Electrons on the Sphere

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Abstract. We investigate the energy of arrangements of N points (charged particles) on the surface of the unit sphere in $\mathbf{R}^3$, interacting through a power law potential $V(r) = r^\alpha$, $-2 < \alpha < 2$, $\alpha \neq 0$ and $V(r) = \log(1/r)$ for $\alpha = 0$. Results of numerical experiments are presented for the three classical cases $\alpha = 0, \pm 1$, for $N = 2, \ldots, 200$. We also investigate the geometric structures of the equilibrium points and their group properties. In the case $\alpha = 0$, we prove that the N points of minimal energy must be well-separated in the sense that any two distinct points are at least $(3/5)(1/\sqrt{N})$ units distance apart.

1. Introduction

Circles and spheres have intrinsic properties that continue to fascinate mathematicians and scientists. Since J. J. Thompson's plum pudding model of the atom, there has been much interest in the equilibrium configurations of charges confined to spheres and disks. With the advent of high speed computers, the investigation of these configurations intensified, especially among physicists, chemists and crystallographers; see, for example, [2], [4], [8], [9], [10], [12], [20]. The discovery of carbon fullerenes (C_{60}, C_{70}, etc.) and its connection to these equilibrium configurations has provided added impetus to these investigations (*cf.* [6], [17], [22]).

To describe our results we begin with some needed notation. A set of $N \geq 2$ points on the unit sphere $S^2 := \{x \in \mathbf{R}^3 : |x| = 1\}$ will be denoted by ω_N. We shall use $|x - y|$ to denote the Euclidean distance in $\mathbf{R}^3 = \{x_1, \ldots, x_N\}$ between two points $x, y \in S^2$. For each real α, the α-*energy* associated with ω_N is defined by

$$E(\alpha, \omega_N) := \begin{cases} \displaystyle\sum_{1 \leq i < j \leq N} \log \frac{1}{|x_i - x_j|}, & \text{if } \alpha = 0 \\ \displaystyle\sum_{1 \leq i < j \leq N} |x_i - x_j|^\alpha, & \text{if } \alpha \neq 0. \end{cases}$$

Our concern is then with the *extremal* α-energy for N points on the sphere:

$$\mathcal{E}(\alpha, N) := \begin{cases} \displaystyle\inf_{\omega_N \subset S^2} E(\alpha, \omega_N) & \text{if } \alpha \leq 0 \\ \displaystyle\sup_{\omega_N \subset S^2} E(\alpha, \omega_N) & \text{if } \alpha > 0. \end{cases}$$

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Since S^2 is compact, it is clear that for each $N \geq 2$, the extremal α-energy is attained by some point set, which we denote by $\omega_N^{(\alpha)}$. Such equilibrium points are not unique, but we use $\omega_N^{(\alpha)}$ to denote any particular determination of them.

The outline of our paper is as follows. In Section 2, we prove that for $\alpha = 0$, the equilibrium points are well-separated in the sense that

$$|x_i - x_j| \geq \frac{3}{5}\frac{1}{\sqrt{N}} \qquad \text{for } x_i \neq x_j, \;\; x_i, x_j \in \omega_N^{(0)}.$$

A similar result for $\alpha = -1$ was proved by Dahlberg [7]. We remark that on partitioning the sphere into $N-1$ parts as described in [15], §2, it follows by the pigeon hole principle that any $\omega_N \subset S^2$ contains at least 2 points with distance $\leq 7/\sqrt{N-1}$.

In Section 3, we discuss our numerical experiments for determining the extremal α-energy and characterizing the equilibrium point sets $\omega_N^{(\alpha)}$. Table 1 lists the extremal energies and their point groups for $\alpha = 0, \pm 1, \quad 2 \leq N \leq 200$.

In Section 4, we compare the conjectured asymptotic formulas for the extremal energies given by the authors in [15] with the numerically determined values. We also discuss the energy values for all local extrema, which turn out to be very close to the global extremum.

In Section 5, we consider the geometric properties of the extremal point set $\omega_N^{(\alpha)}$. We introduce the Dirichlet cells and discuss the similarity between these cells and the structure of carbon fullerenes.

2. Separation theorem for the logarithmic equilibrium points

It is intuitively clear that, at least for $\alpha \leq 0$, the points of minimal energy should be well-separated. To describe this property, we define

$$\delta(\omega_N) := \inf_{i \neq j} |x_i - x_j|; \qquad \delta_N := \sup_{\omega_N \subset S^2} \delta(\omega_N).$$

The determination of δ_N is called *Tamme's problem* or the *spherical packing problem.* It is known [19] that

$$\delta_N \sim \frac{C}{\sqrt{N}} \;\text{ with }\; C = \sqrt{\frac{8\pi}{\sqrt{3}}} \;\text{ as } N \to \infty. \tag{2.1}$$

For the case $\alpha = -1$, Dahlberg [7] proved that for equilibrium points on a smooth surface in $\mathbf{R}^3$, the separation distance is of order $1/\sqrt{N}$. In particular, for S^2 , we have

$$\delta\left(\omega_N^{(-1)}\right) \geq \frac{C_1}{\sqrt{N}}, \;\text{ for some constant } C_1 > 0. \tag{2.2}$$

A separation theorem for positive values of α was obtained by Stolarsky [18] who showed that

$$\delta_n(\omega_N^{(\alpha)}) \geq \left[\frac{4\alpha}{2^\alpha(2+\alpha)}\right]^{1/(2-\alpha)} \cdot N^{-1/(2-\alpha)}, \quad 0 < \alpha < 2. \tag{2.3}$$

In contrast, for the case $\alpha \geq 2$, it is known that some equilibrium points may coincide (*cf.* [3]).

