



Equilibrium Configurations of N Equal Charges on a Sphere

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Abstract

The emergence of new levels of complexity that often accompanies the transition from few- to many-body systems is clearly illustrated by the progression of equilibrium states of N charges on the surface of a sphere as N increases. The characteristics of these electrostatic equilibrium states in the range $2 \leq N \leq 65$ can be examined in detail by equilibrating 1000 randomized initial configurations for every value of N . As N increases, the equilibrium states undergo a succession of structural changes. For instance, a state with non-zero dipole moment appears at $N = 11$, an enantiomeric or mirror image state appears at $N = 15$, and a robust metastable state appears at $N = 16$. For values of N exceeding 50, clusters of four or more metastable states with energies within 0.01% of each other are the dominant pattern. In analogy with some other complex systems, these energetically similar states have strikingly different asymmetric configurations.



J. J. Thomson's plum pudding model of the atom is nearing its centenary, yet there still is lively interest in the equilibrium configuration of charges confined to spheres and disks. This is partly due to the recent discovery of the carbon fullerenes (C_{60} , C_{70} , etc.[1]), and also is related to the 'magic' stability numbers exhibited by atomic microclusters[2]. But the most persistent interest is concerned with the generation of ring structures and other complex asymmetric charge patterns by the spherically symmetric Coulomb field. Calkin *et al.*[3] cite 19 articles on this topic just in the period '85-'86, and this list is not complete[4]. Thomson[5] and Föppl[6] were the first to show that negative point charges embedded in a sphere of uniform positive charge density—the forerunner of the 'jellium' model of solid-state physics—would tend to arrange themselves in sequences of rings. However, the uniqueness and completeness of these results is still uncertain. Rigorous results are available only for the simpler *surface Coulomb* problem of finding the static equilibrium configurations of N equal point charges constrained to move on the surface of a sphere while repelled by their mutual Coulomb interactions. In this case topological methods yield lower bounds for the number of (not necessarily stable) equilibrium states[7]. In addition, Leech[8] has shown that for the special values $N_L = 2 - 6, 12$, the equilibrium configurations remain invariant if the Coulomb law r^{-2} is replaced by the limiting form r^{-n} , $n \rightarrow \infty$. This 'ultra-repulsive' interaction is the basis of the *Tammes* problem of finding the arrangement of N points on the surface of a sphere with the largest possible minimum distance between any pair[9, 10, 11]. Since exact solutions for the Tammes problem are known for the set $N_T^{ex} = 2 - 12, 24$; Leech's theorem also yields optimum configurations for the surface Coulomb problem for the values $N_{SC}^{ex} = 2 - 6, 12 = N_L$. This equivalence of the Tammes and surface Coulomb problems for small values of N shows that in systems with few degrees of freedom symmetry principles alone may be sufficient to determine the equilibrium states. The emergence of new levels of complexity in larger systems then is illustrated by the divergence between the solution sets of these two problems as N increases.

Fast computers now make it feasible to investigate the equilibrium states of the surface Coulomb problem for particle numbers extending up to $N = 65$. Comparisons with prior studies[4, 12] show that the energies of the states must be known with a precision of at least ten significant figures to discriminate nearly degenerate states and compute meaningful dipole moments. Furthermore, since current numerical algorithms can only locate local minima, computer searches must involve high statistics to identify the metastable states. These criteria are satisfied by the following procedures: The set of N unit vectors $\{\vec{r}_i, 1 \leq i \leq N\}$ completely specifies the position of N points on the surface of a unit sphere. The (dimensionless) Coulomb energy is:

$$E(N) = \sum_{i=1}^N \sum_{j>i}^N \frac{1}{|\vec{r}_i - \vec{r}_j|}; \quad (01)$$

and therefore the Coulomb force acting on the i^{th} point is

$$\vec{F}_i = \sum_{j=1}^N \frac{\vec{r}_i - \vec{r}_j}{|\vec{r}_i - \vec{r}_j|^3}, \quad (i \neq j). \quad (02)$$

It is also interesting to compute the energy associated with a single particle:

$$E_i = \sum_{j=1, j \neq i}^N \frac{1}{|\vec{r}_i - \vec{r}_j|}; \quad E(N) = \frac{1}{2} \sum_{i=1}^N E_i. \quad (03)$$

