quad (73)
\]

This relation holds for all \( \ell = 1, \ldots, N \) and parameters \( \delta \) with \(-1 \leq \delta \leq 1\).

Let \( 0 < \delta \leq 1 \), and pick \( \ell \) such that

\[
(V_s * \Delta^{(1)}_{\omega_N \setminus \{ q^s_\ell \}})(q^s_\ell) \leq v_s(N); \quad (74)
\]

that such a choice of \( \ell \) is possible follows from (64). With these choices of \( \delta \) and \( \ell \), inequality (73) and the monotonicity relation (68) together give

\[
\ddot{v}_s(N) \leq \frac{2 + (N - 2)\delta}{N} v_s(N) - \frac{2 + (N + 1)\delta}{N - 1} v_s(N) + \frac{4\delta}{N} v_s(N)
\]

\[
- \frac{2(1 + \delta)}{s} \frac{1}{N(N - 1)}
\]

\[
= - \frac{2(1 + \delta)}{N(N - 1)} \left( v_s(N) + \frac{1}{s} \right). \quad (75)
\]

So nothing can be gained here.

Let \(-2/(N + 1) \leq \delta < 0\), and now pick \( \ell \) such that

\[
(V_s * \Delta^{(1)}_{\omega_N \setminus \{ q^s_\ell \}})(q^s_\ell) \geq v_s(N); \quad (75)
\]

\[
\]
that such a choice of $\ell$ is possible also follows from (64). With these choices of $\delta$ and $\ell$, inequality (73) and the estimate (70) together give

$$\ddot{v}_s(N) \leq -\frac{2(1 + \delta)}{N(N - 1)} \left( v_s(N) + \frac{1}{s} \right), \quad -\frac{2}{N + 1} \leq \delta < 0,$$

for $2 + (N - 2)\delta \geq 0$ and $2 + (N + 1)\delta \geq 0$. Since $v_s(N) + 1/s < 0$, we obtain for $\delta = -2/(N + 1)$ the upper estimate exhibited in Proposition 6

$$\ddot{v}_s(N) \leq -\frac{2}{(N + 1)N} \left( v_s(N) + \frac{1}{s} \right).$$

On the other hand, the estimates (72) and (74) can be used to get a lower bound for $v_s(N - 1)$,

$$v_s(N - 1) \geq \frac{N}{N + 1} \frac{N - 1}{N - 2} v_s(N) - \frac{2V_s(0)}{(N + 1)(N - 2)}.$$

This estimate and the estimate $v_s(N + 1) \geq v_s(N)$ allow us to estimate the r.h.s. in the definition (12) of $\ddot{v}_s(N)$ to obtain the lower estimate exhibited in Proposition 6.

$$\ddot{v}_s(N) \geq \frac{N}{N + 1} \frac{N - 1}{N - 2} v_s(N) - \frac{2V_s(0)}{(N + 1)(N - 2)} - 2v_s(N) + v_s(N)$$

$$= \frac{2}{(N + 1)(N - 2)} (v_s(N) - V_s(0)).$$

Remark 10. For $\delta \leq -2/(N + 1)$ and $\ell$ as in (75), we obtain from (73) (using $v_s(N) \geq v_s(N - 1)$)

$$\ddot{v}_s(N) \leq \frac{2 + (N - 2)\delta}{N} v_s(N - 1) - \frac{2 + (N + 1)\delta}{N - 1} v_s(N + 1) + \frac{4\delta}{N} v_s(N)$$

$$- \frac{2(1 + \delta)}{s} \frac{1}{N(N - 1)}$$

$$\leq \frac{2 + (N + 2)\delta}{N} v_s(N - 1) - \frac{2 + (N + 1)\delta}{N - 1} v_s(N + 1)$$

$$- \frac{2(1 + \delta)}{s} \frac{1}{N(N - 1)}$$

$$= \frac{2}{N} v_s(N - 1) - \frac{2}{N - 1} v_s(N + 1) - \frac{1}{s N(N - 1)}$$

$$+ \left( \frac{N + 2}{N} v_s(N - 1) - \frac{N + 1}{N - 1} v_s(N + 1) - \frac{2}{s N(N - 1)} \right) \delta.$$
Both factors $2 + (N + 2)\delta$ and $2 + (N + 1)\delta$ are $\leq 0$. As special cases one has

$$\ddot{v}_s(N) \leq -\frac{2}{N(N+1)} \left( v_s(N-1) + \frac{1}{s} \right) \quad \text{if } \delta = -\frac{2}{N+1},$$

$$\ddot{v}_s(N) \leq v_s(N+1) - v_s(N-1) \quad \text{if } \delta = -1;$$

the first of these inequalities is simply Proposition 5, while the second one also allows one to obtain identities relating point energies and the average pair-energy when a single point is removed or added in again, as follows.

Remark 11. The concept of the Riesz potential of an $N$-point configuration also allows one to obtain identities relating point energies and the average pair-energy when a single point is removed or added in again, as follows.

Again inserting a minimizing $N$-point configuration $\omega^s_N = \{q_1^s, \ldots, q_N^s\}$ into (65), and also into (63) with $q = q_{\ell}^s$, but this time not using (4), yields

$$v_s(N) = \frac{N-2}{N} \langle V_s(\omega_{N}^s\backslash\{q_\ell^s\}) \rangle + \frac{2}{N} \langle V_s \ast \Delta_{\omega_{N}^s\backslash\{q_\ell^s\}}(q_{\ell}^s) \rangle,$$

(76)

$$v_s(N) = \frac{N+1}{N-1} \langle V_s(\omega_{N}^s \cup \{q_\ell^s\}) \rangle - \frac{2}{N} \langle V_s \ast \Delta_{\omega_{N}^s\backslash\{q_\ell^s\}}(q_{\ell}^s) \rangle,$$

(77)

for all $\ell = 1, \ldots, N$, meaning we have $2N$ (not necessarily all different) expressions for $v_s(N)$.

Now subtracting (76) “from itself,” with two different $\ell$-values in place, and the same for (77), and the same for the identity r.h.s. (76) = r.h.s. (77), and resorting, yields for all $\ell, \ell' = 1, \ldots, N$ the identities:

$$\frac{N-2}{N} \left[ \langle V_s(\omega_{N}^s\backslash\{q_\ell^s\}) \rangle - \langle V_s(\omega_{N}^s\backslash\{q_{\ell'}^s\}) \rangle \right]$$

$$= \frac{2}{N} \left[ \langle V_s \ast \Delta_{\omega_{N}^s\backslash\{q_{\ell'}^s\}}(q_{\ell}^s) \rangle - \langle V_s \ast \Delta_{\omega_{N}^s\backslash\{q_\ell^s\}}(q_{\ell'}^s) \rangle \right]$$

$$= \frac{N+1}{N-1} \left[ \langle V_s(\omega_{N}^s \cup \{q_{\ell'}^s\}) \rangle - \langle V_s(\omega_{N}^s \cup \{q_\ell^s\}) \rangle \right].$$

In this vein, alternate exact representations of the discrete second derivative of $v_s(N)$ follow; for instance, we offer

$$\ddot{v}_s(N) = v_s(N-1) - \langle V_s(\omega_{N}^s\backslash\{q_\ell^s\}) \rangle + v_s(N+1) - \langle V_s(\omega_{N}^s \cup \{q_{\ell}^s\}) \rangle$$

$$- \frac{2}{N} \left[ \langle V_s \ast \Delta_{\omega_{N}^s\backslash\{q_\ell^s\}}(q_{\ell'}^s) \rangle - \langle V_s(\omega_{N}^s\backslash\{q_\ell^s\}) \rangle \right]$$

$$+ \langle V_s(\omega_{N}^s \cup \{q_{\ell}^s\}) \rangle - \langle V_s \ast \Delta_{\omega_{N}^s\backslash\{q_{\ell'}^s\}}(q_{\ell'}^s) \rangle$$

$$+ \frac{2}{N(N-1)} \left[ \langle V_s(\omega_{N}^s \cup \{q_{\ell'}^s\}) \rangle - V_s(0) \right].$$

Note that from the definition [3] it follows that the first line at the r.h.s. $< 0$.

\[30\] In fact, one can show these hold for all general $N$-point sets $\omega_N$.  

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By the last line in our remark we obtain an upper bound on $\ddot{v}_s(N)$ entirely in terms of expressions involving only the optimal $N$-point configuration, viz.

**Proposition 7.** For $s < 0$ the map $N \mapsto \ddot{v}_s(N)$ is bounded above by

$$
\ddot{v}_s(N) \leq -\frac{2}{N} \left[ (V_s \ast \Delta_N^{(1)}(q^*_t))(-q^*_t) - (V_s \ast \Delta_N^{(1)}(q^*_t'))(q^*_t') + \langle V_s \rangle(\omega_N^s \cup \{q^*_t\}) - \langle V_s \rangle(\omega_N^s \setminus \{q^*_t\}) \right] + \frac{2}{N(N-1)} \left[ \langle V_s \rangle(\omega_N^{s+1} \cup \{p\}) - V_s(0) \right].
$$

4.3 Upper bounds on $\ddot{v}_s(N)$ for $N \in \{4, 6, 12\}$, $s \in (-2, \infty)$

The upper and lower bounds on $\ddot{v}_s(N)$ presented so far are valid for general $N > 2$ and $s < 0$. No structural information about any optimizer was used.

For the $N$-values of the universal configurations, viz. $N = 3, 4, 6, 12$, one can easily get better upper bounds on $\ddot{v}_s(N)$ for any $s$; though for $N = 3$ this is a pointless exercise, because (11) gives the exact expression of $\ddot{v}_s(3)$ for all $s > -2$; cf. Subsection 3.3 where we found that $\ddot{v}_s(3) < 0$ for $s < 9.4$ (approximately). This leaves the cases $N \in \{4, 6, 12\}$.

We begin by noting the obvious inequality

$$
\ddot{v}_s(N) \leq \langle V_s \rangle(\omega_{N-1}) - 2v_s(N) + \langle V_s \rangle(\omega_{N+1});
$$

(78)

here, $\omega_{N-1}$ and $\omega_{N+1}$ are any convenient $(N \pm 1)$-point configurations. Inequality (78) allows us to state an immediate corollary to the results of Section 3.

**Corollary 1.** Since the optimizers for $N \in \{3, 4\}$ are universal, but not the one for $N = 5$, r.h.s. (43) is a rigorous upper bound to $\ddot{v}_s(4)$ for all $s \in (-2, \infty)$.

Since the $N = 6$ optimizer is universal, but not those for $N \in \{5, 7\}$, r.h.s. (46) is a rigorous upper bound to $\ddot{v}_s(6)$ for all $s \in (-2, \infty)$.

Similarly, based on the fact that the $N = 12$ optimizer is universal while those for $N \in \{11, 13\}$ are not, we can obtain rigorous upper bounds on $\ddot{v}_s(12)$.

**Proposition 8.** The map $s \mapsto \ddot{v}_s(12)$ is bounded above by

$$
\ddot{v}_s(12) < \langle V_s \rangle(\omega_{12}^s \cup \{q^*_1\}) - 2v_s(12) + \langle V_s \rangle(\omega_{12}^s \cup \{p\}).
$$

(79)

37 Of course, the $N = 2$ configuration is also universally optimal, but "$\ddot{v}_s(2)$" is ill-defined.

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In particular, choosing the epi-center of a face of the icosahedron for $p$ yields

$$
\ddot{v}_s(12) < \frac{1}{26} \left[ \left( \sqrt{1 - \frac{3 + \sqrt{5}}{2 \sqrt{3 \sin \frac{\pi}{5}}} + \frac{3 + \sqrt{5}}{5 \sin^2 \frac{\pi}{5}}} \right)^{-s} + \left( \sqrt{1 + \frac{3 + \sqrt{5}}{2 \sqrt{3 \sin \frac{\pi}{5}}} + \frac{3 + \sqrt{5}}{5 \sin^2 \frac{\pi}{5}}} \right)^{-s}
+ \left( 2 \sin \left[ \frac{1}{2} \arccos \frac{1}{\sqrt{3 \sin \frac{\pi}{5}}} + \frac{1}{2} \arctan \frac{1}{2} \right] \right)^{-s}
+ \left( 2 \sin \left[ \frac{1}{2} \arcsin \frac{1}{\sqrt{3 \sin \frac{\pi}{5}}} + \frac{1}{2} \arccot \frac{1}{2} \right] \right)^{-s}
- \frac{2}{143} \left[ 5 \left( \frac{1}{\sin \frac{\pi}{5}} \right)^{-s} + 5 \left( \frac{4 \sin^2 \frac{\pi}{5} - 1}{\sin \frac{\pi}{5}} \right)^{-s} + 2^{-s} \right] \right].
$$

(80)

Note that the two trial configurations used to obtain (80) are not local energy minimizers (not even mechanical equilibrium configurations). Unfortunately, we pay a high price for having chosen these configurations which allowed us to compute an upper estimate explicitly: r.h.s. (80) > 0 for all $s$; its minimum $\approx 0.014$ at $s \approx -1.8$. Presumably good upper bounds can only be obtained with the aid of a computer, by optimizing the parameters in some well-chosen multi-parameter family of configurations.

5 An asymptotic point of view

A rigorous proof of the concavity of $N \mapsto v_s(N)$ for some regime of $s$-values (possibly for all $s < s_*$, with $s_*$ conjectured to be in $(-1, 0)$) most likely has to be based on a combination of different strategies. Attempts to rigorously identify all the optimizers and to check for the negativity of $\ddot{v}_s(N)$ by “explicit computation” may be feasible for sufficiently small $N$-values, but clearly are bound to fail even for moderately large $N$-values. On the other hand, the very-large-$N$ regime is to some extent accessible by asymptotic analysis. Ultimately the goal is to determine the complete asymptotic large-$N$ expansion of $N \mapsto v_s(N)$, but at least as many terms as possible. With enough hard work one may be able to extend the asymptotic control down to sufficiently small $N$-values to establish an overlap with some explicitly controlled small-$N$ regime. In the previous section we presented the type of analysis suitable for the small-$N$ regime. This section is devoted to asymptotic analysis.

It has already been mentioned in the introduction that the limit $\lim_{N \to \infty} v_s(N)$ is given by the variational principle (10). Explicitly

$$
\lim_{N \to \infty} v_s(N) = \inf_{\mu \in \mathfrak{P}(S^2)} \int_{S^2 \times S^2} \frac{1}{s} \left( \frac{1}{|p - q|^s} - 1 \right) \mu(dp) \mu(dq),
$$

(81)

where $\mathfrak{P}(S^2)$ is the set of all Borel probability measures supported on $S^2$. By classical potential theory ([Bjo56] for $s < 0$, and [Lan72] for $s > 0$) one knows
that for \( s < 2 \),
\[
J_s[\mu] \equiv \int_{S^2} \int_{S^2} \frac{1}{|p - q|^s} \mu(d p) \mu(d q) \tag{82}
\]
is well-defined and finite for any \( \mu \in \mathcal{P}(S^2) \). On \( \mathcal{P}(S^2) \) the Riesz \( s \)-energy integral has a degenerate maximum with value \( 2|s|^{-1} \) when \( s \leq -2 \), and it has a unique maximum when \(-2 < s < 0\), respectively a unique minimum when \( 0 < s < 2 \), achieved at the normalized surface area measure \( \sigma \) on \( S^2 \subset \mathbb{R}^3 \), with value
\[
J_s[\sigma] = \frac{2^{1-s}}{2 - s} \equiv W_s; \tag{83}
\]
this expression is also valid at \( s = 0 \), with \( J_0[\mu] \equiv 1 \) for all \( \mu \in \mathcal{P}(S^2) \). For \( s \geq 2 \) the energy integral (82) is \(+\infty\) for any \( \mu \in \mathcal{P}(S^2) \). Altogether, therefore,
\[
\lim_{N \to \infty} v_s(N) = \begin{cases} 
\frac{1}{s} \left(2^{-s-1} - 1\right) & \text{if } s \in (-\infty, -2], \\
\frac{1}{s} (W_s - 1) & \text{if } s \in [-2, 2), \\
\infty & \text{if } s \in [2, \infty),
\end{cases} \tag{84}
\]
with the special case \( s = 0 \) included as \( \lim_{s \to 0} \frac{1}{s} (W_s - 1) = \frac{1}{2} + \ln \frac{1}{2} \). We need to know how these limiting “values” are approached by \( v_s(N) \) as \( N \to \infty \).

For the regime \( s < -2 \) we already have an exact formula for \( v_s(N) \) valid for all even \( N \), namely (8). Yet, as mentioned in the introduction, the \( s < -2 \) regime is largely unsettled for odd \( N \), and we have nothing to add to this here. Moreover, the case \( s = -2 \) is completely solved, with \( v_{-2}(N) \) given by (5). Thus, henceforth we will discuss the regime \( s > -2 \). Clearly, we need to further make the distinction between the subregimes \( s \in (-2, 2) \) and \( s \geq 2 \).