Here we prove that, for the case $\alpha = 0$, the following separation property holds:

Theorem 1 *If $\omega_N^{(0)}$ is a set of logarithmic equilibrium points, then*

$$\delta\left(\omega_N^{(0)}\right) \geq \frac{3}{5} \cdot \frac{1}{\sqrt{N}}, \quad N \geq 2. \tag{2.4}$$

Proof: Letting $\omega_N^{(0)} = \{x_1^*, x_2^*, \ldots, x_N^*\}$, it suffices to show that $|x_1^* - x_j^*| \geq (3/5)/\sqrt{N}$ for all $2 \leq j \leq N$. For any $\omega_N = \{x_1, \ldots, x_N\} \subset S^2$, it follows from the extremal property of $\omega_N^{(0)}$ that

$$\sum_{i<j} \log \frac{1}{|x_i^* - x_j^*|} \leq \sum_{i<j} \log \frac{1}{|x_i - x_j|},$$

which is equivalent to

$$\prod_{i<j} |x_i - x_j| \leq \prod_{i<j} |x_i^* - x_j^*|. \tag{2.5}$$

Consequently,

$$\prod_{i=2}^{N} |x - x_i^*| \cdot \prod_{2 \leq i < j \leq N} |x_i^* - x_j^*| \tag{2.6}$$

attains its maximum over S^2 at $x = x_1^*$.

Let $\mathcal{S} : S^2 \to \mathbf{C}$ be the stereographical projection of S^2 onto the complex plane $\mathbf{C}$ and set $z_i := \mathcal{S}(x_i^*), i = 1, 2, \ldots, N$. Without loss of generality we assume that x_1^* lies at the south pole of S^2 so that $z_1 = \mathcal{S}(x_1^*) = 0$. Then from (2.6), the expression

$$\prod_{i=2}^{N} \left[\frac{|z - z_i|}{\sqrt{1 + |z|^2}}\right] = \prod_{i=2}^{N} |z - z_i| \cdot \left(1 + |z|^2\right)^{-(N-1)/2}$$

attains its maximum over $\mathbf{C}$ at $z = z_1 = 0$. Setting $p(z) := \prod_{i=2}^{N}(z - z_i)$, we obtain

$$|p(0)| = \sup_{z \in \mathbf{C}} \left\{|p(z)| \cdot \left(1 + |z|^2\right)^{-(N-1)/2}\right\},$$

so that

$$|p(z)| \leq |p(0)| \cdot \left(1+|z|^2\right)^{(N-1)/2} \leq |p(0)| \left(1+|z|^2\right)^{N/2}, \text{ for } z \in \mathbf{C}. \qquad (2.7)$$

By Cauchy's formula, we have for $|z| \leq r < R$,

$$p'(z) = \frac{1}{2\pi i} \int_{|\zeta|=R} \frac{p(\zeta)}{(\zeta - z)^2}\, d\zeta$$

and so, from (2.7),

$$\begin{aligned} |p'(z)| &\leq \frac{1}{2\pi} \left| \int_{|\zeta|=R} \frac{p(z)}{(\zeta - z)^2}\, d\zeta \right| \\ &\leq \frac{1}{2\pi} \int_0^{2\pi} \frac{|p(0)|(1+R^2)^{N/2} R d\theta}{(R-r)^2} \\ &= \frac{R\,|p(0)|}{(R-r)^2} \left(1+R^2\right)^{N/2}. \end{aligned} \qquad (2.8)$$

Setting $r := 1/(3\sqrt{N})$ and $R := 4r$ we thus obtain

$$\begin{aligned} |p'(z)| &\leq \tfrac{4}{3\sqrt{N}} \tfrac{|p(0)|}{(1/N)} \left(1 + \tfrac{16}{9N}\right)^{N/2} \\ &\leq \tfrac{4\sqrt{N}}{3} |p(0)|\, e^{8/9} \quad \text{ for } |z| \leq 1/(3\sqrt{N}). \end{aligned} \qquad (2.9)$$

We next verify the following

Claim: If z' is any of the points $\{z_i\}_{i=2}^N$, then $|z'| \geq 3e^{-8/9}/(4\sqrt{N})$.

Indeed, if $|z'| > 1/(3\sqrt{N})$, then since $1/3 > 3e^{-8/9}/4$, there is nothing to prove. So we assume that $|z'| \leq 1/(3\sqrt{N})$. Since

$$0 = p(z') = p(0) + \int_0^{z'} p'(\zeta) d\zeta,$$

we have

$$|p(0)| = \left| \int_0^{z'} p'(\zeta) d\zeta \right|,$$

and so from (2.9), we obtain

$$|p(0)| \leq \frac{4\sqrt{N}}{3} |p(0)|\, e^{8/9}\, |z'|\,.$$

Thus $|z'| \geq 3e^{-8/9}/(4\sqrt{N})$, as claimed.

Finally, if $z \in \mathbf{C}$ satisfies $|z| = 3e^{-8/9}/(4\sqrt{N})$ and $x = \mathcal{S}^{-1}(z)$, then the Euclidean distance from x to the south pole is

$$
\begin{aligned}
|x - x_1^*| &= \frac{2|z-0|}{\sqrt{1+|z|^2}} = \frac{3e^{-8/9}/2\sqrt{N}}{\sqrt{1+\left(3e^{-8/9}/4\sqrt{N}\right)^2}} \\
&\geq \frac{3e^{-8/9}/2\sqrt{N}}{\sqrt{1+\left(3e^{-8/9}/4\sqrt{2}\right)^2}} \approx 0.6025\frac{1}{\sqrt{N}} > \frac{3}{5}\frac{1}{\sqrt{N}},
\end{aligned}
$$

which completes the proof. ■

Remark: Clearly the constant $3/5$ in Theorem 1 cannot be replaced by any number greater than or equal to the constant $\sqrt{8\pi/\sqrt{3}} \approx 3.809$ in (2.1). In fact, on considering the case $N = 5$, it is not difficult to prove (by reason of contradiction) that there is at least one pair of points with distance $\leq \sqrt{2}$; hence the constant $3/5$ cannot be replaced by a number $> \sqrt{2}\sqrt{5} = \sqrt{10} \approx 3.162$.