As to the regime \( s \in (-2, 2) \), to find the large-\( N \) asymptotic expansion of \( v_s(N) \) one seeks the powers \( \alpha_s \in \mathbb{R} \) and \( \beta_s \in \mathbb{R} \) for which a nontrivial limit
\[
\lim_{N \to \infty} N^{\alpha_s} (\ln N)^{\beta_s} \left(v_s(N) - \frac{1}{s} (W_s - 1)\right) = \tilde{C}_s \tag{85}
\]
exists; then subtracts \( \tilde{C}_s \) from the expression under the limit in (83), multiplies by \( N^{\alpha'_s} (\ln N)^{\beta'_s} \) with new powers \( \alpha'_s \) and \( \beta'_s \), and repeats the procedure; etc. This strategy has to some extent been carried out in the literature, see [BHS12] for a recent account. We will call upon the results of [BHS12] in a moment. To pave the way for our discussion we first recall the definition (8) of \( v_s(N) \), involving our standardized Riesz pair-energy \( V_s(r) \) given in (1), and note that the additive term \( \frac{1}{s} \) in the difference \( v_s(N) - \frac{1}{s} (W_s - 1) \) cancels out. This motivates the definition of the \( S^2 \)-adjusted Riesz pair-energy
\[
U_s(r) \equiv s^{-1} \left(r^{-s} - W_s\right), \quad s < 2, \quad s \neq 0, \tag{86}
\]
and its $s \to 0$ limit

$$U_0(r) \equiv -\log r - W_{\log},$$

(87)

where

$$W_{\log} \equiv \inf \left\{ \int_{S^2} \int_{S^2} \log \frac{1}{|p-q|} \mu(dp) \mu(dq) : \mu \in \mathfrak{P}(S^2) \right\}$$

is the $s$-derivative of

$$W_s = 1 + \left( \frac{1}{2} - \log 2 \right) s + O(s^2) \quad \text{as} \quad s \to 0,$$

evaluated at $s = 0$, with value $W_{\log} (= W'_0) = \frac{1}{2} + \log \frac{1}{2} = -0.193147... < 0$.

We define the average $S^2$-adjusted Riesz pair-energy of a configuration by

$$\langle U_s \rangle(\omega_N) \equiv \frac{2}{N(N-1)} \sum_{1 \leq j < k \leq N} U_s(|q_j - q_k|), \quad s \in (-2,2),$$

(88)

and the minimal average $S^2$-adjusted Riesz pair-energy by

$$u_s(N) \equiv \inf_{\omega_N \subset S^2} \langle U_s \rangle(\omega_N), \quad s \in (-2,2).$$

(89)

We note that for each $s \in (-2,2)$ the map $N \mapsto u_s(N)$ is monotonically increasing and that, by construction, the limit is 0. Hence $u_s(N) \leq 0$ for all $N$.

As for the regime $s \geq 2$, since $v_s(N) \to \infty$ as $N \to \infty$, it would seem that the asymptotic analysis has to be set up in a somewhat different manner. In fact, this is true for $s = 2$ (see below). However, it is worth noting that r.h.s.\(^{[83]}\) is defined on the complex $s$-plane except at the single and simple pole at $s = 2$ and thus gives the analytic continuation of $W_s$ to the complex $s$-plane. We will denote this meromorphic function by the same symbol, $W_s$.

Understood in this analytically extended way, (85) and the ensuing description, the definition (86), as well as (88) and (89), all make sense also for the regime $s > 2$. Note, though, that for $s > 2$ the map $N \mapsto u_s(N)$ diverges monotonically to $+\infty$ as $N \to \infty$ (hence $u_s(N) \leq 0$ for most $N$ when $s > 2$), so that the power $\alpha_s \leq 0$ for $s > 2$ (and if $\alpha_s = 0$, then $\beta_s < 0$), while for $s < 2$ the power $\alpha_s \geq 0$ (and if $\alpha_s = 0$, then $\beta_s > 0$). While all this may seem just like a convenient coincidence, we shall see in Subsection 5.2 that the analytic continuation to $s > 2$ actually seems to have some deeper significance for the asymptotic problem; cf. [BHS12].

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\(^{38}\)The energy functionals $\langle U_s \rangle(\omega_N)$ (without the normalization $1/(N(N-1))$) were studied by Wagner [Wa90, Wa92] who first derived two-sided bounds for optimal $N$-point configurations in terms of the correct order of decay of $N$ for the complete range $-2 < s < 2$. 

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As to the singular case \( s = 2 \), it obviously makes no sense to subtract the infinite term \( \frac{1}{2} W_2 \) from \( v_2(N) \), or from \( V_2(r) \). Yet, if one replaces (85) by

\[
\lim_{N \to \infty} N^{\alpha_2} (\ln N)^{\beta_2} \left( v_2(N) + \frac{1}{2} \right) = \hat{C}_2;
\]

the ensuing description remains valid, with the definitions (88) and (89) extended to \( s = 2 \) with the help of the definition \( U_s(r) \equiv \frac{1}{2} r^2 \). Note that \( N \mapsto u_2(N) \) diverges monotonically to \( +\infty \) as \( N \to \infty \), so the same remarks apply as for the hypersingular regime \( s > 2 \) regarding the powers \( \alpha_s \) and \( \beta_s \).

Clearly, for each \( s \in (-2, \infty) \), \( s \neq 2 \), the \( S^2 \)-adjusted pair-energy \( U_s(r) \) on \( S^2 \) and the standardized pair-energy \( V_s(r) \) differ only by a constant, viz.

\[
U_s(r) = V_s(r) + s^{-1}(1 - W_s), \quad r > 0,
\]

with the case \( s = 0 \) understood as limit \( s \to 0 \), viz. \( U_0(r) = V_0(r) + W_{\log} \). As a consequence, all their discrete \( N \)-derivatives coincide; in particular,

**Lemma 1.** For all \( s > -2 \) (\( s \neq 2 \)) we have

\[
\dot{u}_s(N) = \dot{v}_s(N), \quad (92)
\]

\[
\ddot{u}_s(N) = \ddot{v}_s(N). \quad (93)
\]

In the remaining subsections we will elaborate on the asymptotic expansion of \( N \mapsto u_s(N) \) and its implications for the asymptotic expansion of \( N \mapsto \dot{v}_s(N) \). Subsection 5.1 is concerned with the potential regime \( s \in (-2, 2) \), Subsection 5.2 with the hypersingular regime \( s > 2 \), and Subsection 5.3 with the singular case \( s = 2 \). As mentioned earlier, a discussion of the “degeneracy regime” \( s \leq -2 \) has to be left for some future work.

### 5.1 The potential-theoretical regime \(-2 < s < 2\)

#### 5.1.1 The non-logarithmic cases

In the non-logarithmic cases one has the following bounds for \( u_s(N) \).

**Proposition 9.** Let \( -2 < s < 2 \) with \( s \neq 0 \). Then there exist positive \( s \)-dependent constants \( C > c > 0 \) such that for all sufficiently large \( N \geq 2 \)

\[
\frac{1}{s} \frac{W_s - c N^{s/2}}{N - 1} \leq u_s(N) \leq \frac{1}{s} \frac{W_s - C N^{s/2}}{N - 1} \quad \text{if } -2 < s < 0,
\]

\[
\frac{1}{s} \frac{W_s - c N^{s/2}}{N - 1} \leq u_s(N) \leq \frac{1}{s} \frac{W_s - c N^{s/2}}{N - 1} \quad \text{if } 0 < s < 2.
\]
Proof. We will call upon the results of [BHS12] and references cited therein. To facilitate the identification of the relevant results in the pertinent literature, we introduce the optimal Riesz s-energy of N points on $S^2$, defined for $s \not= 0$ by

$$E_s(S^2, N) \equiv \text{sign} (s) \inf \left\{ \frac{1}{2} \sum_{1 \leq j < k \leq N} \frac{\text{sign} (s)}{|q_j - q_k|^s} : \{q_1, \ldots, q_N\} \subset S^2 \right\},$$

cf. [HaSa04]. Then it is known\(^{39}\) (cf. [BHS12]) that there are s-dependent constants $C > c > 0$ such that

$$-CN^{1+s/2} \leq E_s(S^2, N) - W_s N^2 \leq -cN^{1+s/2}$$

for all sufficiently large $N \geq 2$. Hence

$$-C \frac{N^{1+s/2}}{N(N-1)} \leq \frac{E_s(S^2, N)}{N(N-1)} - W_s + \left(1 - \frac{N^2}{N(N-1)}\right) W_s \leq -c \frac{N^{1+s/2}}{N(N-1)},$$

or, equivalently,

$$\frac{W_s - C N^{s/2}}{N-1} \leq \frac{E_s(S^2, N)}{N(N-1)} - W_s \leq \frac{W_s - c N^{s/2}}{N-1}.$$

The desired relations follow by multiplying the last relations with $1/s$ and using the definition of the $s$-adjusted Riesz pair-energy.

From the bounds in Proposition 9 we get estimates for the discrete second derivative of $u_s(N)$ (and by means of Lemma 1 for $v_s(N)$).

Proposition 10. Let $s \in (-2, 2)$, $s \not= 0$. Let $c$ and $C$ be the constants from Proposition 4. For $s \in (-2, 0)$ the discrete second derivative of $u_s(N)$ satisfies

$$\ddot{u}_s(N) \leq -\frac{2(C - c)}{s} N^{s/2} \frac{1}{N-1} + \frac{W_s}{s} \frac{1}{N(N-1)(N-2)} - \frac{C}{s} \frac{N^{s/2} H_s(N)}{N(N-1)(N-2)},$$

where $H_s(N) \rightarrow (2 - s)(4 - s) > 0$ as $N \rightarrow \infty$. The right-hand side becomes a lower bound by interchanging $c$ and $C$.

The bounds for $0 < s < 2$ are obtained by interchanging $c$ and $C$ in the bounds for $\ddot{u}_s(N)$ with $-2 < s < 0$.

\(^{39}\)It is furthermore well-known that for a sequence $\{\omega_N^s\}_{N \geq 2}$ of optimal N-point configurations with $-2 < s < 2$ ($s \not= 0$) one has the limit relation

$$\lim_{N \rightarrow \infty} \frac{2}{N(N-1)} \sum_{1 \leq j < k \leq N} |q_j^s - q_k^s|^{-s} = W_s. \quad (94)$$

The reciprocal of the quantity under the limit symbol is also known as the $N$-th generalized diameter of $S^2$. It converges monotonically to the generalized transfinite diameter of $S^2$, introduced by Pólya and Szegő in [PoSz31], which equals the so-called $s$-capacity $1/W_s$ of $S^2$. Incidentally, it should also be noted that $-|p - q|^{-s}$ is a conditionally positive definite function of order 1 for $-2 < s < 0$; cf. [SSS88].
Proof. Let \(-2 < s < 0\). First, we consider the upper bound. By the definition of \(\tilde{u}_s(N)\) and Proposition \[10\]

\[
\tilde{u}_s(N) \leq \frac{1}{s} \left( W_s - C(N-1)^{s/2} - \frac{2}{s} W_s - cN^{s/2} \right) \frac{s}{N-1} + \frac{1}{s} W_s - C(N+1)^{s/2} \frac{N}{N-1}
\]

\[
= \frac{W_s}{s} \left( \frac{1}{N-2} - \frac{2}{N-1} + \frac{1}{N} \right)
\]

\[
- \frac{1}{s} \left\{ \frac{C(N-1)^{s/2}}{N-2} - \frac{2cN^{s/2}}{N-1} + \frac{C(N+1)^{s/2}}{N} \right\}
\]

\[
= -\frac{2(C - c)}{s} \frac{N^{s/2}}{N-1} + \frac{W_s}{s} \frac{1}{N(N-1)(N-2)}
\]

\[
- \frac{1}{s} \left\{ \frac{(N-1)^{s/2}}{N-2} - \frac{2N^{s/2}}{N-1} + \frac{(N+1)^{s/2}}{N} \right\}
\]

Since the function (using the integral representation of the gamma function)

\[
f(x) \equiv \frac{x^{s/2}}{x-1} = \sum_{n=0}^{\infty} \frac{1}{x^{n+1-s/2}} = \int_{0}^{\infty} e^{-xt} \sum_{n=0}^{\infty} \frac{t^{n-s/2}}{\Gamma(n+1-s/2)} dt, \quad x > 1,
\]

is strictly monotonically decreasing and convex, the last expression in braces is strictly positive. Series expansion (assisted by MATHEMATICA) reveals

\[
\frac{(N-1)^{s/2}}{N-2} - \frac{2N^{s/2}}{N-1} + \frac{(N+1)^{s/2}}{N} = \frac{N^{s/2}}{N(N-1)(N-2)} \left\{ (2-s)(4-s) - \frac{s(s-4)}{2} N^{-1} + \cdots \right\}
\]

Thus

\[
\tilde{u}_s(N) \leq -\frac{2(C - c)}{s} \frac{N^{s/2}}{N-1} + \frac{W_s}{s} \frac{1}{N(N-1)(N-2)} - \frac{C}{s} \frac{N^{s/2}H_s(N)}{N(N-1)(N-2)}
\]

where \(H_s(N) \rightarrow (2-s)(4-s) > 0\) as \(N \rightarrow \infty\).

For a lower bound one has to interchange \(C\) and \(c\).

For \(s \in (0, 2)\), the above computations hold with \(c\) and \(C\) interchanged. \(\square\)

Proposition \[10\], although much weaker than Proposition \[6\], clearly shows that one needs more information about the asymptotic behavior of \(u_s(N)\) for large \(N\).

The investigation of the asymptotic behavior of \(E_s(S^2, N)\) for large \(N\) yields the following fundamental conjecture. (We refer the interested reader to \[BHS12\] and papers cited therein.)

**Conjecture 1.** Let \(-2 < s < 2\) and \(s \neq 0\). Then there exists a constant \(C_s\) and a function \(\Omega_s(N)\) such that

\[
u_s(N) = \frac{1}{s} \frac{C_s}{(4\pi)^{s/2}} N^{s/2-1} + \frac{W_s}{s} N^{-1} + \Omega_s(N) \quad \text{for all} \quad N \geq 2
\]
and $N^{1-s/2} \Omega_s(N) \to 0$ as $N \to \infty$.

It should be noted that the $N^{-1}$-term may be dominated by the function $\Omega_s(N)$ for $0 < s < 2$. Indeed, at presence it is unclear how fast $N^{1-s/2} \Omega_s(N)$ tends to zero as $N \to \infty$. One suggestion is that $N^{(s-1)/2-1}$ (or even $N^{s/2-2}$) is the correct order of $N$ for the next term. The numerical evidence is inconclusive in this regard. Worse, the properly normalized $\Omega_s(N)$ may be oscillating with bounded non-zero amplitude as $N$ becomes large.

**Motivation of Conjecture 1.** For $-2 < s < 2$ and $s \neq 0$, the following conjecture for the large-$N$ behavior of $\mathcal{E}_s(S^2, N)$ is known (cf. [BHS12] for a most recent account)

$$\mathcal{E}_s(S^2, N) = W_s N^2 + \frac{C_s}{(4\pi)^{s/2}} N^{1+s/2} + \mathcal{R}_s(N),$$

where $\mathcal{R}_s(N)/N^{1+s/2} \to 0$ as $N \to \infty$. Hence,

$$u_s(N) = \frac{1}{s} \left\{ \frac{\mathcal{E}_s(S^2, N)}{N(N-1)} - W_s \right\} = \frac{1}{s} \left\{ \left( \frac{N}{N-1} - 1 \right) W_s + \frac{C_s}{(4\pi)^{s/2}} N^{1+s/2} + \frac{\mathcal{R}_s(N)}{N(N-1)} \right\}$$

$$= \frac{1}{s} \left\{ \frac{C_s}{(4\pi)^{s/2}} N^{s/2-1} + W_s N^{-1} + \frac{W_s + \frac{C_s}{(4\pi)^{s/2}} N^{s/2} + \mathcal{R}_s(N)}{N(N-1)} \right\}$$

$$= \frac{1}{s} \frac{C_s}{(4\pi)^{s/2}} N^{s/2-1} + \frac{W_s}{s} N^{-1} + \Omega_s(N),$$

where

$$\Omega_s(N) = \frac{1}{N(N-1)} \left\{ \frac{W_s}{s} + \frac{1}{s} \frac{C_s}{(4\pi)^{s/2}} N^{s/2} + \frac{1}{s} \frac{\mathcal{R}_s(N)}{N^{1+s/2}} \right\}.$$ 

By the assumption on $\mathcal{R}_s(N)$ it follows that $N^{1-s/2} \Omega_s(N) \to 0$ as $N \to \infty$. □

Conjecture 1 imposes the following large-$N$ behavior for the discrete second derivative of $u_s(N)$.