3. Numerical experiments and the table of energies

To numerically determine extremal α-energies we begin by mapping the sphere onto the extended complex plane via stereographical projection. This allows the use of methods of unconstrained optimization.

We began with the case $\alpha = 0$. As a first step, the Steepest Descent method was examined. To make this algorithm faster for our particular case, we extracted an explicit formula for the descent step so as to avoid the expensive part of this algorithm, *i.e.* , the line minimization to calculate the step size in each iteration. However, we found convergence was slow near the extremal points when high precision was desired. To accelerate the convergence, we mimicked Newton's method, using first-order linear approximation to avoid calculating the inverse of a Jacobian matrix. When we combined the two algorithms, using the Steepest Descent for rough calculation and then switching to the second Newton-type algorithm we obtained a robust and fast algorithm. Unfortunately, this technique was successful only for the case $\alpha = 0$.

To get a general method to optimize the energy, we investigated the Downhill Simplex method, the Conjugate Gradient method and the Quasi-Newton method (or Variable Metric method). We refer the reader to [13], [14] for more information about these algorithms. We found that for the energy problem, the Quasi-Newton method worked best. We implemented this method so that it would calculate the extremal α-energy for any α. A few observations are in order from our calculations.

First, when N is large, say larger than 75, there are a lot of local extrema. To make things even more difficult, all the local extrema have very close energies.

To maximize the possibility that the extremal points found were actual global extremal points, we tried different iteration schemes and at least 1000 different random start positions. We also examined the geometric and group structure of the extremal points and used the appropriate asymptotic approximation formula (see (4.3)) to inspect any suspicious energy values obtained. We also ran cross-checks in the following way. For each N, we compared the symmetry groups for the extremal points for $\alpha = 0, \pm 1$. If these groups were different, for example, if the symmetry groups for $\omega_N^{(0)}$ and $\omega_N^{(-1)}$ were not the same, we would plug in $\omega_N^{(0)}$ as the starting position to find $\omega_N^{(-1)}$, and then compare the final energy values and group properties. A similar procedure was employed in all possible cases. Second, we found that the extremal points for different values of α's are usually very close; typically they give even better energy values than many of the corresponding local extrema.

There have been many attempts at finding the extremal energies. Most of them have focused on the case $\alpha = -1$ and attempted by researchers from physics, chemistry, biology and crystallography; see [1], [2], [4], [5], [8], [10], [12], [20], [21] and the references therein. From what we can find, our numerical results are more extensive and more accurate than those now in the literature. We remark that (as announced by the usenet news group *sci.math.research*) Hardin, Sloane and Smith did extensive calculations for spherical codes, packings, coverings and optimal energy. We compared their results for the cases $\alpha = \pm 1$ and found that they agreed with ours for all the $\mathbf{R}^3$ cases considered. Their tables are available via *netlib.att.com*

Table 1 lists the extremal energies that we found and the corresponding point group character for the cases $\alpha = 0, \pm 1$ and $2 \le N \le 200$. We refer the reader to [16] for more information about the point group notation.

N	Newton Points		Logarithmic Points		Extremal Sum	
	(-1)-Energy	PG	0-Energy	PG	1-Energy	PG
2	0.500000000	$D_{\infty h}$	-0.693147181	$D_{\infty h}$	2.000000000	$D_{\infty h}$
3	1.732050808	D_{3h}	-1.647918433	D_{3h}	5.196152423	D_{3h}
4	3.674234614	T_d	-2.942487759	T_d	9.797958971	T_d
5	6.474691495	D_{3h}	-4.420507155	D_{3h}	15.681433797	D_{3h}
6	9.985281374	O_h	-6.238324625	O_h	22.970562749	O_h
7	14.452977414	D_{5h}	-8.182477864	D_{5h}	31.530925729	C_2
8	19.675287861	D_{4d}	-10.428017781	D_{4d}	41.473091069	D_{4d}
9	25.759986531	D_{3h}	-12.887752726	D_{3h}	52.743634159	D_{3h}
10	32.716949460	D_{4d}	-15.563123389	D_{4d}	65.349740387	D_{4d}
11	40.596450508	C_{2v}	-18.420479721	C_{2v}	79.274738603	C_{2v}
12	49.165253058	I_h	-21.606145231	I_h	94.582915228	I_h
13	58.853230612	C_{2v}	-24.866721876	C_{2v}	111.170400367	C_{2v}
14	69.306363297	D_{6h}	-28.407813009	D_{6h}	129.120384120	D_{6h}
15	80.670244114	D_3	-32.147876284	D_3	148.400623449	D_3

16	92.911655303	T	-36.106152162	T	169.019120242	T
17	106.050404829	D_{5h}	-40.273066961	D_{5h}	190.972276822	D_{5h}
18	120.084467448	D_{4h}	-44.650287259	D_{4h}	214.261010695	D_{4h}
19	135.089467557	C_{2v}	-49.199891566	C_{2v}	238.872314927	C_{2v}
20	150.881568334	D_{3h}	-54.011129975	D_{3h}	264.836151018	D_{3h}
21	167.641622399	C_{2v}	-59.000912135	C_{2v}	292.125643198	C_{2v}
22	185.287536149	T_d	-64.206007762	T_d	320.752927535	T_d
23	203.930190663	D_3	-69.578382593	D_3	350.703055942	D_3
24	223.347074052	O	-75.213984789	O	382.004840435	O
25	243.812760299	C_s	-80.997509990	C_s	414.624638234	C_s
26	265.133326317	C_2	-87.009423057	C_2	448.585640735	C_2
27	287.302615033	D_{5h}	-93.251986400	D_{5h}	483.888307515	D_{5h}
28	310.491542358	T	-99.658609384	T	520.514876245	T
29	334.634439920	D_3	-106.254571171	C_2	558.472198025	C_{2v}
30	359.603945904	C_{2v}	-113.089255497	C_{2v}	597.772969974	C_{2v}
31	385.530838063	D_3	-120.110346639	D_3	638.402930774	D_3
32	412.261274651	I_h	-127.378867615	I_h	680.378893329	I_h
33	440.204057448	C_s	-134.747820824	C_s	723.664658824	C_1
34	468.904853281	C_{2v}	-142.375852271	C_{2v}	768.298034095	C_{2v}
35	498.569872491	C_2	-150.192058511	C_2	814.262256769	C_s
36	529.122408375	C_{2v}	-158.224068426	C_{2v}	861.563951327	C_{2v}
37	560.618887731	D_{5h}	-166.450697524	D_{5h}	910.197927572	D_{5h}
38	593.038503567	D_{6h}	-174.880197152	D_{6h}	960.166478128	D_{6h}
39	626.389009017	D_{3h}	-183.509225712	D_{3h}	1011.468379374	D_{3h}
40	660.675278835	T_d	-192.337689917	T_d	1064.104220573	T_d
41	695.916744342	D_{3h}	-201.359206649	D_{3h}	1118.072491255	D_{3h}
42	732.078107544	D_{5h}	-210.584511558	D_{5h}	1173.375392867	D_{5h}
43	769.190846459	C_{2v}	-220.003477052	C_{2v}	1230.010677519	D_{2d}
44	807.174263085	O_h	-229.641801488	O_h	1287.983871724	O_h
45	846.188401061	D_3	-239.453698253	D_3	1347.286313191	D_3
46	886.167113639	T	-249.455847901	T	1407.920471173	T
47	927.059270680	C_s	-259.661759853	C_s	1469.888840611	C_s
48	968.713455344	O	-270.117949959	O	1533.201032999	O
49	1011.557182654	C_3	-280.701903118	C_3	1597.833364652	C_3
50	1055.182314726	D_{6h}	-291.528600658	D_{6h}	1663.807762158	D_{6h}
51	1099.819290319	D_3	-302.533673455	D_3	1731.111978303	D_3
52	1145.418964319	C_3	-313.732371935	C_3	1799.749277102	C_3
53	1191.922290416	C_{2v}	-325.138234695	C_{2v}	1869.721471573	C_2
54	1239.361474729	C_2	-336.745464397	C_2	1941.028321457	C_2
55	1287.772720783	C_2	-348.541796281	C_2	2013.666898463	C_2
56	1337.094945276	C_{2v}	-360.545899244	C_2	2087.641190319	C_2
57	1387.383229253	D_3	-372.741200618	D_3	2162.947618213	D_3
58	1438.618250640	C_{2v}	-385.132829792	C_{2v}	2239.587371641	C_{2v}
59	1490.773335279	C_2	-397.728149661	C_2	2317.561595973	C_2
60	1543.830400976	D_3	-410.533162793	D_3	2396.871796975	D_3

61	1597.941830199	C_1	-423.507635991	C_1	2477.510554009	C_1
62	1652.909409898	C_{5v}	-436.703979238	C_{5v}	2559.487475604	C_{5v}
63	1708.879681503	D_3	-450.081239177	D_3	2642.794690003	D_3
64	1765.802577927	C_{2v}	-463.654432989	C_{2v}	2727.435316863	C_{2v}
65	1823.667960264	C_2	-477.426426069	C_2	2813.409669853	C_2
66	1882.441525304	C_2	-491.407470034	D_3	2900.720101300	D_3
67	1942.122700405	C_{5v}	-505.592612503	C_{5v}	2989.364523851	C_{5v}
68	2002.874701749	C_{2v}	-519.946642286	C_{2v}	3079.338280647	C_{2v}
69	2064.533483235	D_3	-534.508186181	D_3	3170.647315121	D_3
70	2127.100901551	D_{2d}	-549.275055846	D_{2d}	3263.290940842	C_{2v}
71	2190.649906426	C_2	-564.231694734	C_2	3357.267031049	C_2
72	2255.001190975	I	-579.420345773	I	3452.582333378	I
73	2320.633883745	C_2	-594.728698429	C_2	3549.219062869	C_2
74	2387.072981838	C_2	-610.267071410	C_2	3647.194636734	C_2
75	2454.369689040	D_3	-626.023462685	D_3	3746.506709423	D_3
76	2522.674871841	C_2	-641.963150518	C_2	3847.150291717	C_2
77	2591.850152354	C_{5v}	-658.117809839	C_{5v}	3949.130169686	C_{5v}
78	2662.046474566	T_d	-674.452994190	D_3	4052.441072676	D_3
79	2733.248357479	C_s	-690.974900936	C_s	4157.084301899	C_s
80	2805.355875981	D_{4h}	-707.703346180	D_{4h}	4263.062515153	D_{4h}
81	2878.522829664	C_2	-724.604469337	C_2	4370.370662592	C_2
82	2952.569675287	C_{2v}	-741.717922456	C_{2v}	4479.014655900	C_{2v}
83	3027.528488921	C_2	-759.035354755	C_2	4588.992879403	C_2
84	3103.465124431	C_2	-776.545431564	C_2	4700.304386584	C_2
85	3180.361442939	C_2	-794.250312284	C_2	4812.949204545	C_2
86	3258.211605713	C_2	-812.151321866	D_3	4926.927492794	D_3
87	3337.000750015	C_2	-830.251915153	C_2	5042.239537538	C_2
88	3416.720196758	C_{2v}	-848.553426918	C_{2v}	5158.885719439	C_{2v}
89	3497.439018625	C_2	-867.042516404	C_2	5276.864357178	C_2
90	3579.091222723	D_3	-885.731821765	D_3	5396.176934707	D_3
91	3661.713699320	C_2	-904.614412440	C_2	5516.822641458	C_2
92	3745.291636241	C_{2v}	-923.692636330	C_{2v}	5638.801684482	C_{2v}
93	3829.844338421	C_2	-942.963958073	C_2	5762.113935722	C_2
94	3915.309269620	C_{2v}	-962.439132146	C_{2v}	5886.760543315	C_{2v}
95	4001.771675565	C_2	-982.102678320	C_2	6012.739719604	C_2
96	4089.154010056	C_2	-1001.969533966	C_2	6140.053338966	D_3
97	4177.533599622	C_2	-1022.023977757	C_2	6268.699217104	C_2
98	4266.822464156	C_2	-1042.284690399	C_2	6398.680119684	C_2
99	4357.139163132	C_2	-1062.726669939	C_2	6529.992426643	C_2
100	4448.350634331	T	-1083.377140539	T	6662.639917807	T
101	4540.590051694	D_3	-1104.208757815	D_3	6796.618809138	D_3
102	4633.736565899	D_3	-1125.246488904	D_3	6931.932549575	D_3
103	4727.836616833	C_2	-1146.481260096	C_2	7068.579950074	C_2
104	4822.876522749	T	-1167.915837173	T	7206.561396622	T
105	4919.000637616	D_3	-1189.520301973	D_3	7345.872974890	D_3