**Corollary 2.** Let $-2 < s < 2$ with $s \neq 0$. Under the assumption that Conjecture 1 is true, there holds

$$\ddot{u}_s(N) = \frac{(1-s/2)(2-s/2)}{s} \frac{C_s}{(4\pi)^{s/2}} N^{s/2-3} + \frac{2}{s} W_s N^{-3} + \ddot{\Omega}_s(N) + F_s(N) \quad (95)$$

with $N^{4-s/2} F_s(N) \to 0$ as $N \to \infty$. 54
Proof. By the definition of the discrete second derivative (cf. (12))

\[
\ddot{u}_s(N) = \frac{1}{s} \frac{C_s}{(4\pi)^{s/2}} N^{s/2-1} \left\{ \left(1 - \frac{1}{N}\right)^{s/2-1} - 2 - \left(1 + \frac{1}{N}\right)^{s/2-1} \right\}
+ \frac{W_s}{s} N^{-1} \left\{ \left(1 - \frac{1}{N}\right)^{-1} - 2 - \left(1 + \frac{1}{N}\right)^{-1} \right\} + \ddot{\Omega}_s(N).
\]

Series expansion gives (here \((a)_n\) is the Pochhammer symbol or rising factorial)

\[
\left(1 - \frac{1}{N}\right)^{s/2-1} - 2 - \left(1 + \frac{1}{N}\right)^{s/2-1} = \sum_{n=1}^{\infty} \frac{(1-s/2)_n}{n!} \frac{1+(-1)^n}{N^n}
\]
and simplification yields

\[
\left(1 - \frac{1}{N}\right)^{-1} - 2 - \left(1 + \frac{1}{N}\right)^{-1} = \frac{2}{N^2 - 1}.
\]

Hence

\[
\ddot{u}_s(N) = \frac{(1-s/2)_2}{s} \frac{C_s}{(4\pi)^{s/2}} N^{s/2-3} + \frac{2}{s} W_s N^{-3} + \ddot{\Omega}_s(N) + F_s(N),
\]
where

\[
F_s(N) \equiv \frac{1}{s} \frac{C_s}{(4\pi)^{s/2}} N^{s/2-1} \left[ \left(1 - \frac{1}{N}\right)^{s/2-1} - 2 - \left(1 + \frac{1}{N}\right)^{s/2-1} - \frac{(1-s/2)_2}{N^2} \right]
+ \frac{W_s}{s} \frac{2}{N^3(N^2 - 1)}
\]
and \(N^{4-s/2}F_s(N) \to 0\) as \(N \to \infty\), since \(-2 < s < 2\).

Remark 12. For \(-2 < s < 0\) the dominant term in (95) is \((2W_s/s)N^{-3}\) or possibly \(\ddot{\Omega}_s(N)\). Thus, for sufficiently large \(N\) the sign of \(\ddot{u}_s(N)\) is negative or interference from higher order terms in the conjectured asymptotic expansion of \(u_s(N)\) forces a positive sign. The numerical evidence for \(s = -1\) (no exceptional \(N < 200\) with non-negative discrete second derivative of \(v_{-1}(N)\)) discussed earlier supports a negative sign of \(\ddot{v}_{-1}(N)\), viz. \(\ddot{v}_{-1}(N)\). In fact, if \(\ddot{u}_s(N) \geq 0\) for infinitely many growing \(N_k\), then (95) would imply that

\[
\ddot{\Omega}_s(N_k) = \Omega_s(N_{k-1}) - 2\Omega_s(N_k) + \Omega_s(N_{k+1}) \geq -\frac{2}{s} W_s N_{k}^{-3} > 0.
\]

Remark 13. For \(0 < s < 2\) the dominant term in (95) is the \(C_s\)-term or possibly \(\ddot{\Omega}_s(N)\). It is not even known that the constant \(C_s\) appearing in Conjecture 7 and thus in (95) exists. Results for the hypersingular case discussed
below suggest that $C_s$ is related to the Epstein zeta function for the hexagonal lattice in the plane. An inspection of the graph of the conjectured value of $C_s$, analytically continued, shows that it is negative in the interval $(0, 2)$! Asymptotically seen, higher-order terms in the large-$N$ expansion of $u_s(N)$, $0 < s < 2$ cause the appearance of “large” magic numbers $N$. Indeed, analysis of the putatively minimal average $S^2$-adjusted Riesz pair-energy up to $N = 200$ for $s = 1$ gives a sequence of $N$’s for which $\tilde{u}_s(N)$ is not negative.

5.1.2 The logarithmic case

In the logarithmic case one has the following bounds for $u_0(N)$.

**Proposition 11.** There exist positive constants $C > c > 0$ such that for all sufficiently large $N$

$$\frac{W_{\log} - \frac{1}{2} \log N - C N}{N(N-1)} \leq u_0(N) \leq \frac{W_{\log} - \frac{1}{2} \log N - c N}{N(N-1)}.$$  

**Proof.** Let $\mathcal{E}_{\log}(S^2, N)$ be defined by

$$\mathcal{E}_{\log}(S^2, N) \equiv \inf \left\{ 2 \sum_{1 \leq j < k \leq N} \log \frac{1}{|q_j - q_k|} : \{q_1, \ldots, q_N \} \subset S^2 \right\}.$$  

Then it is known\(^{40}\) that there are constants $C > c > 0$ such that (cf. \cite{BHS12})

$$-C N \leq \mathcal{E}_{\log}(S^2, N) - W_{\log} N^2 + \frac{1}{2} N \log N \leq -c N$$  

for all sufficiently large $N \geq 2$. Hence

$$\frac{-\frac{1}{2} \log N - C N}{N(N-1)} \leq \mathcal{E}_{\log}(S^2, N) - W_{\log} - \frac{1}{N-1} W_{\log} \leq \frac{-\frac{1}{2} \log N - c N}{N(N-1)}.$$  

The desired bounds follow. \(\square\)

Proposition\(\square\) provides the following weak bounds for the discrete second derivative of $u_0(N)$ (and by means of Lemma\(\square\) for $v_s(N)$).

\(^{40}\)It is also well-known that, for a sequence $\{\omega_N^\log\}_{N \geq 2}$ of optimal $N$-point configurations,

$$\lim_{N \to \infty} \frac{2}{N(N-1)} \sum_{1 \leq j < k \leq N} \log \frac{1}{|q_{j,N}^{\log} - q_{k,N}^{\log}|} = W_{\log}.$$  

The reciprocal of the exponential function of the quantity under the limit symbol is also known as the $N$-th diameter of $S^2$ in the logarithmic case. It converges monotonically to the transfinite diameter of $S^2$ (in the logarithmic case), introduced in \cite{PoSz31}, which equals the logarithmic capacity $\exp(-W_{\log})$ of $S^2$; see \cite{Pri11} for a recent account.
Proposition 12. Let \( c \) and \( C \) be the constants from Proposition 11. Then
\[
\tilde{u}_0(N) \leq \frac{2(C - c)}{N - 1} - \frac{2c}{N(N - 1)(N - 2)}
- \frac{3 \log N}{(N + 1)N(N - 1)(N - 2)} + \frac{6W \log + H_0(N)}{(N + 1)N(N - 1)(N - 2)},
\]
where \( H_0(N) \to \frac{5}{2} \) as \( N \to \infty \).

For the corresponding lower bound one has to interchange \( c \) and \( C \).

Proof. First we consider the upper bound. By the definition of \( \tilde{u}_0(N) \) and Proposition 11
\[
\tilde{u}_0(N) \leq \frac{W \log - \frac{1}{2} \log(N - 1) - c(N - 1)}{(N - 1)(N - 2)} - 2 \frac{W \log - \frac{1}{2} \log N - C N}{N(N - 1)}
+ \frac{W \log - \frac{1}{2} \log(N + 1) - c(N + 1)}{(N + 1)N}
= W \log \left( \frac{1}{(N - 1)(N - 2)} - 2 \frac{1}{N(N - 1)} + \frac{1}{(N + 1)N} \right)
- \frac{1}{2} \left[ \frac{\log(N - 1)}{(N - 1)(N - 2)} - 2 \frac{\log N}{N(N - 1)} + \frac{\log(N + 1)}{(N + 1)N} \right]
- \left\{ \frac{c}{N - 2} - 2 \frac{C}{N - 1} + \frac{c}{N} \right\}.
\]
Simplification (assisted by MATHEMATICA) gives for the expression in parenthesis
\[
\frac{6}{(N + 1)N(N - 1)(N - 2)},
\]
for the expression in braces
\[
-2 \frac{C - c}{N - 1} + c \left( \frac{1}{N - 2} - \frac{2}{N - 1} + \frac{1}{N} \right) = -2 \frac{C - c}{N - 1} + \frac{2c}{N(N - 1)(N - 2)}
\]
and for the square-bracketed expression (using series expansion)
\[
\frac{6 \log N}{(N + 1)N(N - 1)(N - 2)} + \frac{\log(1 - \frac{1}{N})}{(N - 1)(N - 2)} + \frac{\log(1 + \frac{1}{N})}{(N + 1)N}
= \frac{6 \log N}{(N + 1)N(N - 1)(N - 2)} + \frac{-\frac{5}{N^2} + \frac{8}{N^3} + \cdots}{(N - 1)(N - 2)}.
\]
Putting everything together, we arrive at
\[
\tilde{u}_0(N) \leq \frac{2(C - c)}{N - 1} - \frac{2c}{N(N - 1)(N - 2)}
- \frac{3 \log N}{(N + 1)N(N - 1)(N - 2)} + \frac{6W \log + \frac{5}{2} - \frac{3}{2N} + \cdots}{(N + 1)N(N - 1)(N - 2)}.
\]
For the corresponding lower bound one has to interchange $c$ and $C$. □

The investigation of the asymptotic behavior of $E_{\log}(S^2, N)$ provides the following conjecture.

**Conjecture 2.** There exists a constant $C_{\log}$ and a function $\Omega_0(N)$ such that

$$u_0(N) = -\frac{1}{2} \log N + \frac{W_{\log} + C_{\log}}{N} - \frac{1}{2} \frac{\log N}{N^2} + \frac{W_{\log} + C_{\log}}{N^2} + \Omega_0(N) \quad \forall N \geq 2,$$

where $N\Omega_0(N) \rightarrow 0$ (or in its stronger form $N^2\Omega_0(N) \rightarrow c_0 \neq 0$) as $N \rightarrow \infty$.

The constant $C_{\log}$ is given by

$$C_{\log} = 2 \log 2 + \frac{1}{2} \log \frac{2}{3} + 3 \log \frac{\sqrt{\pi}}{\Gamma(1/3)} = -0.05560530494339251850 \ldots < 0.$$

**Motivation of Conjecture 2.** The following conjecture for the large-$N$ behavior of $E_{\log}(S^2, N)$ is known (cf. [BHS12] for a most recent account)

$$E_{\log}(S^2, N) = W_{\log} N^2 - \frac{1}{2} N \log N + C_{\log} N + R_{\log}(N),$$

where $R_{\log}(N)/N \rightarrow 0$ as $N \rightarrow \infty$. A stronger form states that $R_{\log}(N)$ converges to a non-zero constant. Hence

$$u_0(N) = \frac{E_{\log}(S^2, N)}{N(N-1)} - W_{\log}$$

$$= \left(\frac{N^2}{N(N-1)} - 1\right) W_{\log} - \frac{1}{2} \frac{\log N}{N-1} + \frac{C_{\log}}{N-1} + \frac{R_{\log}(N)}{N(N-1)}$$

$$= -\frac{1}{2} \frac{\log N}{N} + \frac{W_{\log} + C_{\log}}{N} - \frac{1}{2} \frac{\log N}{N^2} + \frac{W_{\log} + C_{\log}}{N^2} + \Omega_0(N),$$

where we used that

$$\frac{1}{N-1} = \frac{1}{N} + \frac{1}{N(N-1)} = \frac{1}{N} + \frac{1}{N^2} + \frac{1}{N^2(N-1)}$$

and

$$\Omega_0(N) \equiv \frac{1}{N(N-1)} \left\{ R_{\log}(N) - \frac{1}{2} \frac{\log N}{N} + \frac{W_{\log}}{N} \right\}.$$

From the assumptions on $R_{\log}(N)$ it follows that $N\Omega_0(N) \rightarrow 0$ (or in its stronger form $N^2\Omega_0(N) \rightarrow c_0 \neq 0$) as $N \rightarrow \infty$. □

Conjecture 2 implies the following large-$N$ behavior for the discrete second derivative of $u_0(N)$. 

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Corollary 3. Under the assumption that Conjecture 2 is true, there holds

\[ \ddot{u}_0(N) = -\frac{\log N}{N^3} + \frac{3/2 + W_{\log} + C_{\log}}{N^3} + \ddot{O}_0(N) + F_0(N), \quad (96) \]

with \( N^{4-\epsilon}F_0(N) \to 0 \) as \( N \to \infty \) for any \( \epsilon > 0 \).

Note that \( 3/2 + W_{\log} + C_{\log} > 0 \).

Proof. By the definition of the discrete second derivative (cf. (12))

\[
\ddot{u}_0(N) = -\frac{1}{2} \left( \frac{\log(N-1)}{N-1} - \frac{2 \log N}{N} + \frac{\log(N+1)}{N+1} \right) \\
+ (W_{\log} + C_{\log}) \left[ \frac{1}{N-1} - \frac{2}{N} + \frac{1}{N+1} \right] \\
- \frac{1}{2} \left( \frac{\log(N-1)}{(N-1)^2} - \frac{2 \log N}{N^2} + \frac{\log(N+1)}{(N+1)^2} \right) \\
+ (W_{\log} + C_{\log}) \left[ \frac{1}{(N-1)^2} - \frac{2}{N^2} + \frac{1}{(N+1)^2} \right] + \ddot{O}_0(N).
\]

The series expansions

\[
\left(1 - \frac{1}{N}\right)^{-\alpha} = \sum_{n=0}^{\infty} \frac{(\alpha)_n}{n!} \frac{1}{N^n}
\]

and

\[
\log \left(1 - \frac{1}{N}\right) \left(1 - \frac{1}{N}\right)^{-\alpha} = -\sum_{k=1}^{\infty} \sum_{n=0}^{\infty} \frac{1}{k} \frac{(\alpha)_n}{n!} \frac{1}{N^{k+n}}
= -\sum_{\ell=1}^{\infty} \left\{ \sum_{n=0}^{\ell-1} \frac{1}{\ell - n} \frac{(\alpha)_n}{n!} \right\} \frac{1}{N^\ell}
\]

yield

\[
\frac{1}{N-1} - \frac{2}{N} + \frac{1}{N+1} = \frac{1}{N} \left( \frac{1}{1 - \frac{1}{N}} - 2 + \frac{1}{1 + \frac{1}{N}} \right) = \frac{1}{N} \sum_{n=2}^{\infty} \frac{1 + (-1)^n}{N^n}
\]

and thus

\[
\frac{\log(N-1)}{N-1} - \frac{2 \log N}{N} + \frac{\log(N+1)}{N+1}
= \log N \left[ \frac{1}{N-1} - \frac{2}{N} + \frac{1}{N+1} \right] + \frac{1}{N} \left[ \log(1 - \frac{1}{N}) + \log(1 + \frac{1}{N}) \right]
= \frac{\log N}{N^3} \sum_{n=0}^{\infty} \frac{1 + (-1)^n}{N^n} - \sum_{\ell=2}^{\infty} \frac{H_\ell}{N^{\ell+1}} \frac{1 + (-1)^\ell}{N^{\ell+1}},
\]

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where $H_\ell$ denotes the $\ell$-th Harmonic number $H_\ell \equiv \sum_{k=1}^{\ell} \frac{1}{k}$; furthermore
\[
\frac{1}{(N-1)^2} - 2 \frac{1}{N^2} + \frac{1}{(N+1)^2} = \frac{1}{N^2} \left( \frac{1}{(1-\frac{1}{N})^2} - 2 + \frac{1}{(1+\frac{1}{N})^2} \right)
\]
\[
= \frac{1}{N^2} \sum_{n=2}^{\infty} \frac{(2)_n}{n!} \frac{1 + (-1)^n}{N^n} = \sum_{n=2}^{\infty} \frac{(n+1)(1 + (-1)^n)}{N^{n+2}}
\]
and thus
\[
\log\left(\frac{N-1}{N-1}\right) - 2 \frac{\log N}{N^2} + \frac{\log(N+1)}{(N+1)^2}
\]
\[
= \log N \left( \frac{1}{(N-1)^2} - 2 \frac{1}{N^2} + \frac{1}{(N+1)^2} \right)
\]
\[
+ \frac{1}{N^2} \left( \frac{\log(1-\frac{1}{N})}{(1-\frac{1}{N})^2} + \frac{\log(1+\frac{1}{N})}{(1+\frac{1}{N})^2} \right)
\]
\[
= \frac{\log N}{N^4} \sum_{n=0}^{\infty} (n+3) \frac{1 + (-1)^n}{N^n} - \sum_{\ell=2}^{\infty} \left\{ \sum_{n=0}^{\ell-1} \frac{1}{\ell-n} \frac{(2)_n}{n!} \right\} \frac{1 + (-1)^\ell}{N^{\ell+2}}.
\]
Combining everything (and shifting indices of summations), we arrive at
\[
\ddot{u}_0(N) = -\frac{1}{2} \left( \frac{\log N}{N^3} \sum_{n=0}^{\infty} \frac{1 + (-1)^n}{N^n} - \frac{1}{N^3} \sum_{\ell=0}^{\infty} H_{\ell+2} \frac{1 + (-1)^\ell}{N^{\ell}} \right)
\]
\[
+ \frac{W_{\log} + C_{\log}}{N^3} \sum_{n=0}^{\infty} \frac{1 + (-1)^n}{N^n}
\]
\[
- \frac{\log N}{2N^4} \sum_{n=0}^{\infty} (n+3) \frac{1 + (-1)^n}{N^n}
\]
\[
+ \frac{1}{2N^4} \sum_{\ell=0}^{\infty} \left\{ \sum_{n=0}^{\ell+1} \frac{n+1}{\ell+2-n} \right\} \frac{1 + (-1)^\ell}{N^{\ell}}
\]
\[
+ \frac{W_{\log} + C_{\log}}{N^4} \sum_{n=0}^{\infty} (n+3) \frac{1 + (-1)^n}{N^n}
\]
\[
+ \ddot{\Omega}_0(N).
\]
Rearranging the terms gives
\[
\ddot{u}_0(N) = -\frac{\log N}{N^3} + \frac{3/2 + W_{\log} + C_{\log}}{N^3} + \ddot{\Omega}_0(N) + F_0(N),
\]
where

$$F_0(N) \equiv -\frac{1}{2} \log N \sum_{n=2}^{\infty} \frac{1 + (-1)^n}{N^n} + \frac{1}{2} \sum_{\ell=2}^{\infty} H_{\ell+2} \frac{1 + (-1)^\ell}{N^\ell}$$

$$+ W_{\log} + C_{\log} \sum_{n=2}^{\infty} \frac{1 + (-1)^n}{N^n}$$

$$- \log N \sum_{n=0}^{\infty} \frac{(n+3)}{N^n}$$

$$+ \frac{1}{2N^4} \sum_{\ell=0}^{\infty} \left\{ \sum_{n=0}^{\ell+1} \frac{n+1}{\ell+2-n} \right\} \frac{1 + (-1)^\ell}{N^\ell}$$

$$+ \frac{W_{\log} + C_{\log}}{N^4} \sum_{n=0}^{\infty} (n+3) \frac{1 + (-1)^n}{N^n}$$

with $N^{4-\epsilon} F_0(N) \to 0$ as $N \to \infty$ for any $\epsilon > 0$.