106	5015.984595705	C_{2v}	-1211.341059880	C_{2v}	7486.520457533	C_{2v}
107	5113.953547714	C_2	-1233.351922242	C_2	7628.500739294	C_2
108	5212.813507831	C_2	-1255.571131869	C_2	7771.816125988	D_3
109	5312.735079920	C_2	-1277.966926891	C_2	7916.462521093	C_2
110	5413.549294192	T	-1300.571089557	T	8062.444047253	T
111	5515.293214587	D_3	-1323.375216776	D_3	8209.759347324	D_3
112	5618.044882326	C_{5v}	-1346.366613690	C_{5v}	8358.407118805	C_{5v}
113	5721.824978027	D_3	-1369.541472775	D_3	8508.387038733	D_3
114	5826.521572163	C_2	-1392.919494322	C_2	8659.701175163	C_2
115	5932.181285777	C_3	-1416.491607946	C_3	8812.348552364	C_2
116	6038.815593578	C_2	-1440.258465197	C_{2v}	8966.329411418	C_2
117	6146.342446579	C_2	-1464.232642918	C_2	9121.645065544	C_2
118	6254.877027790	C_2	-1488.392870531	C_2	9278.292910398	C_2
119	6364.347317479	C_2	-1512.753571720	C_2	9436.274838453	C_2
120	6474.756324980	C_2	-1537.312676422	C_2	9595.590553763	C_2
121	6586.121949585	C_3	-1562.068597381	C_3	9756.239732194	C_3
122	6698.374499261	I_h	-1587.032194015	I_h	9918.223675550	I_h
123	6811.827228174	C_{2v}	-1612.152971295	C_{2v}	10081.537287715	C_{2v}
124	6926.169974193	C_{2v}	-1637.479110028	C_{2v}	10246.185131492	C_{2v}
125	7041.473264023	C_2	-1663.001445804	C_2	10412.166497524	C_2
126	7157.669224867	C_{4v}	-1688.730136051	C_{4v}	10579.482453484	C_{4v}
127	7274.819504675	C_{5v}	-1714.654740337	C_{5v}	10748.131844929	C_{5v}
128	7393.007443068	C_2	-1740.762592566	C_2	10918.113328937	C_2
129	7512.107319268	C_2	-1767.074137949	C_2	11089.429241270	C_2
130	7632.167378912	C_2	-1793.581783669	C_2	11262.078698041	C_2
131	7753.205166941	C_2	-1820.282173304	C_2	11436.061217693	C_2
132	7875.045342797	I	-1847.205544897	I	11611.380466342	I
133	7998.179212898	C_3	-1874.266565339	C_3	11788.026381995	C_3
134	8122.089721194	C_2	-1901.555126737	C_2	11966.009479378	C_2
135	8246.909486992	D_3	-1929.047938796	D_3	12145.327013586	D_3
136	8372.743302539	T	-1956.727046585	T	12325.976926500	T
137	8499.534494781	C_{5v}	-1984.602697192	C_{5v}	12507.960464867	C_{5v}
138	8627.406389880	C_2	-2012.654078683	C_2	12691.275252719	C_2
139	8756.227056953	C_2	-2040.902595645	C_2	12875.923619485	C_2
140	8885.980609041	C_1	-2069.352260415	C_1	13061.906293508	C_2
141	9016.615349190	C_{2v}	-2098.009276077	C_{2v}	13249.223341972	C_{2v}
142	9148.271579993	C_2	-2126.853298666	C_2	13437.873191965	C_2
143	9280.839851192	C_2	-2155.899524571	C_2	13627.857056746	C_2
144	9414.371794460	C_{2v}	-2185.142440882	C_{2v}	13819.174689974	C_{2v}
145	9548.928837232	C_2	-2214.568874024	C_2	14011.824280757	C_2
146	9684.381825575	C_{2v}	-2244.202659774	C_{2v}	14205.808742993	C_{2v}
147	9820.932378373	C_2	-2274.010595028	C_2	14401.124458642	C_2
148	9958.406004270	C_2	-2304.019778666	C_2	14597.774256334	C_2
149	10096.859907397	C_1	-2334.221781315	C_1	14795.757120103	C_1
150	10236.196436701	O	-2364.632242592	O	14995.074954692	O