**Remark 14.** The dominant term in (96) is the negative $-(\log N)/N^3$ term or possibly $\tilde{\Omega}_0(N)$. An increasing infinite sequence of magic numbers $(N_k)$ with $\tilde{u}_0(N_k) \geq 0$ would be caused by higher-order terms in the conjectured asymptotic expansion of $u_0(N)$ and thus would, for example, exclude the hypothetical expansion $\Omega_0(N) = c_0 + \tilde{\Omega}_0(N)$ with $\tilde{\Omega}_0(N)/[(\log N)/N] \to 0$ as $N \to \infty$.

### 5.2 The hypersingular regime $s > 2$

For $s > 2$ it is proved in Hardin and Saff [HaSa05] that

$$\lim_{N \to \infty} \frac{E_s(S^2, N)}{N^{1+s/2}} = \frac{C_s}{(4\pi)^{s/2}}$$

for some constant $C_s$ depending on $s$. In [KuSa98] it is shown that, for $s > 2$,

$$\limsup_{N \to \infty} \frac{E_s(S^2, N)}{N^{1+s/2}} \leq \frac{(\sqrt{3}/2)^{s/2} \zeta_A(s)}{(4\pi)^{s/2}},$$

and it is conjectured in [KuSa98] that for $s > 2$,

$$C_s = \left( \sqrt{3}/2 \right)^{s/2} \zeta_A(s),$$

(97)

where $\zeta_A$ is the zeta function associated with the hexagonal lattice. The zeta function associated with the hexagonal lattice admits the factorization

$$\zeta_A(s) = 6 \zeta \left( \frac{s}{2} \right) L_{-3} \left( \frac{s}{2} \right), \quad \text{Re } s > 2,$$
where \( \zeta(s) \) is the Riemann zeta function and \( L_{-3}(s) \) a Dirichlet L-Series, viz.

\[
\zeta(s) = 1 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{4^s} + \frac{1}{5^s} + \frac{1}{6^s} + \cdots, \quad \text{Re } s > 1,
\]

\[
L_{-3}(s) = 1 - \frac{1}{2^s} + \frac{1}{4^s} - \frac{1}{5^s} + \frac{1}{7^s} - \frac{1}{8^s} + \cdots, \quad \text{Re } s > 1.
\]

For computational purposes it is more convenient to express this Dirichlet L-series in terms of the Hurwitz zeta function

\[
\zeta(s, a) \equiv \sum_{k=0}^{\infty} \frac{1}{(k + a)^s}, \quad \text{Re } s > 1,
\]

by means of

\[
L_{-3}(s) = 3^{-s} \left[ \zeta(s, \frac{1}{3}) - \zeta(s, \frac{2}{3}) \right].
\]

Using these representations we computed the graph of r.h.s.\( (97) \), see Fig. 18.

![Figure 18: The graph of the right-hand side of (97).](image)

The fundamental conjecture for the asymptotic expansion of \( \mathcal{E}_s(S^2, N) \), \( s \in (2, 4) \), as \( N \) becomes large states that

**Conjecture 3.** For \( s \in (2, 4) \) the asymptotic expansion of \( \mathcal{E}_s(S^2, N) \) reads

\[
\mathcal{E}_s(S^2, N) \sim \left( \sqrt{3/8\pi} \right)^{s/2} \zeta(s) N^{1+s/2} + W_s N^2 + o(N^2) \quad \text{as } N \to \infty.
\]

Note the appearance of (the analytically continued) \( W_s \) as coefficient of the \( O(N^2) \)-term, which now is the next-to-leading-order term.
The fundamental conjecture motivates the introduction of the following $S^2$-re-adjusted pair-energy
\[
\tilde{U}_s(r) \equiv s^{-1} \left( r^{-s} - W_s - \left( \sqrt{3}/8\pi \right)^{s/2} \zeta_A(s) N^{s/2-1} \right), \quad s \in (2, 4),
\]
the associated average $S^2$-re-adjusted pair-energy of a configuration $\omega_N$,
\[
\langle \tilde{U}_s \rangle(\omega_N) \equiv \frac{2}{N(N-1)} \sum_{1 \leq j < k \leq N} \tilde{U}_s(|q_j - q_k|), \quad s \in (2, 4),
\]
and the minimal average $S^2$-re-adjusted Riesz pair-energy, given by
\[
\tilde{u}_s(N) \equiv \inf_{\omega_N \subset S^2} \langle \tilde{U}_s \rangle(\omega_N), \quad s \in (2, 4).
\]
According to the fundamental conjecture, $\tilde{u}_s(N)$ would be bounded above and tend to 0 when $N \to \infty$, for all $2 < s < 4$.

However, since $N \mapsto N^{s/2-1}$ is a concave, increasing function for $s \in (2, 4)$, it is neither clear whether $N \mapsto \tilde{u}_s(N) = u_s(N) - \left( \sqrt{3}/8\pi \right)^{s/2} \zeta_A(s) N^{s/2-1}$ is increasing (whereas $N \mapsto u_s(N)$ is), nor whether $N \mapsto \tilde{u}_s(N)$ is concave whenever $N \mapsto u_s(N)$ is. These are interesting open problems for future study.

5.3 The singular case $s = 2$

Kuijlaars and Saff [KuSa98] showed that
\[
\lim_{N \to \infty} \frac{E_2(N)}{N^2 \log N} = \frac{1}{4}.
\]
A conjecture of Brauchart, Hardin and Saff [BHS12] is that
\[
E_2(N) \sim \frac{1}{4} N^2 \log N + C_2 N^2 + o(N^2) \quad \text{as} \quad N \to \infty,
\]
where
\[
C_2 = \frac{1}{4} \left[ \gamma - \log(2\sqrt{3}\pi) \right] + \frac{\sqrt{3}}{4\pi} \left[ \gamma_1 \left( \frac{2}{3} \right) - \gamma_1 \left( \frac{1}{3} \right) \right] = -0.08576841030090... < 0.
\]
This motivates the introduction of the following $S^2$-re-adjusted pair-energy,
\[
\tilde{U}_2(r) \equiv \frac{1}{2} \left( r^{-2} - C_2 - \frac{1}{4} \log N \right),
\]
its associated average $S^2$-re-adjusted pair-energy of a configuration $\omega_N$,
\[
\langle \tilde{U}_2 \rangle(\omega_N) \equiv \frac{2}{N(N-1)} \sum_{1 \leq j < k \leq N} \tilde{U}_2(|q_j - q_k|),
\]
and the minimal average $S^2$-re-adjusted Riesz pair-energy at $s = 2$, given by

$$\tilde{u}_2(N) \equiv \inf_{\omega_N \subset S^2} \langle \tilde{U}_2 \rangle (\omega_N).$$

(103)

By the above conjecture, $\tilde{u}_2(N)$ would be bounded and tend to 0 when $N \to \infty$.

However, since $N \to \log N$ is a concave, increasing function, it is neither clear whether $N \to \tilde{u}_2(N) = u_2(N) - C_2 - \frac{1}{4} \log N$ is increasing (whereas $N \to u_2(N)$ is) nor whether $N \to \tilde{u}_2(N)$ is concave whenever $N \to u_2(N)$ is. Also these are interesting open problems for future study.

6 Summary and Outlook

In this paper we have inquired into the local concavity properties of the map $N \to v_s(N)$, where $v_s(N)$ is the minimal average standardized Riesz pair-energy for $N$-point configurations on the unit 2-sphere $S^2 \subset R^3$. Here, by “standardized” Riesz pair energy we mean $V_s(r) = s^{-1} (r^{-s} - 1)$, with $s \in \mathbb{R}$, where $r$ is the chordal distance between the points of the pair. The map $s \to V_s(r)$ defines a real analytical family of pair energies; in particular, it includes the logarithmic interactions $-\ln r = \lim_{s \to 0} V_s(r)$.

We have readily seen analytically that $N \to v_{-2}(N)$ is strictly locally concave, and restricted to even numbers $N = 2n$, we have seen that the results of [Bjö56] imply the strict local concavity of $N \to v_s(N)$ also for $s < -2$. Yet, given the very limited amount of knowledge about true minimizers, we have studied mostly the $N$-dependence of putatively minimal average standardized Riesz pair-energies $v_s^*(N)$, obtained numerically in computer experiments. Our empirical findings indicate that also for $s = -1$ the minimal average standardized Riesz pair energy could be locally strictly concave function of $N$, without any “convex anomalies.” However, when $s \in \{0, 1, 2, 3\}$ we have found that $N \to v_s^*(N)$ is not strictly concave. Based on our empirical findings we have conjectured that there exists an $s_* \in (-1, 0)$ such that $N \to v_s^*(N)$ is locally strictly concave for all $s < s_*$, while local strict concavity is violated at some $N$-values whenever $s \geq s_*$. We presented some rigorous (but rough), and some quasi-rigorous (yet more promising) upper bounds on $s_*$. We also presented various rigorous bounds on the second discrete derivative, $\ddot{v}_s(N)$, of $N \to v_s(N)$, in parts aided by an asymptotic analysis of the large-$N$ regime. Our control of $\ddot{v}_s(N)$ is not good enough to prove strict local concavity for any $s$ other than $s = -2$, yet we expect that our analysis will serve as a stepping stone along the way to a concavity proof for $s < s_*$. We also presented various rigorous bounds on the second discrete derivative, $\ddot{v}_s(N)$, of $N \to v_s(N)$, in parts aided by an asymptotic analysis of the large-$N$ regime. Our control of $\ddot{v}_s(N)$ is not good enough to prove strict local concavity for any $s$ other than $s = -2$, yet we expect that our analysis will serve as a stepping stone along the way to a concavity proof for $s < s_*$. We also presented various rigorous bounds on the second discrete derivative, $\ddot{v}_s(N)$, of $N \to v_s(N)$, in parts aided by an asymptotic analysis of the large-$N$ regime. Our control of $\ddot{v}_s(N)$ is not good enough to prove strict local concavity for any $s$ other than $s = -2$, yet we expect that our analysis will serve as a stepping stone along the way to a concavity proof for $s < s_*$. We also presented various rigorous bounds on the second discrete derivative, $\ddot{v}_s(N)$, of $N \to v_s(N)$, in parts aided by an asymptotic analysis of the large-$N$ regime. Our control of $\ddot{v}_s(N)$ is not good enough to prove strict local concavity for any $s$ other than $s = -2$, yet we expect that our analysis will serve as a stepping stone along the way to a concavity proof for $s < s_*$. We also presented various rigorous bounds on the second discrete derivative, $\ddot{v}_s(N)$, of $N \to v_s(N)$, in parts aided by an asymptotic analysis of the large-$N$ regime. Our control of $\ddot{v}_s(N)$ is not good enough to prove strict local concavity for any $s$ other than $s = -2$, yet we expect that our analysis will serve as a stepping stone along the way to a concavity proof for $s < s_*$. We also presented various rigorous bounds on the second discrete derivative, $\ddot{v}_s(N)$, of $N \to v_s(N)$, in parts aided by an asymptotic analysis of the large-$N$ regime. Our control of $\ddot{v}_s(N)$ is not good enough to prove strict local concavity for any $s$ other than $s = -2$, yet we expect that our analysis will serve as a stepping stone along the way to a concavity proof for $s < s_*$. We also presented various rigorous bounds on the second discrete derivative, $\ddot{v}_s(N)$, of $N \to v_s(N)$, in parts aided by an asymptotic analysis of the large-$N$ regime. Our control of $\ddot{v}_s(N)$ is not good enough to prove strict local concavity for any $s$ other than $s = -2
introduction, it is of special interest to prove, or disprove, the empirically suggested local strict concavity of $N \mapsto v_{-1}(N)$. Since the optimizers of the $s = -1$ Fekete problem are related to spherical digital nets, it is of interest to raise our concavity questions also for these average standardized Riesz pair-energies computed for such nets; see our Appendix B.

For each studied $s$-value, the $N$-values at which the map $N \mapsto v_s^x(N)$ is strictly convex were collected into a set $C^x_+(s)$. We have found that the empirical map $s \mapsto C^x_+(s)$ is set-theoretically monotonic increasing, based on which we conjecture that the actual map $s \mapsto C_+(s)$ is set-theoretically monotonic increasing, indeed. Inspired by this conjecture we suspected, and then verified (by finding lower-energy configurations), that the $N = 177$ and $N = 197$ data points in the computer-experimental tables of putatively minimal Riesz pair-energies for $s \in \{2, 3\}$ in [Ca09] are non-optimal. This makes it plain that a-priori knowledge of any monotonicity property of the map $s \mapsto C_+(s)$ will also furnish valuable test criteria for the accuracy of empirical maps $N \mapsto v_s^x(N)$.

We have also discovered yet another empirical monotonicity: the percentage of odd numbers in $C^x_+(s)$ increases monotonically with $s \in \{0, 1, 2, 3\}$. Based on this finding it is reasonable to conjecture that the percentage of odd numbers in $C_+(s)$ increases monotonically with $s > s^*$, if such $s^*$ exists.

So far we have not been able to detect any algebraic generating rule for any $C^x_+(s)$ pertinent to $s \in \{0, 1, 2, 3\}$, and with increasing $s$ it seems increasingly unlikely (another monotonicity property!) to detect any such rule, because the sets $C^x_+(s)$ appear more and more random as $s$ increases. On the other hand, the set $C^x_+(0)$ exhibits some intriguing quasi-regular patterns which reminded us of the periodic table of the chemists, or the “magic” numbers in nuclear physics; incidentally, note that the $s = 0$ problem can be viewed as the electric ground state energy problem for a system of $N$ “two-dimensional” point charges on $S^2$. Thus we decided to call the $N$-values in $C^x_+(0)$ the “Magic Numbers of Smale’s 7th problem.” We have speculated that those “magic” numbers are perhaps associated with “optimally symmetric” endpoints of families of more-and-more symmetric configurations, based on our observation that the first few configurations associated with $C^x_+(0)$ are in fact highly symmetric.

We hope that our paper triggers future research into the regime of concavity of the minimal average standardized Riesz pair-energies on $S^2$, and the structure of its convexity sets as functions of $s$. As a preliminary guide into such future inquiries, we have formulated a list of 14 interesting questions. It would also be interesting to try to answer analogues of our questions formulated for the $s$-Fekete problem on other compact manifolds. In particular, we ourselves plan to answer the analogues of our list of question for the $s$-Fekete problem on $S^1$, for which all the optimizers are explicitly known.

Furthermore, even though the paper [Mettel77] contains many numerically computed bifurcation diagrams, we noticed the absence of any proper bifurca-
tion analyses in the literature on the $s$-Fekete problems. To assist our inquiries we have begun such a bifurcation analysis, so far numerically, for a few small $N$-values. In the process we discovered a previously undetected bifurcation in the $N = 7$-point problem at $s = 0$, where the local minimality is exchanged between the pentagonal bi-pyramid and a $C_2(1^{123})(f = 5)$ configuration. We have not confirmed that this family is truly globally minimizing for the interval $-2 < s < 0$, neither did we confirm that the pentagonal bi-pyramid is globally minimizing for $0 < s < 1$; yet we strongly suspect that all this is true. We are planning a more detailed bifurcation analysis, with special attention given to the 7-point problem, to be reported on in a future publication. We emphasize that a bifurcation analysis will be practically feasible only for moderate $N$ values because the eigenvalue problems involve nontrivial $2N \times 2N$ matrices which will become difficult to handle when $N$ gets too large.

In the introduction we mentioned that computer-experimental evidence suggests that the number of non-globally minimizing configurations (modulo rotations on $S^2$), is growing exponentially with $N$; cf. [ErHo97]. It would be nice to have a rigorous proof, together with a determination of the growth rate. But to the best of our knowledge, there is no rigorous estimate even of their number being finite! This reminds one of Smale’s 6-th problem, viz. the celestial-mechanical counterpart of such a finiteness proof.

An exponential growth rate of the number of locally minimizing configurations (or perhaps of the number of equilibrium configurations) is reminiscent of “the complexity of the energy landscape,” see [Wal04]. As far as we know, not much is known about the $s$-Riesz energy landscape for $N$-point configurations on $S^2$. With the help of catalogs of non-globally minimizing configurations and their energies it should be feasible to determine the experimental number counts of the local minimizers below a certain energy $E$; see [Cetal13] for a most recent study and additional references.

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Appendix A

In this appendix we supply the proofs of relations (7) and (8) which control the limit \( s \to \infty \).

Proof of Relation (7)

Suppose \( \omega_N = \{ q_1, \ldots, q_N \} \subset \mathbb{S}^2 \) is a fixed \( N \)-point set, with separation distance \( \rho(\omega_N) = \min_{1 \leq i < j \leq N} |q_i - q_j| \). Then using that the function \( f(x) \equiv x - 1/s \) is strictly decreasing for \( s > 0 \), we find that

\[
\left[ \langle V_s \rangle(\omega_N) + \frac{1}{s} \right]^{-1/s} = \left[ \frac{1}{s N(N-1)} \sum_{1 \leq i < j \leq N} \frac{1}{|q_i - q_j|^s} \right]^{-1/s}
\]

\[
= \rho(\omega_N) \left[ \frac{1}{s N(N-1)} \sum_{1 \leq i < j \leq N} \left( \frac{\rho(\omega_N)}{|q_i - q_j|} \right)^s \right]^{-1/s}
\]

\[
\geq \rho(\omega_N) \left( \frac{1}{s} \right)^{-1/s}
\]

\[
\geq \rho(\omega_N).
\]

On the other hand, retaining only one of the least distance pairs in the double sum yields

\[
\left[ \langle V_s \rangle(\omega_N) + \frac{1}{s} \right]^{-1/s} \leq \left( \frac{1}{s N(N-2)} \frac{1}{\rho(\omega_N)^s} \right)^{-1/s}
\]

\[
= \rho(\omega_N) \left( \frac{1}{s} \right)^{-1/s} \left( \frac{2}{N(N-2)} \right)^{-1/s}
\]

\[
\to \rho(\omega_N) \quad \text{as} \quad s \to \infty.
\]

This completes the proof of (7).

Proof of Relation (8)

Let \( \omega_N^s = \{ q_1^s, \ldots, q_N^s \} \subset \mathbb{S}^2 \) denote a minimizing \( N \)-point set, and suppose \( \omega_N^\infty \) is a best-packing configuration with \( \rho(\omega_N^\infty) = \rho(N) \).

Then, first of all,

\[
\langle V_s \rangle(\omega_N^s) \leq \langle V_s \rangle(\omega_N^\infty);
\]

but \( \langle V_s \rangle(\omega_N^s) = v_s(N) \), and so, by (7), we have

\[
\lim_{s \to \infty} \inf \left[ v_s(N) + \frac{1}{s} \right]^{-1/s} \geq \rho(\omega_N^\infty) \equiv \rho(N).
\]
On the other hand, using that $|q_i^s - q_j^s| = \rho(\omega_N^s)$ for at least one pair $(i, j)$, and furthermore that $\rho(\omega_N^s) \leq \rho(N)$, we obtain

\[
\langle V_s \rangle(\omega_N^s) + \frac{1}{s} = \frac{1}{sN(N-1)} \sum_{1 \leq i < j \leq N} |q_i^s - q_j^s|^{-s}
\]

\[
= [\rho(N)]^{-s} \frac{2}{sN(N-1)} \sum_{1 \leq i < j \leq N} \left[ \frac{\rho(N)}{|q_i^s - q_j^s|} \right]^s
\]

\[
\geq [\rho(N)]^{-s} \frac{2}{sN(N-1)} > 0.
\]

Hence,

\[
\left[ \langle V_s \rangle(\omega_N^s) + \frac{1}{s} \right]^{-1/s} \leq \rho(N)s^{1/s} (N(N-1)/2)^{1/s} = \rho(N) 
\]

as $s \to \infty$;

but again, $\langle V_s \rangle(\omega_N^s) = v_s(N)$, and so we get

\[
\limsup_{s \to \infty} \left[ v_s(N) + \frac{1}{s} \right]^{-1/s} \leq \rho(N). \tag{105}
\]

By (104) and (105)

\[
\lim_{s \to \infty} \left[ v_s(N) + \frac{1}{s} \right]^{-1/s} = \rho(N).
\]

This completes the proof of (8).
Appendix B

Spherical digital nets

Maximal sum-of-distance points (i.e. optimal configurations \( \omega^s_N \) for \( s = -1 \)) provide optimal integration nodes for equal-weight numerical integration rules on the sphere; see [BrDi13] and [BSSW12, BrWo]. In general, such configurations are obtained by solving a highly non-linear optimization problem which makes them impractical for large number of points.

Digital nets and sequences introduced in [Ni87] are efficiently computable so-called low-discrepancy point systems in the unit square that define effective Quasi-Monte Carlo rules for integrating functions on the unit square

\[
\frac{1}{N} \sum_{j=1}^{N} f(x_j) \approx \int_{[0,1]^2} f(x) \, dx.
\]

Informally speaking, the points of a digital net in \([0,1]^2\) are distributed in such a way that a large number of elementary rectangles contain precisely the fraction of all points that corresponds to their area; cf. [DiPi10] and Fig. 19.

![Figure 19: 2048 Sobol' points in the unit square generated using a method by JoKu03.](image)

This distribution property remains unchanged when lifting a digital net and elementary rectangles (now called spherical rectangles) to \( S^2 \) using the area-preserving Lambert transformation of the map makers. These spherical digital nets are studied in [BrDi12] and [AiBrDi12]. Of particular interest is that numerically they are comparable with maximal sum-of-distance points.
It is conjectured\footnote{Numerical results based on the Sobol’ points implemented in Matlab for $N$ up to 4 Million points support this conjecture (J.B., manuscript in preparation ).} that $\langle V_{-1} \rangle(\omega_N^{\text{sphDN}})$ will approach the same limit as $v_{-1}(N)$ with the same rate of convergence as $N \to \infty$.

We tested for local concavity a sequence of $N$-point spherical digital nets formed by the first $N$ points of a Sobol’ sequence lifted to the sphere. For the implementation of the Sobol’ points we used \cite{JoKu03}; cf. Fig. 19. The graph of $N \mapsto \langle V_{-1} \rangle(\omega_N^{\text{sphDN}})$ (Fig. 20) shows an overall concave shape.

Yet, some irregularities are clearly discernible in Fig. 20, in fact, the discrete second derivative of $N \mapsto \langle V_{-1} \rangle(\omega_N^{\text{sphDN}})$ reveals that $N \mapsto \langle V_{-1} \rangle(\omega_N^{\text{sphDN}})$ for this sequence of spherical digital nets is locally highly non-concave; see Fig. 21.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure20.png}
\caption{\footnotesize $\langle V_{-1} \rangle(\omega_N^{\text{sphDN}})$ based on the 2048 Sobol’ points given in Fig. 19.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure21.png}
\caption{\footnotesize Discrete second derivative of $\langle V_{-1} \rangle(\omega_N^{\text{sphDN}})$ based on the 2048 Sobol’ points given in Fig. 19. The discrete points are joint by lines to guide the eyes.}
\end{figure}
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“Magic” numbers in Smale’s 7th problem: Supplement

This supplementary section lists the standardized \( s \)-Riesz energy data used in the main part of our paper.

6.1 Tables for \( s = -1 \)

Putatively minimal average standardized Riesz pair-energy \( v_{-1}^x(N) \) and its second derivative \( \ddot{v}_{-1}^x \) converted from computer-experimental data \( E_{-1}^x(N) \) in [RSZ95].

| \( N \) | \( v_{-1}^x(N) \) | \( \ddot{v}_{-1}^x(N) \) |
|-------|----------------|----------------|
| 2     | -1.0000000000  | -0.1688915465 |
| 3     | -0.7320508077  | -0.0342078637 |
| 4     | -0.6329931618  | -0.0280772524 |
| 5     | -0.5681433797  | -0.0068743336 |
| 6     | -0.5313708499  | -0.0096073663 |
| 7     | -0.5014726538  | -0.0042099548 |
| 8     | -0.4811818239  | -0.0031963792 |
| 9     | -0.4651009489  | -0.0025731588 |
| 10    | -0.4522164530  | -0.0020269265 |
| 11    | -0.4413588837  | -0.0025731588 |
| 12    | -0.4330744732  | -0.0004714806 |
| 13    | -0.4252615432  | -0.0014567068 |
| 14    | -0.4189053200  | -0.0007901741 |
| 15    | -0.4133392709  | -0.0007194468 |
| 16    | -0.4084926687  | -0.0005618514 |
| 17    | -0.4042079178  | -0.0004755958 |
| 18    | -0.4003987627  | -0.0003245148 |
| 19    | -0.3969141224  | -0.0004449970 |
| 20    | -0.3938744790  | -0.0002396557 |
| 21    | -0.3910744914  | -0.0002663080 |
| 22    | -0.3885408118  | -0.0001709545 |
| 23    | -0.3861780867  | -0.0002601472 |
| 24    | -0.3840755088  | -0.0001091965 |
| 25    | -0.3820821274  | -0.0001747639 |

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|   |                  |                  |
|---|------------------|------------------|
| 26 | -0.3802635100   | -0.0001542742   |
| 27 | -0.3785991667   | -0.0000886587   |
| 28 | -0.3770234821   | -0.0000994882   |
| 29 | -0.3755472858   | -0.0001196462   |
| 30 | -0.3741907356   | -0.0000753432   |
| 31 | -0.3729095285   | -0.0001033183   |
| 32 | -0.3717316398   | -0.0000232543   |
| 33 | -0.3705770053   | -0.0000928414   |
| 34 | -0.3695152123   | -0.0000545753   |
| 35 | -0.3685079946   | -0.0000610507   |
| 36 | -0.3675618275   | -0.0000478945   |
| 37 | -0.3666635549   | -0.0000476311   |
| 38 | -0.3658129134   | -0.0000422886   |
| 39 | -0.3650045606   | -0.0000399725   |
| 40 | -0.3642361802   | -0.0000352382   |
| 41 | -0.3635030381   | -0.0000354383   |
| 42 | -0.3628053343   | -0.0000304398   |
| 43 | -0.3621380703   | -0.0000343435   |
| 44 | -0.3615051498   | -0.0000230366   |
| 45 | -0.3608952658   | -0.0000242521   |
| 46 | -0.3603096340   | -0.0000251566   |
| 47 | -0.3597491588   | -0.0000320904   |
| 48 | -0.3592207739   | -0.0000094516   |
| 49 | -0.3587018407   | -0.0000275106   |
| 50 | -0.3582104181   | -0.0000158895   |
| 51 | -0.3577348849   | -0.0000176294   |
| 52 | -0.3572769812   | -0.0000179846   |
| 53 | -0.3568370621   | -0.0000167784   |
| 54 | -0.3564139214   | -0.0000138648   |
| 55 | -0.3560046454   | -0.0000157930   |
| 56 | -0.3556111625   | -0.0000126576   |
| 57 | -0.3552303372   | -0.0000127819   |
| 58 | -0.3548622938   | -0.0000128192   |
| 59 | -0.3545070695   | -0.0000130118   |
| 60 | -0.3541648570   | -0.0000082593   |

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|    |                |                |
|----|----------------|----------------|
| 61 | -0.3538309038  | -0.0000130841  |
| 62 | -0.3535100347  | -0.0000083204  |
| 63 | -0.3531974859  | -0.0000095653  |
| 64 | -0.3528945024  | -0.0000092839  |
| 65 | -0.3526008028  | -0.0000099603  |
| 66 | -0.3523170635  | -0.0000085228  |
| 67 | -0.3520418471  | -0.0000061002  |
| 68 | -0.3517727307  | -0.0000084551  |
| 69 | -0.3515120695  | -0.0000077804  |
| 70 | -0.3512591888  | -0.0000065818  |
| 71 | -0.3510128898  | -0.0000089700  |
| 72 | -0.3507755608  | -0.0000017464  |
| 73 | -0.3505399783  | -0.0000083169  |
| 74 | -0.3503127126  | -0.0000070610  |
| 75 | -0.3500925079  | -0.0000049921  |
| 76 | -0.3498772953  | -0.0000064646  |
| 77 | -0.3496685474  | -0.0000044272  |
| 78 | -0.3494642267  | -0.0000047166  |
| 79 | -0.3492646225  | -0.0000053979  |
| 80 | -0.3490704162  | -0.0000036243  |
| 81 | -0.3488798341  | -0.0000053146  |
| 82 | -0.3486945667  | -0.0000046236  |
| 83 | -0.3485139228  | -0.0000041813  |
| 84 | -0.3483374603  | -0.0000040455  |
| 85 | -0.3481650433  | -0.0000039518  |
| 86 | -0.3479965781  | -0.0000038940  |
| 87 | -0.3478320068  | -0.0000038600  |
| 88 | -0.3476712956  | -0.0000032965  |
| 89 | -0.3475138808  | -0.0000035676  |
| 90 | -0.3473600336  | -0.0000032498  |
| 91 | -0.3472094363  | -0.0000031976  |
| 92 | -0.3470620364  | -0.0000030669  |
| 93 | -0.3469177035  | -0.0000032350  |
| 94 | -0.3467766057  | -0.0000027273  |
| 95 | -0.3466382351  | -0.0000030607  |

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|   |                 |                  |
|---|----------------|------------------|
| 96| -0.3465029252  | -0.0000024914   |
| 97| -0.3463701068  | -0.0000030062   |
| 98| -0.3462402945  | -0.0000021599   |
| 99| -0.3461126421  | -0.0000028725   |
|100| -0.3459878622  | -0.0000020284   |
|101| -0.3458651107  | -0.0000026513   |
|102| -0.3457450106  | -0.0000023449   |
|103| -0.3456272511  | -0.0000015587   |
|104| -0.3455118366  | -0.0000025700   |
|105| -0.3453979807  | -0.0000019386   |
|106| -0.3452866950  | -0.0000019386   |
|107| -0.3451773478  | -0.0000022877   |
|108| -0.3450702883  | -0.0000015216   |
|109| -0.3449647504  | -0.000001798    |
|110| -0.3448613924  | -0.0000018916   |
|111| -0.3447599259  | -0.0000016306   |
|112| -0.3446600899  | -0.0000015411   |
|113| -0.3445617950  | -0.0000018275   |
|114| -0.3444653276  | -0.0000016283   |
|115| -0.3443704885  | -0.0000016236   |
|116| -0.3442772731  | -0.0000017758   |
|117| -0.3441858334  | -0.0000013487   |
|118| -0.3440957425  | -0.0000015893   |
|119| -0.3440072409  | -0.0000015063   |
|120| -0.3439202456  | -0.0000014235   |
|121| -0.3438346739  | -0.0000015652   |
|122| -0.3437506673  | -0.0000008439   |
|123| -0.3436675047  | -0.0000014344   |
|124| -0.3435857765  | -0.0000013062   |
|125| -0.3435053545  | -0.0000014107   |
|126| -0.3434263433  | -0.0000012300   |
|127| -0.3433485620  | -0.0000010363   |
|128| -0.3432718170  | -0.0000012992   |
|129| -0.3431963713  | -0.0000011613   |
|130| -0.3431220868  | -0.0000010782   |

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|   |         |         |
|---|---------|---------|
| 131 | -0.3430488805 | -0.0000014789 |
| 132 | -0.3429771532 | -0.000002910 |
| 133 | -0.3429057168 | -0.0000014821 |
| 134 | -0.3428357625 | -0.0000011364 |
| 135 | -0.3427669446 | -0.0000008849 |
| 136 | -0.3426990116 | -0.0000010022 |
| 137 | -0.3426320808 | -0.0000007288 |
| 138 | -0.3425658788 | -0.0000009612 |
| 139 | -0.3425006380 | -0.0000010152 |
| 140 | -0.3424364125 | -0.0000009987 |
| 141 | -0.3423731856 | -0.0000008186 |
| 142 | -0.3423107773 | -0.0000009224 |
| 143 | -0.3422492915 | -0.0000008783 |
| 144 | -0.3421886840 | -0.0000006861 |
| 145 | -0.3421287625 | -0.0000009504 |
| 146 | -0.3420697915 | -0.0000005912 |
| 147 | -0.3420114117 | -0.0000008435 |
| 148 | -0.3419538754 | -0.0000007333 |
| 149 | -0.3418970724 | -0.0000008899 |
| 150 | -0.3418411593 | -0.0000005652 |
| 151 | -0.3417858113 | -0.0000008084 |
| 152 | -0.3417312717 | -0.0000007905 |
| 153 | -0.3416775227 | -0.0000005462 |
| 154 | -0.3416243199 | -0.0000007311 |
| 155 | -0.3415718481 | -0.0000005965 |
| 156 | -0.3415199729 | -0.0000007574 |
| 157 | -0.3414688550 | -0.0000006272 |
| 158 | -0.3414183644 | -0.0000006462 |
| 159 | -0.3413685199 | -0.0000005827 |
| 160 | -0.3413192581 | -0.0000005710 |
| 161 | -0.3412705674 | -0.0000006268 |
| 162 | -0.341225034 | -0.0000005491 |
| 163 | -0.3411749886 | -0.0000005855 |
| 164 | -0.3411280593 | -0.0000005656 |
| 165 | -0.3410816956 | -0.0000005625 |