151	10376.571469275	C_2	-2395.223454116	C_2	15195.724313035	C_2
152	10517.867592878	C_{2v}	-2426.017592613	C_{2v}	15397.708074533	C_2
153	10660.082748237	D_3	-2457.015181903	D_3	15601.026233832	D_3
154	10803.372421141	C_2	-2488.190876449	C_2	15805.676112445	C_2
155	10947.574692279	C_2	-2519.568633738	C_2	16011.660007325	C_2
156	11092.798311456	C_2	-2551.133177676	C_2	16218.976471980	C_2
157	11238.903041157	C_2	-2582.905106818	C_2	16427.627598938	C_2
158	11385.990186197	C_2	-2614.869900531	C_2	16637.611973455	C_2
159	11534.023960956	C_2	-2647.032315746	C_2	16848.929978448	C_2
160	11683.054805550	C_{2v}	-2679.385135324	C_{2v}	17061.580963354	C_{2v}
161	11833.084739465	C_2	-2711.928008296	C_2	17275.564907705	C_2
162	11984.050335813	D_3	-2744.670230669	D_3	17490.882667332	D_3
163	12136.013053220	C_2	-2777.602750486	C_2	17707.533374511	C_2
164	12288.930105320	C_{2v}	-2810.731799771	C_{2v}	17925.517640426	C_{2v}
165	12442.804451373	C_2	-2844.056720503	C_2	18144.835341402	C_2
166	12597.649071324	D_{2d}	-2877.576867676	D_{2d}	18365.486574436	D_{2d}
167	12753.469429750	C_2	-2911.288645747	C_2	18587.470832804	C_2
168	12910.212672268	D_3	-2945.203677659	D_3	18810.789295472	D_3
169	13068.006451127	C_2	-2979.300376733	C_2	19035.439875459	C_2
170	13226.682823953	C_2	-3013.605076433	C_{2v}	19261.425233809	C_{2v}
171	13386.355930717	D_3	-3048.099114048	D_3	19488.743344225	D_3
172	13547.018108787	C_{2v}	-3082.784657234	C_{2v}	19717.394556501	C_{2v}
173	13708.635243035	C_2	-3117.667409139	C_2	19947.379404870	C_2
174	13871.187092293	O	-3152.750082143	O	20178.698345747	O
175	14034.781306929	C_2	-3188.015721848	C_2	20411.349195589	C_2
176	14199.354775632	C_1	-3223.475044956	C_1	20645.333519975	C_1
177	14364.837545298	C_{5v}	-3259.137161265	C_{5v}	20880.651951627	C_{5v}
178	14531.309552588	C_{2v}	-3294.990498454	C_{2v}	21117.303439355	C_{2v}
179	14698.754594220	C_1	-3331.038315813	C_1	21355.288321825	C_1
180	14867.099927526	C_{2v}	-3367.291624923	D_3	21594.607773936	D_3
181	15036.467239769	C_2	-3403.729564056	C_2	21835.259391988	C_2
182	15206.730610906	C_{5v}	-3440.373706455	C_{5v}	22077.245597998	C_{5v}
183	15378.166571028	C_1	-3477.183558898	C_1	22320.562506933	C_1
184	15550.421450311	T	-3514.208923509	T	22565.214740435	T
185	15723.723463950	C_1	-3551.418165874	C_1	22811.199322475	C_1
186	15897.897437048	C_1	-3588.835434011	C_1	23058.518537118	C_1
187	16072.975186320	C_{5v}	-3626.456172212	C_{5v}	23307.171959094	C_{5v}
188	16249.250131462	C_2	-3664.239977217	C_2	23557.155883564	C_2
189	16426.371938864	C_2	-3702.235296431	C_2	23808.474738381	C_2
190	16604.428338500	C_3	-3740.429815446	C_3	24061.127363604	C_3
191	16783.452219362	C_1	-3778.818018467	C_1	24315.113162430	C_1
192	16963.338386460	I	-3817.417956180	I	24570.434193082	I
193	17144.564740880	C_2	-3856.160361559	C_2	24827.083723606	C_2
194	17326.616136471	C_1	-3895.116946540	C_1	25085.068457771	C_1
195	17509.489303931	D_3	-3934.288802721	D_3	25344.388445898	D_3

196	17693.476356930	C_2	-3973.636580943	C_2	25605.040025602	C_2
197	17878.340162571	C_{5v}	-4013.187189799	C_{5v}	25867.025762759	C_{5v}
198	18064.262177195	C_2	-4052.924591023	C_2	26130.344362812	C_2
199	18251.082495640	C_1	-4092.864570639	C_1	26394.996914806	C_1
200	18438.842717531	C_{2v}	-4133.003079528	C_{2v}	26660.983213139	C_{2v}
212	20768.053085964	I	-4629.781535732	I	29956.817677683	I
272	34515.193292687	I_h	-7533.180190868	I_h	49316.045521553	I_h
282	37147.294418462	I	-8085.027739960	I	53009.259186708	I

Table 1. Extremal energies and point groups

Remark: Note that Table 1 contains the three additional entries $N = 212, 272$ and 282 for each $\alpha = 0, \pm 1$. These values of N are part of the "icosahedral group sequence", *i.e.* , integers N of the form $N = 20i + 30j + 60k$, with $i = 0$ or 1, $j = 0$ or 1, $k \geq 0$. For this sequence, Table 1 includes the values $N = 12, 32, 72, 122, 132, 192, 212, 272, 282$. Notice that these values of N yield substantially lower values for $\mathcal{E}(\alpha, N) - f(\alpha, N)$; see Figures 1–3. Also we found that for these special values of N, the global extremum of energy was significantly less than all other local extrema. The icosahedral group sequence was also numerically investigated on [11].