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|    |          |          |
|----|----------|----------|
| 166 | -0.3410358944 | -0.0000005158 |
| 167 | -0.3409906091 | -0.0000005912 |
| 168 | -0.3409459150 | -0.0000004328 |
| 169 | -0.3409016537 | -0.0000006121 |
| 170 | -0.3408580044 | -0.0000004603 |
| 171 | -0.3408148156 | -0.0000004770 |
| 172 | -0.3407721037 | -0.0000005051 |
| 173 | -0.3407298968 | -0.0000005265 |
| 174 | -0.3406882164 | -0.0000003733 |
| 175 | -0.3406469094 | -0.0000004704 |
| 176 | -0.3406060727 | -0.0000005030 |
| 177 | -0.3405657391 | -0.0000004271 |
| 178 | -0.3405258325 | -0.0000004416 |
| 179 | -0.3404863676 | -0.0000005073 |
| 180 | -0.34044474099 | -0.0000003502 |
| 181 | -0.3404088025 | -0.0000004928 |
| 182 | -0.3403706878 | -0.0000002503 |
| 183 | -0.3403328233 | -0.0000005234 |
| 184 | -0.3402954823 | -0.0000003383 |
| 185 | -0.3402584796 | -0.0000004666 |
| 186 | -0.3402219435 | -0.0000004336 |
| 187 | -0.3401858409 | -0.0000002152 |
| 188 | -0.3401499536 | -0.0000004637 |
| 189 | -0.3401145299 | -0.0000003905 |
| 190 | -0.3400794967 | -0.0000003512 |
| 191 | -0.3400448147 | -0.0000004582 |
| 192 | -0.3400105908 | -0.0000000862 |
| 193 | -0.3399764531 | -0.0000004471 |
| 194 | -0.3399427626 | -0.0000004414 |
| 195 | -0.3399095134 | -0.0000002415 |
| 196 | -0.3398765058 | -0.0000003723 |
| 197 | -0.3398438704 | -0.0000002997 |
| 198 | -0.3398115348 | -0.0000003509 |
| 199 | -0.3397795500 | -0.0000003349 |
| 200 | -0.3397479002 |          |
6.2 Tables for $s = 0$

Putatively minimal average standardized Riesz pair-energy $v_0^s(N)$ and its second derivative $\ddot{v}_0^s$ converted from computer-experimental data $E_0^s(N)$ in [RSZ95,Ca09]

| $N$ | $v_0^s(N)$ | $\ddot{v}_0^s(N)$  |
|-----|-------------|---------------------|
| 2   | -0.6931471806 | -0.08494951843776   |
| 3   | -0.54930614433405 | -0.01052760684652   |
| 4   | -0.49041462650586 | -0.00220150379344   |
| 5   | -0.44205071552419 | -0.0036773970446    |
| 6   | -0.41588830833597 | 8.40980789335588E-05|
| 7   | -0.38964180306881 | -0.00093390867908   |
| 8   | -0.37242920648072 | -0.00277652137846   |
| 9   | -0.35799313127109 | -0.00029013036125   |
| 10  | -0.34584718642271 | -0.00012165715347   |
| 11  | -0.33491781310909 | -0.00033773970446   |
| 12  | -0.32736583684007 | 0.001009733962      |
| 13  | -0.31880412660905 | -0.0019313529543    |
| 14  | -0.31217376933233 | -0.00062683826669   |
| 15  | -0.30617025032223 | -0.00071787003732   |
| 16  | -0.30088460134959 | -0.00052653998475   |
| 17  | -0.29612549236163 | -0.0004655949713    |
| 18  | -0.29183194287079 | -0.0001802707487    |
| 19  | -0.28771866412865 | -0.0006371974506    |
| 20  | -0.28426910513158 | -0.0001371831788    |
| 21  | -0.28095672445238 | -0.0003037417766    |
| 22  | -0.27794808554978 | -7.39232856201699E-05|
| 23  | -0.27501336933281 | -0.00043578332413   |
| 24  | -0.27251443763996 | 2.3805380444275E-05|
| 25  | -0.26999169996667 | -0.00025233942062   |
| 26  | -0.26772130171399 | -0.00022427146747   |
| 27  | -0.26567517492879 | -1.80666292328713E-05|
| 28  | -0.26364711477282 | -9.1718141883222E-05|
| 29  | -0.26171076643103 | -0.00020088193085   |
| 30  | -0.2599752999931  | -6.1987138598565E-05|
| 31  | -0.25830182072903 | -0.00018389162935   |

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|    |            |            |
|----|------------|------------|
| 32 | -0.25681223309431 | 0.00011843935354 |
| 33 | -0.25520420610606 | -0.00019321886972 |
| 34 | -0.25378939798752 | -4.90378805957925E-05 |
| 35 | -0.25242362774958 | -9.14574502674514E-05 |
| 36 | -0.2511493149619 | -5.0970084028344E-05 |
| 37 | -0.24992597225826 | -6.00975463840858E-05 |
| 38 | -0.248762727101 | -5.1294955380482E-05 |
| 39 | -0.24765077693927 | -4.79551673250311E-05 |
| 40 | -0.24658678194487 | -3.72211580642046E-05 |
| 41 | -0.24556000810854 | -4.80799643073904E-05 |
| 42 | -0.24458131423651 | -3.35668470362871E-05 |
| 43 | -0.24363618721152 | -5.92585111488242E-05 |
| 44 | -0.24275031869767 | -7.97229394605692E-06 |
| 45 | -0.24187242247778 | -2.56166416358061E-05 |
| 46 | -0.24102014289952 | -3.72799285126846E-05 |
| 47 | -0.24020514324977 | -7.61240941284103E-05 |
| 48 | -0.23946626769415 | 3.52976504339186E-05 |
| 49 | -0.2386920944881 | -6.46098671298889E-05 |
| 50 | -0.23798253114917 | -8.34470347785277E-06 |
| 51 | -0.23728131251373 | -2.04882748124635E-05 |
| 52 | -0.23660058215309 | -2.95202648709358E-05 |
| 53 | -0.23594937205733 | -2.36160936392393E-05 |
| 54 | -0.23532177805521 | -1.40962708229109E-05 |
| 55 | -0.23470828032391 | -2.5931202199847E-05 |
| 56 | -0.23412071379481 | -1.3970915995838E-05 |
| 57 | -0.23354711181817 | -1.6695091408836E-05 |
| 58 | -0.23299021766001 | -2.03062754731143E-05 |
| 59 | -0.23245362341379 | -2.26108284711313E-05 |
| 60 | -0.23193963999605 | 7.18878297334413E-07 |
| 61 | -0.2314249377 | -2.7881591285861E-05 |
| 62 | -0.23093811699524 | -5.04737413728473E-06 |
| 63 | -0.2304563466462 | -1.27476168964025E-05 |
| 64 | -0.22998731795089 | -1.36433729289731E-05 |
| 65 | -0.2295319356101 | -1.78383549429839E-05 |
| 66 | -0.22909439162424 | -1.46188939495751E-05 |
|   |            |            |
|---|------------|------------|
| 67| -0.22867146653234 | 1.55185044292683E-06 |
| 68| -0.22824698958999  | -1.55888787838065E-05 |
| 69| -0.22783810152643  | -1.38738439675878E-05 |
| 70| -0.22744308730683  | -6.93485401087601E-06 |
| 71| -0.22705500794125  | -2.33475483877588E-05 |
| 72| -0.22669027612405  | 2.08645393496298E-05  |
| 73| -0.2263046797675   | -2.0759411346805E-05  |
| 74| -0.22594115935209  | -1.64016705273828E-05 |
| 75| -0.22559404060721  | -3.30638960721608E-06 |
| 76| -0.22525022825193  | -1.42299813379876E-05 |
| 77| -0.22492064587799  | -2.00815429066137E-06 |
| 78| -0.22459307165834  | -4.1880322580734E-06  |
| 79| -0.22426968547095  | -1.04558366928464E-05 |
| 80| -0.22395675512025  | 4.70035913385791E-07  |
| 81| -0.22363435473364  | -1.17868321321268E-05 |
| 82| -0.22334174117916  | -8.75711084366571E-06 |
| 83| -0.22304888473553  | -5.13968401155696E-06 |
| 84| -0.2227611679759   | -5.62785486868389E-06 |
| 85| -0.22247907907115  | -5.83387355199139E-06 |
| 86| -0.22220282403995  | -6.58125936803255E-06 |
| 87| -0.22193315026811  | -6.60772472819408E-06 |
| 88| -0.221670174221    | -3.04605593015594E-06 |
| 89| -0.22141024422983  | -6.1955634545151E-06  |
| 90| -0.221156509804    | -4.28504674476748E-06 |
| 91| -0.22090706042491  | -4.74832589339447E-06 |
| 92| -0.22066235937172  | -4.02426048681792E-06 |
| 93| -0.22042168257901  | -6.3957705141393E-06  |
| 94| -0.2201840154335   | -2.6865068587234E-06 |
| 95| -0.21995580701456  | -5.94847179991032E-06 |
| 96| -0.21973016095756  | -2.5317439198357E-06 |
| 97| -0.2195068607496   | -6.28182405801314E-06 |
| 98| -0.21928985701641  | -8.8521900634686E-07 |
| 99| -0.21907373117687  | -6.46345842683638E-06 |
|100| -0.21886406879576  | -7.93152682282416E-07 |
|101| -0.21865519956733  | -5.71565295034993E-06 |

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|   | -0.21845204599185 | -3.77464931103355E-06 |
|---|------------------|-----------------------|
| 102| -0.2182566706568 | -4.1870682880305E-06 |
| 103| -0.2180574520034 | 1.4221677929138E-06 |
| 104| -0.21786086116722| -7.102350180588E-06 |
| 105| -0.21767134948428| -2.190123833706E-06 |
| 106| -0.21748402790372| -5.3241145300531E-06 |
| 107| -0.21730203043769| 2.696535636467E-07 |
| 108| -0.21711976331821| -5.1378892570215E-06 |
| 109| -0.21694263378766| -3.5730198860162E-06 |
| 110| -0.21676907727699| -1.4248080854883E-06 |
| 111| -0.21659694557432| -8.2974063129636E-07 |
| 112| -0.21642564361173| -3.9248191232019E-06 |
| 113| -0.21625826646825| -2.4147970263613E-06 |
| 114| -0.2160930403448 | -2.4627666566352E-06 |
| 115| -0.21593080437736| -4.262759661926E-06 |
| 116| -0.21577256747981| -1.0352776545858E-06 |
| 117| -0.21561536585992| -3.1050549168534E-06 |
| 118| -0.21546126929497| -2.7259285149128E-06 |
| 119| -0.21530989865854| -2.4358044693508E-06 |
| 120| -0.21516096382658| -3.848801744471E-06 |
| 121| -0.21501587779637| 3.0093731113178E-06 |
| 122| -0.21486778239304| -3.5112830346073E-06 |
| 123| -0.21472319827275| -2.2175641857524E-06 |
| 124| -0.21458083171665| -3.4568776829668E-06 |
| 125| -0.21444192203822| -2.0420505243978E-06 |
| 126| -0.2143050541032 | -4.3927146264888E-07 |
| 127| -0.21416862605389| -2.9449804793135E-06 |
| 128| -0.21403514267793| -1.95234087436E-06 |
| 129| -0.21390361164806| -1.515768462767E-06 |
| 130| -0.21377359635907| -4.9898615124832E-06 |
| 131| -0.21364857100359| 4.91205787697679E-06 |
| 132| -0.21351863355423| -5.4377450932618E-06 |
| 133| -0.21339413384996| -2.6642286552451E-06 |
| 134| -0.21327229837435| -6.3150049725688E-07 |
| 135| -0.21315109439924| -1.74302284844385E-06 |
| 136| -0.21302989043572| -4.30842850244477E-06 |

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|   |   |   |   |
|---|---|---|---|
| 137 | -0.21303163344697 | 4.95917642923116E-07 |
| 138 | -0.212911676577707 | -1.79459218507816E-06 |
| 139 | -0.21279351429934 | -2.16703439157029E-06 |
| 140 | -0.21267751905601 | -2.73921437016211E-06 |
| 141 | -0.21256426302705 | -6.20672131720834E-07 |
| 142 | -0.21245163307022 | -2.13000696466792E-06 |
| 143 | -0.21234113312036 | -1.53863234181317E-06 |
| 144 | -0.21223217180284 | -2.44880969918482E-07 |
| 145 | -0.21212345536628 | -2.51754395819148E-06 |
| 146 | -0.21201725647369 | 6.48949280507294E-07 |
| 147 | -0.21191040863181 | -1.89781145781831E-06 |
| 148 | -0.2118054586014 | -3.03896148842843E-06 |
| 149 | -0.21170159453247 | -2.47021583343887E-06 |
| 150 | -0.21160020067937 | 4.70809362607127E-08 |
| 151 | -0.21149875974534 | -1.91372729152596E-06 |
| 152 | -0.2113992325386 | -1.9098988734776E-06 |
| 153 | -0.21130161523074 | 2.90559403481883E-07 |
| 154 | -0.21120370736347 | -1.7525558348963E-06 |
| 155 | -0.21110755205178 | -4.59130073517972E-07 |
| 156 | -0.2110118426531 | -2.13449161656776E-06 |
| 157 | -0.21091826774604 | -9.05849328844899E-07 |
| 158 | -0.2108255986883 | -1.2727163832903E-06 |
| 159 | -0.2107342023522 | -6.7946534526571E-07 |
| 160 | -0.21064348548145 | -6.48182475859738E-07 |
| 161 | -0.21055341679317 | -1.3578738045561E-06 |
| 162 | -0.21046470597876 | -6.4275778021919E-07 |
| 163 | -0.21037663792214 | -1.10541287440258E-06 |
| 164 | -0.21028967527839 | -1.03610910762164E-06 |
| 165 | -0.21020374874375 | -9.70611329143001E-07 |
| 166 | -0.21011879282045 | -6.94936569872739E-07 |
| 167 | -0.21003453183371 | -1.51683901841726E-06 |
| 168 | -0.20995178768599 | 3.98236263132734E-08 |
| 169 | -0.20986900371464 | -1.81203067386776E-06 |
| 170 | -0.20978803177396 | -4.81552880238212E-07 |
| 171 | -0.20970754138617 | -6.28672096575356E-07 |

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|    |            |            |
|----|------------|------------|
| 172| -0.20962767967047| -1.00642611994273E-06 |
| 173| -0.2095488243809  | -1.16785260270702E-06 |
| 174| -0.20947113694392  | -2.97605704802084E-08 |
| 175| -0.20939347926752  | -7.3976966222445E-07 |
| 176| -0.20931656136078  | -1.3145110071956E-06 |
| 177| -0.20924095796514  | -5.50239363683591E-07 |
| 178| -0.20916590480886  | -7.5062053070893E-07 |
| 179| -0.20909160227312  | -1.4231080628039E-06 |
| 180| -0.20901872283818  | -1.0896361599122E-07 |
| 181| -0.20894595236685  | -1.42841684058759E-06 |
| 182| -0.20887461031237  | 1.0368942854333E-06 |
| 183| -0.2088022313636   | -1.96770331067908E-06 |
| 184| -0.20873182011814  | -5.7982430315286E-08 |
| 185| -0.20866146685511  | -1.47193601873763E-06 |
| 186| -0.2085925855281   | -1.17488648110342E-06 |
| 187| -0.20852487908757  | 1.14936697975798E-06 |
| 188| -0.20845602328007  | -1.6255270476592E-06 |
| 189| -0.20838879299961  | -8.99850945978997E-07 |
| 190| -0.20832246257009  | -5.787145888914E-07 |
| 191| -0.20825671085517  | -1.55592193121223E-06 |
| 192| -0.20819251506217  | 2.22030766108827E-06 |
| 193| -0.20812609896152  | -1.68921007370759E-06 |
| 194| -0.20806137207094  | -1.70547896297113E-06 |
| 195| -0.20799835065932  | 3.9565570589261E-07 |
| 196| -0.20793493359199  | -1.01998206419873E-06 |
| 197| -0.20787253650673  | -1.7647982364366E-07 |
| 198| -0.2078103159013   | -9.81940776911827E-07 |
| 199| -0.20774907723664  | -7.58389227834E-07 |
| 200| -0.20768859696121  |
6.3 Tables for $s = 1$

Putatively minimal average standardized Riesz pair-energy $v^*_x(N)$ and its second derivative $\ddot{v}^*_x$ converted from computer-experimental data $\mathcal{E}^*_x(N)$ in [RSZ95, Ca09].