4. Asymptotic behavior of the extremal energies

Now let's consider the asymptotic behavior (as $N \to \infty$) of the extremal energies. From the theoretical estimates described by the authors in [15], we know that there exist constants $C_{1,\alpha}, C_{2,\alpha}$ such that for all $N \geq 2$

$$C_{1,0}N \leq \mathcal{E}(0,N) + \frac{1}{4}\log\left(\frac{4}{e}\right)N^2 + \frac{1}{4}N\log N \leq C_{2,0}N \quad \text{if } \alpha = 0 \tag{4.1}$$

$$C_{1,\alpha}N^{1-\alpha/2} \leq \mathcal{E}(\alpha,N) - \frac{2^\alpha}{2+\alpha}N^2 \leq C_{2,\alpha}N^{1-\alpha/2} \quad \text{if } \alpha \neq 0. \tag{4.2}$$

These estimates lend support to the following conjecture stated in [15]:

Conjecture 1 *For $-2 < \alpha < 2$, there exist absolute constants B_α, C_α, depending only on α, such that*

$$\mathcal{E}(\alpha,N) = \begin{cases} -\frac{1}{4}\log\left(\frac{4}{e}\right)N^2 - \frac{1}{4}N\log N + B_\alpha N + C_\alpha \log N + O(1) & \text{if } \alpha = 0, \\ \frac{2^\alpha}{2+\alpha}N^2 + B_\alpha N^{1-\alpha/2} + C_\alpha N^{-\alpha/2} + O\left(N^{-1-\alpha/2}\right) & \text{if } \alpha \neq 0. \end{cases} \tag{4.3}$$

Using the conjectured formulas (4.3) (with the O-term deleted)[1] we obtained a best fit to the data of Table 1 with the discrepancy being measured in the

[1]For the case $\alpha = 0$, we ignored the $\log N$ term in obtaining a best fit.

ℓ_1 sense. We used the ℓ_1 norm so as to minimize the effect caused by some extraordinary N values ($N \leq 12$ and $N = 32, 72, 122, 132, 192$, etc. are such examples). We obtained the following asymptotic approximations $f(\alpha, N)$ to the actual values of $\mathcal{E}(\alpha, N)$:

$$f(-1, N) = \frac{N^2}{2} - 0.55230N^{3/2} + 0.0689N^{1/2}, \tag{4.4}$$

$$f(0, N) = -\frac{1}{4}\log\left(\frac{4}{e}\right)N^2 - \frac{1}{4}N\log N - 0.026422N + 0.13822, \tag{4.5}$$

$$f(1, N) = \frac{2}{3}N^2 - 0.40096N^{1/2} - 0.188N^{-1/2}. \tag{4.6}$$

To see how good our approximation formulas (4.4), (4.5), (4.6) are, we plot the difference $\mathcal{E}(\alpha, N) - f(\alpha, N)$ for $\alpha = 0, \pm 1$ and $4 \leq N \leq 200$ in Figures 1, 2, and 3. We used the gnuplot program with the impulse plot-style, which simply draws vertical lines from the N-axis to the points being plotted. It is important to note that, as follows from the inequalities (4.1), (4.2), the growth of $\mathcal{E}(\alpha, N)$ is of order N^2, and that Figures 1–3 suggest that the differences $\mathcal{E}(\alpha, N) - f(\alpha, N)$ are bounded by a very small constant times $N^{-\alpha/2}$.

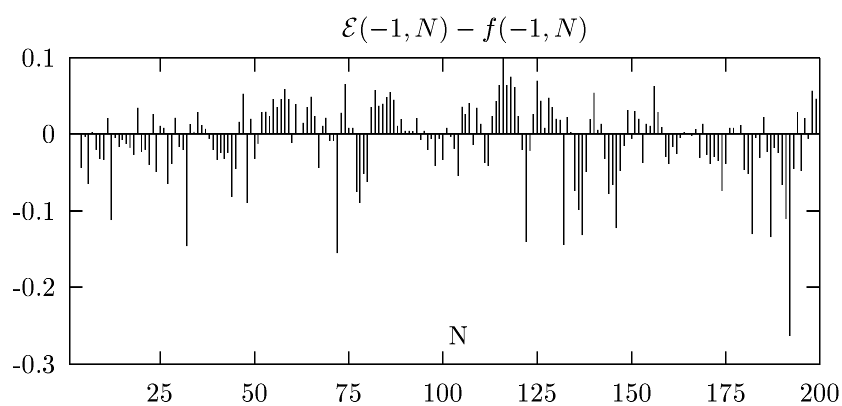

Figure 1. Error in Approximating Extremal Newton Energy

As we mentioned earlier, when N is large, the number of equilibrium meta-stable states increases dramatically. Furthermore, all these meta-stable states have very close energies. To give a rough idea, we plot in Figure 4 the energy value difference $E(0, \omega_N) - \mathcal{E}(0, N)$ for all the equilibrium states that we found for $\alpha = 0, 4 \leq N \leq 122$, where $E(0, \omega_N)$ is the energy for a particular local extremal point set ω_N. The horizontal axis represents values of N. Each point