| $N$ | $v^*_x(N)$ | $\ddot{v}^*_x(N)$ |
|-----|------------|-------------------|
| 2   | -0.5       |                   |
| 3   | -0.42264973066667 | -0.04232810533333 |
| 4   | -0.38762756666667 | 7.45526666666508E-05 |
| 5   | -0.35253085  | -0.01688044       |
| 6   | -0.33431457333333 | 0.00433531571429 |
| 7   | -0.31176298095238 | -0.0080975785714 |
| 8   | -0.29731114642857 | -0.00158550753968 |
| 9   | -0.28444481944444 | -0.00137818531746 |
| 10  | -0.27295667777778 | -0.00041418207071 |
| 11  | -0.26188271818182 | -0.00426316411411 |
| 12  | -0.25507192272727 | 0.00278972470862 |
| 13  | -0.2454714025641  | -0.00252072968968 |
| 14  | -0.23839161208791 | -0.00040013934066 |
| 15  | -0.23171196095238 | -0.00070389601648 |
| 16  | -0.22573620583333 | -0.0004516105042 |
| 17  | -0.22021761176471 | -0.00043518230392 |
| 18  | -0.2151342       | 4.76747850017833E-05 |
| 19  | -0.2100311345029 | -0.001014455731 |
| 20  | -0.20588648247368 | 6.32914970759568E-05 |
| 21  | -0.20170656      | -0.00036281636979 |
| 22  | -0.1978894538961 | 0.00012053221909 |
| 23  | -0.19395181557312 | -0.00075729358319 |
| 24  | -0.19077147083333 | 0.00030032709354 |
| 25  | -0.187290799     | -0.00039502261795 |
| 26  | -0.18420514978462 | -0.00035453068433 |
| 27  | -0.18147403125356 | 0.00014910944208 |
| 28  | -0.17853830328042 | -6.36662690692846E-05 |
| 29  | -0.17577724157635 | -0.00036358242656 |
| 30  | -0.17332426229885 | -3.0140505350701E-05 |
| 31  | -0.17090142352688 | -0.00034949054751 |

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|---|----------------|----------------|
| 32| -0.16882807530242 | 0.00047453285447 |
| 33| -0.16628019422348 | -0.00043015872711 |
| 34| -0.16416247187166 | -2.26916734467064E-05 |
| 35| -0.162067441119328 | -0.00015075078669 |
| 36| -0.16012316130159 | -5.10168934061417E-05 |
| 37| -0.1582298983033 | -8.08560605566333E-05 |
| 38| -0.15641749136558 | -6.56186490742838E-05 |
| 39| -0.154670707037692 | -5.64969681400296E-05 |
| 40| -0.15298041175641 | -3.09230519075498E-05 |
| 41| -0.1513210434878 | -7.33915171534649E-05 |
| 42| -0.14973506673635 | -3.38043008132338E-05 |
| 43| -0.14818289428571 | -0.0001195286089 |
| 44| -0.14675025044397 | 5.33652486994773E-05 |
| 45| -0.14526424135354 | -2.16579398023553E-05 |
| 46| -0.14379989020929 | -7.03160078679987E-05 |
| 47| -0.14240585506013 | -0.00019965584505 |
| 48| -0.14121147576241 | 0.00018476878612 |
| 49| -0.13983232767857 | -0.00017350225833 |
| 50| -0.13862668185306 | 2.44009844140303E-05 |
| 51| -0.13739663504314 | -1.82048889588726E-05 |
| 52| -0.13618479312217 | -6.16711355130306E-05 |
| 53| -0.13503626233672 | -3.48533194521883E-05 |
| 54| -0.13391930487072 | -8.99523501085575E-06 |
| 55| -0.13281298263973 | -4.98686302196072E-05 |
| 56| -0.13175652903896 | -1.21869364950733E-05 |
| 57| -0.13071226237469 | -2.45326380451383E-05 |
| 58| -0.12969252834846 | -3.94585825060911E-05 |
| 59| -0.12877943447458 | 3.88729843092683E-05 |
| 60| -0.12680774306011 | -7.11879630302947E-05 |
| 61| -0.12590723960867 | 9.13323864926152E-05 |
| 62| -0.12499760291859 | -1.78978935229113E-05 |
| 63| -0.12410586412202 | -2.2432214846948E-05 |
| 64| -0.12323655756731 | -3.7632974317850E-05 |
| 65| -0.12240488331002 | -3.57007573017487E-05 |
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| 67 | -0.12160890981004 | 3.8002925510261E-05 |
| 68 | -0.12077493338455 | -3.6245151990876E-05 |
| 69 | -0.11997720237425 | -3.3405841008749E-05 |
| 70 | -0.11921287720497 | -2.1898359168228E-06 |
| 71 | -0.11845074187928 | -7.3058212219679E-05 |
| 72 | -0.1177616623748 | 0.00011439556059 |
| 73 | -0.11695818730974 | -7.1506992641468E-05 |
| 74 | -0.11622621923732 | -4.8203235101906E-05 |
| 75 | -0.1155424544 | 7.76740127672593E-06 |
| 76 | -0.1148509221614 | -4.0831420324061E-05 |
| 77 | -0.11420022134313 | 1.1883019029901E-05 |
| 78 | -0.11353763750583 | 5.32224366234235E-06 |
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| 80 | -0.11222915317089 | 2.15470341941026E-05 |
| 81 | -0.11156702788272 | -3.4671241648021E-05 |
| 82 | -0.11093957383619 | -2.33227845723243E-05 |
| 83 | -0.1103354425742 | -3.30589089370115E-06 |
| 84 | -0.1097346172031 | -8.6612598618685E-06 |
| 85 | -0.10914245295798 | -1.01474813861691E-05 |
| 86 | -0.10856043619425 | -1.38954558682736E-05 |
| 87 | -0.10799231488639 | -1.56714266911218E-05 |
| 88 | -0.10743986500522 | 2.58841823319589E-06 |
| 89 | -0.10688482670582 | -1.4475583592799E-05 |
| 90 | -0.10634426399001 | -4.9191604736265E-06 |
| 91 | -0.10580862043468 | -8.5242578341548E-06 |
| 92 | -0.10528150113712 | -3.83732358921751E-06 |
| 93 | -0.10475821916316 | -1.8261250519024E-05 |
| 94 | -0.10425319843972 | 1.63249118823039E-06 |
| 95 | -0.10374654522508 | -1.5807537793548E-05 |
| 96 | -0.10325569954825 | 1.45172793653003E-06 |
| 97 | -0.10276340214347 | -1.74573989013549E-05 |
| 98 | -0.1022885621376 | 7.73638239381924E-06 |
| 99 | -0.10180598574933 | -1.98968348971151E-05 |
| 100 | -0.10134330619596 | 7.36955150049123E-06 |
| 101 | -0.10087325709109 | -1.67947511141575E-05 |

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| 107 | -0.09822720019221 | -1.76356269994127E-05 |
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| 110 | -0.09698927536447 | -1.016904812991E-05 |
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| 113 | -0.09579251295354 | -1.21909542836196E-05 |
| 114 | -0.09540109111008 | -4.62733453871E-06 |
| 115 | -0.09501429660107 | -2.84369804537388E-06 |
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| 120 | -0.09317138305602 | -4.8472284530838E-06 |
| 121 | -0.09282066810193 | -1.4195417874901E-05 |
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| 123 | -0.09211952176863 | -1.40567714890238E-05 |
| 124 | -0.09176895171912 | -4.42297296898708E-06 |
| 125 | -0.09142280464258 | -1.29646726877435E-05 |
| 126 | -0.09108962238737 | -4.7769255214064E-06 |
| 127 | -0.0907612167604 | 5.5774078181391E-06 |
| 128 | -0.09042723387426 | -1.00291390614515E-05 |
| 129 | -0.09010320812718 | -3.9319490656493E-06 |
| 130 | -0.08978325832916 | -1.805519360909E-06 |
| 131 | -0.0894650420505 | -2.2144548554486E-05 |
| 132 | -0.08916894022669 | 3.47446343774704E-05 |
| 133 | -0.08883809376851 | -2.49352516719092E-05 |
| 134 | -0.088532182562 | -9.2745829558644E-06 |
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| 136 | -0.0879364594183 | -3.83633506273462E-06 |
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| 137 | -0.08764120923358 | 9.28179083925507E-06 |
| 138 | -0.08733667725801 | -4.96691127305215E-06 |
| 139 | -0.08703711219372 | -6.48071846010012E-06 |
| 140 | -0.08674402784789 | -1.153783651152E-05 |
| 141 | -0.08646247728571 | 2.88057330044555E-06 |
| 142 | -0.08617804615023 | -8.10357186920019E-06 |
| 143 | -0.08590171858662 | -2.83406828316402E-06 |
| 144 | -0.0856282250913  | 3.08765248391296E-06 |
| 145 | -0.08535164394349 | -9.3135028550321E-06 |
| 146 | -0.08508438114596 | 9.77312152317111E-06 |
| 147 | -0.08480734522691 | -6.73755093349993E-06 |
| 148 | -0.0845370468588  | -1.35350460139794E-06 |
| 149 | -0.08426810199528 | -1.01102776257633E-05 |
| 150 | -0.0840092674094  | 3.98419392733107E-06 |
| 151 | -0.08374644862958 | -6.47185117563787E-06 |
| 152 | -0.08349010170094 | -6.46295731676627E-06 |
| 153 | -0.08324021772962 | 6.9215810685916E-06 |
| 154 | -0.08298341217723 | -6.97592395515478E-06 |
| 155 | -0.08273358254881 | 2.22367802815704E-06 |
| 156 | -0.08248152924235 | -9.37420619473493E-06 |
| 157 | -0.08223885014209 | -9.11422094795888E-07 |
| 158 | -0.08199708246392 | -3.78393568656321E-06 |
| 159 | -0.08175909872144 | 2.66358675782286E-07 |
| 160 | -0.08152084862028 | 3.57793971339504E-07 |
| 161 | -0.08128224072516 | -4.5739171544712E-06 |
| 162 | -0.0810482067418  | 1.9512927820906E-07 |
| 163 | -0.08081397763993 | -3.06567351604503E-06 |
| 164 | -0.08058281420619 | -2.78741157611062E-06 |
| 165 | -0.08035443818404 | -1.78951245766168E-06 |
| 166 | -0.08012785167433 | -1.38040567321251E-06 |
| 167 | -0.07990264557031 | -5.14734082346369E-06 |
| 168 | -0.0796825868071  | 3.97994090828302E-06 |
| 169 | -0.07945854810299 | -8.01907032266236E-06 |
| 170 | -0.0792425284692  | 4.29077579244819E-07 |
| 171 | -0.07902607975783 | -5.07074718991696E-07 |

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|   |   |   |   |
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| 172 | -0.07881013812118 | -2.70880987029987E-06 |
| 173 | -0.07859690529439 | -4.00328217031731E-06 |
| 174 | -0.07838767574978 | 3.16258809651693E-06 |
| 175 | -0.07817528361708 | -1.08412407107128E-06 |
| 176 | -0.07796397560844 | -5.57936359946165E-06 |
| 177 | -0.07775824696341 | -3.57159952613095E-07 |
| 178 | -0.0775287547832 | -1.40102088563854E-06 |
| 179 | -0.07734890501412 | -5.90793734966955E-06 |
| 180 | -0.07715084248727 | 1.72040057400125E-06 |
| 181 | -0.07695105955985 | -6.01734425598188E-06 |
| 182 | -0.07675729397669 | 1.07493765258981E-05 |
| 183 | -0.07655277901699 | -1.06424341453915E-05 |
| 184 | -0.07635890649145 | 2.87615567673427E-06 |
| 185 | -0.07616215781022 | -6.84096980885229E-06 |
| 186 | -0.0759725009888 | -5.41068488502106E-06 |
| 187 | -0.07578775307228 | 1.00531148125027E-05 |
| 188 | -0.07559320293094 | -5.38082179846189E-06 |
| 189 | -0.07540403361139 | -4.94420160701559E-06 |
| 190 | -0.07521980849346 | -1.4946266796517E-06 |
| 191 | -0.07503708781819 | -7.21515014479035E-06 |
| 192 | -0.07486156269306 | 1.87730199249225E-05 |
| 193 | -0.07466727434801 | -9.35273588464902E-06 |
| 194 | -0.07448233873885 | -9.26861601924234E-06 |
| 195 | -0.0743066717457 | 5.44473581409743E-06 |
| 196 | -0.07412556001675 | -4.57468066927813E-06 |
| 197 | -0.07394902296846 | 2.40835261167138E-06 |
| 198 | -0.07377007756755 | -5.0053065725475E-06 |
| 199 | -0.07359613747322 | -2.7916899483371E-06 |
| 200 | -0.07342501145829 |   |
### 6.4 Tables for $s = 2$

Putatively minimal average standardized Riesz pair-energy $v_s^x(N)$ and its second derivative $\ddot{v}_s^x$ converted from computer-experimental data $E_s^x(N)$ in [Ca09,Cec]

| $N$ | $v_2^x(N)$ | $\ddot{v}_2^x(N)$ |
|-----|-------------|-------------------|
| 2   | -0.375      |                   |
| 3   | -0.33333333333333 | -0.02083333333333 |
| 4   | -0.3125     | 0.004166666666667 |
| 5   | -0.2875     | -0.0125           |
| 6   | -0.275      | 0.00654761904762  |
| 7   | -0.25595238095238 | -0.00708111160256 |
| 8   | -0.24398587350732 | -0.00057967860454 |
| 9   | -0.23259904466681 | -0.00055045392804 |
| 10  | -0.22176266975433 | 0.00033285517504  |
| 11  | -0.21059343966682 | -0.00512124466615 |
| 12  | -0.20454545454545 | 0.0047362955787   |
| 13  | -0.19376083986662 | -0.00317098031643 |
| 14  | -0.18614720550341 | -0.00010364440555 |
| 15  | -0.17863721554614 | -0.00065340344862 |
| 16  | -0.1717806290375  | -0.00034316587478 |
| 17  | -0.16526720840364 | -0.00034854790081 |
| 18  | -0.15910233567059 | 0.00038063150976  |
| 19  | -0.15255683142778 | -0.00152293973609 |
| 20  | -0.14753426692105 | 0.00042866131909  |
| 21  | -0.14208304109524 | -0.00045522879984 |
| 22  | -0.13708704406926 | 0.00047783137135  |
| 23  | -0.13161321567194 | -0.00129097866742 |
| 24  | -0.12743036594203 | 0.00082264497879  |
| 25  | -0.12242487123333 | -0.00063117898305 |
| 26  | -0.1180505550769  | -0.00057104766809 |
| 27  | -0.11424728745014 | 0.00049490776561  |
| 28  | -0.10994911162698 | 5.65472008196011E-06 |
| 29  | -0.10564528108374 | -0.00065437631007  |
| 30  | -0.10199582685057 | 4.62317141797786E-05 |
| 31  | -0.09830014090323 | -0.00065764181832  |

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|   |                      |                      |
|---|----------------------|----------------------|
| 32| -0.09526209677419   | 0.0012504149463      |
| 33| -0.09097363769886   | -0.0009251275975     |
| 34| -0.08761030622103   | 5.91024322797451E-05 |
| 35| -0.08418787231092   | -0.0002549928849     |
| 36| -0.08102043128571   | -3.3167224807679E-05 |
| 37| -0.0778615748498    | -0.00011337017065    |
| 38| -0.07486525385491   | -7.51279263169202E-05|
| 39| -0.07191947815115   | -5.87632577415675E-05|
| 40| -0.06903246570513   | 2.86269813359885E-06 |
| 41| -0.06614259056098   | -0.00011825042522    |
| 42| -0.06337096584204   | -1.97694361344092E-05|
| 43| -0.06061911055925   | -0.00025016977112    |
| 44| -0.05811742504757   | 0.00024097656619     |
| 45| -0.0553747269697    | 5.2138628396925E-06  |
| 46| -0.05262688702899   | -0.0001562593615     |
| 47| -0.05003527062442   | -0.00050422672429    |
| 48| -0.04794788094415   | 0.00060527859806     |
| 49| -0.04525521266582   | -0.00045806519211    |
| 50| -0.04302060957959   | 0.00013046977964     |
| 51| -0.04065553671373   | 9.33868571739715E-06 |
| 52| -0.03828112516214   | -0.00014110705345    |
| 53| -0.03604782066401   | -4.82038341302893E-05|
| 54| -0.03386272          | 1.7415376398322E-05  |
| 55| -0.0316602039596    | -0.00010261269444    |
| 56| -0.02956030061364   | 7.0258735660178E-06  |
| 57| -0.02745373139411   | -4.07512525181786E-05|
| 58| -0.0253871934271    | -8.35262289764493E-05|
| 59| -0.02340454168907   | -0.0001050587664     |
| 60| -0.02152694582768   | 0.00016769257832     |
| 61| -0.01948165738798   | -0.00018739457367    |
| 62| -0.01762376352195   | 5.47408259087834E-05 |
| 63| -0.01571112883001   | -2.05467919953128E-05|
| 64| -0.01381904093006   | -3.61050203668833E-05|
| 65| -0.01196305805048   | -8.62239386549835E-05|
| 66| -0.01019329910956   | -9.33649851432294E-05|

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| 67 | -0.00851690515378 | 0.00016530091924 |
| 68 | -0.00667521027875 | -9.00022621951962 |
| 69 | -0.00492411562873 | -9.00175016249616E-05 |
| 70 | -0.00326303848033 | 2.51906377677358E-05 |
| 71 | -0.00157677069417 | 0.00043654750963 |
| 72 | 0.00177987334855 | -9.00023064867119 |
| 73 | 0.00344582045354 | -9.0014405338374 |
| 74 | 0.00496771417477 | 5.35525706528706E-05 |
| 75 | 0.00654316046667 | -0.0012329288809 |
| 76 | 0.00799531387047 | 6.57277856631611E-05 |
| 77 | 0.00951319505994 | 5.75274490662858E-05 |
| 78 | 0.01108860369847 | -8.1330778467277E-05 |
| 79 | 0.01258268155854 | 0.00010413254126 |
| 80 | 0.01418089195988 | -0.00010840762017 |
| 81 | 0.01567069474104 | -6.89680790688652E-05 |
| 82 | 0.01709152944314 | 1.477626251012E-05 |
| 83 | 0.01852714037149 | -1.34604538951644E-05 |
| 84 | 0.01994929084594 | -1.8560243783277E-05 |
| 85 | 0.02135288107661 | -3.04430634913144E-05 |
| 86 | 0.02272602824379 | -4.26087560516653E-05 |
| 87 | 0.02405656665491 | 3.2274308983713E-05 |
| 88 | 0.02541937949694 | -3.88368458263955E-05 |
| 89 | 0.0267435549313 | 5.70681608413892E-07 |
| 90 | 0.02806790217094 | -1.67719447810022E-05 |
| 91 | 0.02937567690397 | 6.4641063497059E-06 |
| 92 | 0.03068991574334 | -5.95216588944458E-05 |
| 93 | 0.0319463292382 | 2.69131375872922E-05 |
| 94 | 0.03322626324188 | -4.7686691525503E-05 |
| 95 | 0.03446020686842 | 2.42741077024489E-05 |
| 96 | 0.03571842460266 | -5.37049783949639E-05 |
| 97 | 0.03692293735851 | 4.71981375491648E-05 |
| 98 | 0.03817464825191 | -6.65380220707945E-05 |
| 99 | 0.03935982112323 | 4.45316430658371E-05 |
|100| 0.04058952563762 | -5.40295618385311E-05 |

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| 103 | 0.0429272645355 | -2.43687086123323E-05 |
| 104 | 0.04406495977222 | 8.21308575939266E-05 |
| 105 | 0.04528478589469 | -8.43384376443268E-05 |
| 106 | 0.04642027357951 | 7.58413329604579E-05 |
| 107 | 0.04756334539764 | -6.36426596846151E-05 |
| 108 | 0.04864277455607 | 6.80430404995658E-05 |
| 109 | 0.04979024675501 | -6.0937156617924E-05 |
| 110 | 0.05087678179733 | 2.75757120087317E-05 |
| 111 | 0.05192913264128 | 3.81404359711679E-05 |
| 112 | 0.05300905919723 | -4.13185040168962E-05 |
| 113 | 0.05412712618916 | -1.00696020491897E-05 |
| 114 | 0.05520387476707 | 2.50510293475781E-06 |
| 115 | 0.05627055356293 | -5.2473082764404E-05 |
| 116 | 0.05733973755172 | 1.96518802271228E-05 |
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| 118 | 0.05938726279299 | 2.54941215299676E-05 |
| 119 | 0.06039681067084 | -9.83905057683199E-06 |
| 120 | 0.06138086442717 | -5.636247557115E-05 |
| 121 | 0.06235507913292 | 0.00015092856218 |
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| 123 | 0.06434316461149 | -6.3657849368955E-06 |
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| 125 | 0.0663509097471 | -1.44415809621989E-05 |
| 126 | 0.06729671673333 | 4.04506944298166E-05 |
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| 128 | 0.06920153623831 | -7.7685445403185E-06 |
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|---|---|---|
|137 | 0.07733701534403 | 5.55155963970488E-05 |
|138 | 0.0782645953718 | -1.70098308470701E-05 |
|139 | 0.07917469389949 | -2.21642751551121E-05 |
|140 | 0.08006286398664 | -5.100523672679E-05 |
|141 | 0.08090003355015 | 2.5665607242645E-05 |
|142 | 0.08176286872091 | -3.56716332161611E-05 |
|143 | 0.08259003225845 | -2.4199563383176E-06 |
|144 | 0.08341477583965 | 1.987124105428E-05 |
|145 | 0.08425939063506 | -3.6258013589283E-05 |
|146 | 0.0850677474171 | 5.8903499001811E-05 |
|147 | 0.08593500769313 | -2.9150125351062E-05 |
|148 | 0.0867311784381 | 4.3164608837248E-06 |
|149 | 0.08761554445538 | -4.6035810371375E-05 |
|150 | 0.08841194048591 | 2.4473496811117E-05 |
|151 | 0.08923281001325 | -2.4539113605826E-05 |
|152 | 0.09002914042698 | -2.40588137072617E-05 |
|153 | 0.090801412027 | 4.39663874003404E-05 |
|154 | 0.09161765001443 | -3.16951149688105E-05 |
|155 | 0.09240219288689 | 1.99327377604641E-05 |
|156 | 0.09320666849711 | -4.35444629491855E-05 |
|157 | 0.09396759964437 | 3.22203751190742E-05 |
|158 | 0.09473175282915 | -1.37141092296789E-05 |
|159 | 0.09548219190471 | 8.79071510573315E-06 |
|160 | 0.09624142169536 | 8.82251454399575E-06 |
|161 | 0.09700947402756 | -1.8007166065998E-05 |
|162 | 0.09775951924316 | 7.89535087392016E-06 |
|163 | 0.09851735399682 | -1.04178560480506E-05 |
|164 | 0.09926477089443 | -9.04683195968037E-06 |
|165 | 0.10000314096009 | -1.11980714579476E-06 |
|166 | 0.10074039121833 | -5.4279234323884E-06 |
|167 | 0.10147221355313 | -1.84494793301626E-05 |
|168 | 0.10218558640861 | 2.711870341609E-05 |
|169 | 0.1029260784452 | -3.81989052800069E-05 |
|170 | 0.10362837077515 | 9.0726758542603E-06 |
|171 | 0.10433973618163 | 2.24229295586742E-06 |
| 172 | 0.10505334388107 | -9.13906908106554E-06 |
| 173 | 0.10575781251143 | -1.54236575632405E-05 |
| 174 | 0.10644685748422 | 2.26676546440929E-05 |
| 175 | 0.10715857011166 | 5.9078233182962E-07 |
| 176 | 0.10787087352143 | -2.63275045164768E-05 |
| 177 | 0.10855684942668 | 2.3344125574809E-06 |
| 178 | 0.10924515974449 | -1.09400399017634E-06 |
| 179 | 0.10993237605831 | -2.66541589132308E-05 |
| 180 | 0.11059293821322 | 1.15582399126124E-05 |
| 181 | 0.11126505860804 | -2.673326537923E-05 |
| 182 | 0.11191044167021 | 6.69827539641066E-05 |
| 183 | 0.11262280748634 | -5.68771647287969E-05 |
| 184 | 0.11327829613774 | 2.23036620916606E-05 |
| 185 | 0.11395608845123 | -3.30450971889329E-05 |
| 186 | 0.11460083566754 | -2.81054961135396E-05 |
| 187 | 0.11521747738773 | 6.40038727942605E-05 |
| 188 | 0.11589812298071 | -2.56804432821056E-05 |
| 189 | 0.11655308813042 | -2.45519164336905E-05 |
| 190 | 0.11718350136369 | -5.99227262465529E-06 |
| 191 | 0.11780792232433 | -3.29110832968382E-05 |
| 192 | 0.11839943220168 | 0.00011409688875 |
| 193 | 0.11910503896778 | -5.2031424011334E-05 |
| 194 | 0.11975861430987 | -4.86327746073156E-05 |
| 195 | 0.12036355687735 | 3.55299256605823E-05 |
| 196 | 0.12100402937049 | -2.2219165023796E-05 |
| 197 | 0.12162228269813 | 2.0870138922631E-05 |
| 198 | 0.12226140616469 | -2.72087952620792E-05 |
| 199 | 0.122873320836 | -1.23590826804909E-05 |
| 200 | 0.12347287642462 | |
6.5 Tables for $s = 3$

Putatively minimal average standardized Riesz pair-energy $v_3^x(N)$ and its second derivative $\ddot{v}_3^x$ converted from computer-experimental data $\mathcal{E}_3^x(N)$ in [Ca09,Cec]

| $N$ | $v_3^x(N)$ | $\ddot{v}_3^x(N)$ |
|-----|------------|-------------------|
| 2   | -0.29166666666667 | -0.01008684444444 |
| 3   | -0.269183 | -0.00983913333333 |
| 4   | -0.25678677777778 | 0.00517927555556 |
| 5   | -0.23921198 | -0.29166666666667 |
| 6   | -0.23071909555556 | -0.2691833 |
| 7   | -0.21485553015873 | -0.01008684444444 |
| 8   | -0.20507438690476 | 0.00517927555556 |
| 9   | -0.19505499351852 | 0.00015172161376 |
| 10  | -0.18488387851852 | -0.00983913333333 |
| 11  | -0.17371759939394 | -0.00983913333333 |
| 12  | -0.168437346969697 | -0.00983913333333 |
| 13  | -0.15641525512821 | -0.00983913333333 |
| 14  | -0.14823084945055 | -0.00983913333333 |
| 15  | -0.13979041015873 | -0.00983913333333 |
| 16  | -0.13188856083333 | -0.00983913333333 |
| 17  | -0.12418507230392 | -0.00983913333333 |
| 18  | -0.11663774422658 | 0.00104769691618 |
| 19  | -0.10824518265107 | 0.00104769691618 |
| 20  | -0.10208243089474 | 0.00104769691618 |
| 21  | -0.09487198222222 | -0.00983913333333 |
| 22  | -0.08826499864358 | -0.00983913333333 |
| 23  | -0.08056499337286 | -0.00983913333333 |
| 24  | -0.07500716728261 | -0.00983913333333 |
| 25  | -0.06769667003333 | -0.00983913333333 |
| 26  | -0.06139214204103 | -0.00983913333333 |
| 27  | -0.05600264963913 | 0.001151036925697 |
| 28  | -0.04946212457672 | 0.001151036925697 |
| 29  | -0.04277319302956 | -0.00983913333333 |
| 30  | -0.03723403350192 | 0.001151036925697 |
| 31  | -0.03147298915412 | -0.00983913333333 |

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|   |   |   |   |   |
|---|---|---|---|---|
| 32 | -0.02691829964382 | 0.00280037730523 |
| 33 | -0.01956323282828 | -0.00188481440318 |
| 34 | -0.01409298041592 | 0.00025763185791 |
| 35 | -0.00836509614566 | -0.00042633428334 |
| 36 | -0.00306354615873 | 4.2583899529677E-05 |
| 37 | 0.00228058772773 | -0.00017826218792 |
| 38 | 0.00744645942627 | -3.56287001576465E-05 |
| 39 | 0.01257670242465 | -4.8327427307978E-05 |
| 40 | 0.01765861799573 | 0.00010472418523 |
| 41 | 0.02284525775203 | -0.00019360091523 |
| 42 | 0.02783829659311 | 3.51409925407678E-05 |
| 43 | 0.03286647642673 | -0.00051981849079 |
| 44 | 0.03737483776956 | 0.00073780197852 |
| 45 | 0.04262100109091 | 9.2143136521367E-05 |
| 46 | 0.04795930754911 | -0.00035398032246 |
| 47 | 0.05294363368486 | -0.00121438817462 |
| 48 | 0.05761357164598 | 0.0016791584031 |
| 49 | 0.0621626680102 | -0.00115421019211 |
| 50 | 0.06645755418231 | 0.0004243123044 |
| 51 | 0.07117675265882 | 0.00011958393757 |
| 52 | 0.0760155350729 | -0.00032546670807 |
| 53 | 0.08052885077891 | -5.61197833050947E-05 |
| 54 | 0.08498604670161 | 0.00011398397277 |
| 55 | 0.08955722659708 | -0.00021864014624 |
| 56 | 0.09390976634632 | 8.3101054175451E-05 |
| 57 | 0.09834540714703 | -7.21014484539179E-05 |
| 58 | 0.10270894649929 | -0.00018594031678 |
| 59 | 0.1068564553478 | -0.0002206671527 |
| 60 | 0.11084207785499 | 0.00054714300148 |
| 61 | 0.11534475317668 | -0.00048653601821 |
| 62 | 0.11936089248017 | 0.000180273365 |
| 63 | 0.12355730412016 | 4.326346725222E-06 |
| 64 | 0.12775804209491 | -5.15173597218366E-05 |
| 65 | 0.13190726209994 | -0.00019978950367 |
| 66 | 0.13585669382129 | -0.00024366441101 |
|   |       |       |
|---|-------|-------|
| 67 | 0.13956246052163 | 0.00055550923398 |
| 68 | 0.14382373645596 | -0.00022708593816 |
| 69 | 0.14785792645212 | -0.00024535484855 |
| 70 | 0.15164676159972 | 0.00013100204677 |
| 71 | 0.15556659878941 | -0.00066592521513 |
| 72 | 0.15882051077334 | 0.00143510479688 |
| 73 | 0.16350952754947 | -0.00070960675555 |
| 74 | 0.16748893757004 | -0.0004133927858 |
| 75 | 0.1710549548048 | 0.00021124809025 |
| 76 | 0.1748322012982 | -0.00036314952753 |
| 77 | 0.17824633592732 | 0.00024507688991 |
| 78 | 0.18190552861472 | 0.00026234373412 |
| 79 | 0.18582706503624 | -0.0002459406304 |
| 80 | 0.18950266099473 | 0.0003869692721 |
| 81 | 0.19356522622531 | -0.0003383314012 |
| 82 | 0.19728947831577 | -0.00018854494634 |
| 83 | 0.20082514545989 | 8.91076541672253E-05 |
| 84 | 0.2044992025818 | -1.67607390024194E-05 |
| 85 | 0.20805793431746 | -2.9490780758069E-05 |
| 86 | 0.21163645759599 | -6.9839552229306E-05 |
| 87 | 0.21514514132228 | -0.0001165745907 |
| 88 | 0.21853725058952 | 0.0001498369889 |
| 89 | 0.22207919685563 | -0.00010861201564 |
| 90 | 0.22551253110612 | 3.5637838353475E-05 |
| 91 | 0.22898150319495 | -3.2585384919031E-05 |
| 92 | 0.23241788898887 | 6.1263695399891E-05 |
| 93 | 0.23591554024233 | -0.00019466580045 |
| 94 | 0.23921852478533 | 0.00013426626295 |
| 95 | 0.2426557615528 | -0.00014976206544 |
| 96 | 0.2459433654598 | 0.00012888508606 |
| 97 | 0.24935963985037 | -0.0001696671728 |
| 98 | 0.25260631752637 | 0.00020921463468 |
| 99 | 0.25605320983165 | -0.00022261889586 |
| 100 | 0.25927748324377 | 0.00019225679823 |
| 101 | 0.26269401345413 | -0.0001765310158 |
|   | 0.26593401264868 | -1.82619993290833E-05 |
|---|-----------------|------------------------|
| 102| 0.2691557498439 | -6.26353506716915E-05 |
| 103| 0.27231485168845 | 0.00032375670265 |
| 104| 0.27579771023565 | -0.00028172388738 |
| 105| 0.27899884489548 | 5.158728064907E-05 |
| 106| 0.28225156683595 | -0.0002268305527 |
| 107| 0.28527745822372 | 0.00029510069715 |
| 108| 0.28859845030864 | -0.0001385262691 |
| 109| 0.29170122137059 | -0.00017153871193 |
| 110| 0.29469013980562 | 0.00013750345979 |
| 111| 0.29781656170045 | 0.00013796399609 |
| 112| 0.3011452230721 | -2.08736037944357E-05 |
| 113| 0.30427451891787 | 3.81762178164879E-05 |
| 114| 0.30741364192474 | -0.0002228574694 |
| 115| 0.31059094114943 | 9.62420288364019E-05 |
| 116| 0.3135695462717 | -7.14383650260997E-05 |
| 117| 0.31663721013376 | -8.89888952134462E-05 |
| 118| 0.31963701080732 | -1.67171852707981E-05 |
| 119| 0.32254758582166 | -0.000210883099063 |
| 120| 0.32544196718274 | 0.00066944307554 |
| 121| 0.32812524755318 | 0.00017153871193 |
| 122| 0.33147797099916 | 0.00013796399609 |
| 123| 0.33456215224233 | 6.41573772408588E-06 |
| 124| 0.33765274922323 | -4.9005694251042E-05 |
| 125| 0.34053100768254 | 2.82856096472939E-05 |
| 126| 0.34336236057243 | 0.00020195688012 |
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| 134| 0.36632252767864 | 0.00010516120896 |
| 135| 0.36910664377269 | -2.1922376047645E-05 |

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|---|---|---|
|   | 0.3718688374907 | 0.00026705962559 |
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|   | 0.38075030867044 | -0.0002112555359 |
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|   | 0.421597732503 | 0.00011045146252 |
|   | 0.4243615343482 | -0.00019248156826 |
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|   | 0.4320883573569 | 5.73596687816202E-05 |
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|   | 0.43736290299068 | -7.2164600769975E-05 |
|   | 0.43995600851136 | 5.09445660059615E-05 |
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|   | 0.45037232278447 | -2.46402004429602E-05 |
|   | 0.45293729300363 | -6.64396903324871E-05 |
|   | 0.45543582353246 | 0.0001430025502 |
|   | 0.45807735611149 | -0.00017571816366 |
|   | 0.46054317152686 | 6.17658464966975E-05 |
|   | 0.4630707228873 | 2.14594050894634E-05 |
|   |            |            |            |
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| 177| 0.47823800814437 |            | 1.42237316299032E-05 |
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| 194| 0.51972378534996 |            | -0.00023549816973 |
| 195| 0.5219862089162  |            | 0.00019285863599 |
| 196| 0.52444149111844 |            | -0.0001048140132 |
| 197| 0.52679195930747 |            | 0.00012282712877 |
| 198| 0.52926525462527 |            | -0.00013765031158 |
| 199| 0.53160089963149 |            | -5.55293841086879E-05 |
| 200| 0.5338810152536  |            |            |