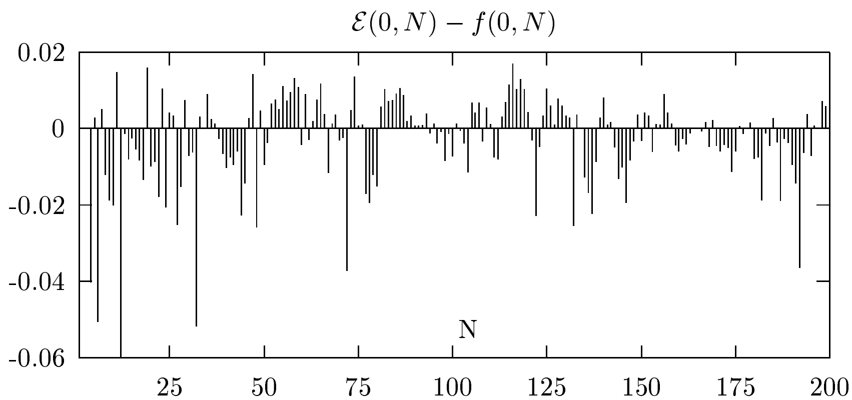

Figure 2. Error in Approximating Extremal Logarithmic Energy

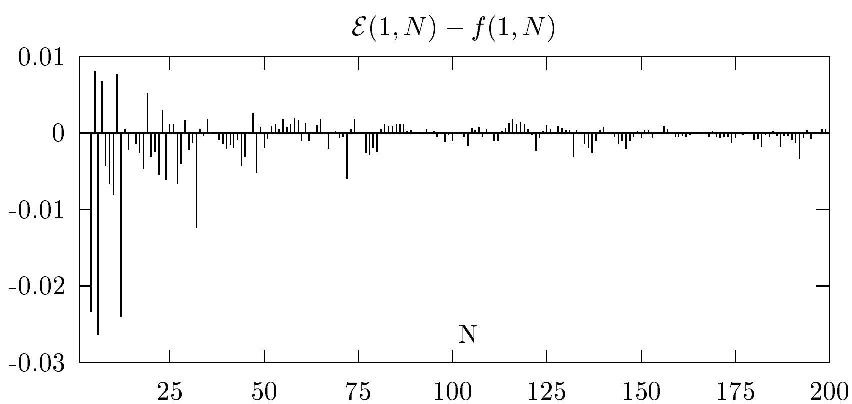

Figure 3. Error in Approximating Extremal Sums

represents a local extremum. As one can see from the scale, even as N gets larger, all the local extremal points have very close energies. Therefore, it is increasingly difficult to find a global extremum as N becomes large.

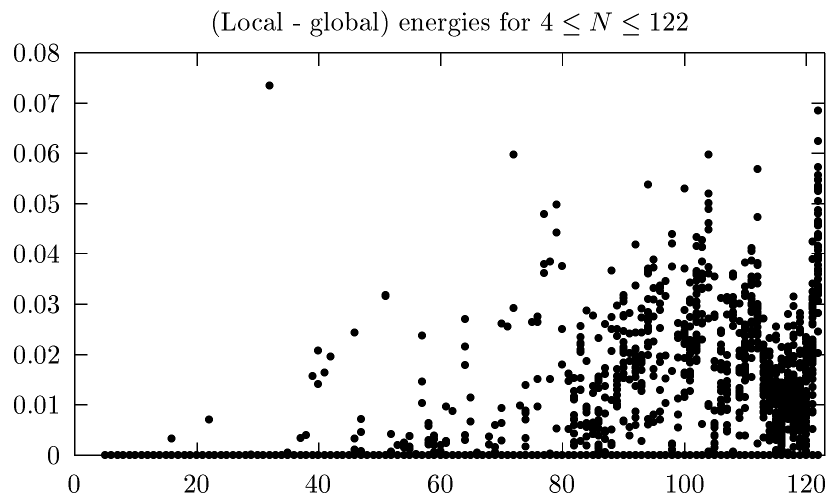

Figure 4. Distributions for the local extremal energies

5. The geometry of extremal points and the carbon fullerenes

As one can see from the table in Section 3, most of the extremal point sets have symmetry properties. We now look at these points from another perspective. Let $\omega_N = \{x_1, x_2, \ldots, x_N\}$ be a set of N points on S^2. Define

$$D_i := \{x \in S^2 : |x - x_i| \leq |x - x_j|, \ \forall j\}.$$

Then D_i is called the *Dirichlet cell* of x_i. In other words, D_i is the region on the sphere consisting of points that are closer to x_i than to any other points of ω_N. It is easy to prove that each D_i is a spherical polygon, *i.e.* , the boundary of D_i consists of finitely many pieces of great circle arcs. We say D_i is a *spherical r-gon* if the boundary of D_i consists of r great circle arcs.

Conjecture 2 *If $N \geq 6$, then the Dirichlet cells of $\omega_N^{(\alpha)}$ consist only of spherical 4-gons, 5-gons and 6-gons, i.e. , quadrilaterals, pentagons and hexagons.*

If the Dirichlet cells for $\omega_N^{(\alpha)}$ consist only of pentagons and hexagons it is an easy consequence of Euler's identity that there are exactly 12 pentagons, provided that exactly 3 edges emanate from each vertex. The total number of vertices is $2(N-2)$.

Our computations suggest that the 12 points whose Dirichlet cells are pentagons tend to distribute themselves as far apart from each other as possible. While they usually do not form the vertices of an icosahedron, the arrangement is quite close to that. Figure 5 depict 37 and 122 electrons in equilibrium on the surface of the sphere and their Dirichlet cells for the case $\alpha = -1$. The pentagons in the case $N = 37$ yield nearly an icosahedral arrangement, while the pentagons in the case $N = 122$ are numerically indistinguishable from an exact icosahedral arrangement.

As one can see, the cell structure of 37-electrons resembles the C_{70} fullerene. In fact, they are very close. Zhang, et al. [22] combined this idea with some Chemist's Principles, to determine the structures for C_{20} up to C_{70}.

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