Starting from an initial distribution of points randomly distributed on the sphere, an equilibrium state may be found by allowing the points to move in the direction of the forces acting on them subject to the constraint of remaining on the surface of the sphere. The steepest descent method of iterating: $\vec{r}_i \rightarrow \vec{r}_i' = (\vec{r}_i + \gamma \vec{F}_i) / |\vec{r}_i + \gamma \vec{F}_i|$, with γ chosen to maximize convergence, was used on this problem by Claxton[13]. It turns out that if $\gamma \rightarrow \infty$ the update formula becomes simply $\vec{r}_i \rightarrow \vec{r}_i' = \vec{F}_i / |\vec{F}_i|$, which is an over-relaxed update step with good convergence. If this step is so large that $\{\vec{r}_i'\}$ has a higher energy than $\{\vec{r}_i\}$ then the γ is automatically adjusted downward for that step until the energy does decrease. The iteration is terminated when the energies stabilize within the machine precision of one part in 2^{-48} . It should be noted

that this calculation involves the cancellation of large forces so it is important to use at least 48-bit precision. Conjugate-gradient methods do not improve this technique because the energy surface is far from quadratic.

A survey of the equilibrium configurations of the surface Coulomb problem is given in Table 1. The first column lists the number of charges N . The next column shows the average number of iterations required to reach an equilibrium state. The frequency of occurrence, or 'capture basin,' of each state is indicated in the third column. The asterisks mark enantiomeric states. The percentages in column 3 are based on a statistical sample of a thousand random starts for every value of N and therefore are presumably accurate to within 3%. Column 4 lists the dimensionless energy $E(N)$ of each state. The 'center of charge,' or dipole moment $d(N) = |\sum_{i=1}^N \vec{r}_i|$ of every configuration is given in column 5. Column 6 shows the minimum angular separation between pairs of points of the surface Coulomb states. A corresponding set of values for the Tammes problem, compiled by Professor T. Tarnai, is listed in column 7.

It is apparent that the configurations become more complex as N increases. Specifically for $N = 7$ the surface Coulomb distribution is given by the vertices of a pentagonal dipyramid, while the Tammes solution corresponds to two triangles asymmetrically positioned about the equator with the remaining point at a pole. Since the Tammes configuration also has a dipole moment ≈ 0.433762 , this split of the solutions is due to dynamic symmetry breaking[13, 14]. The first non-vanishing dipole moment for a surface Coulomb state appears at $N = 11$. The symmetries of this configuration[15], and more complicated examples, can be inferred from the set of partial energies (E_i in eq.(3)), the angular separations $\cos^{-1}(\vec{r}_i \cdot \vec{r}_j)$, and computer graphics. Enantiomeric states appear at $N = 15$ both in the Coulomb and Tammes problems[10]. The first robust metastable Coulomb state occurs at $N = 16$. Since it is possible for the algorithm to converge to saddle points from certain rare initial

configurations, results are only reported for states found for more than one random start. Clusters of metastable states become more common as the number of charges increases beyond 50. In particular, the patterns for $N = 56$ and $N = 60$ show that in complex systems the ground state may have low statistical weight[16]. It is also interesting that the 'bucky ball' (truncated icosahedron) configuration associated with C_{60} is *not* a solution of either the Tammes or surface Coulomb problems for $N = 60$, but rather is similar to the *dual* of the most common state for the Coulomb problem at $N = 32$.

Finally we note that the simple empirical formula $E(N) \approx (N^2/2) - 0.5510N^{3/2}$ provides a good fit for the energies listed in the Table. This expression can be interpreted in two ways: (i) $N^2/2$ is the energy of a uniform charge density on a sphere. In order to recover the energy of a distribution of point charges it is necessary to subtract the self-energies of a set of N uniformly charged disks, which can be shown to be proportional to $N^{3/2}$. (ii) Alternatively, $N^2/2$ can be identified with the average energy of a set of N charges randomly distributed over the surface of a sphere. In this case the $N^{3/2}$ term represents the correlation energies of the surface Coulomb equilibrium states.

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Table 1: Equilibrium configurations for the surface Coulomb problem						
N	Average iterations	Frequency (percent)	Coulomb energy	Dipole moment	Coulomb angle (rad.)	Tammes angle (rad.)
2	1	100	0.50000000	0	3.141592	3.141592
3	14	100	1.73205081	0	2.094395	2.094395
4	16	100	3.67423461	0	1.910633	1.910633
5	78	100	6.47469149	0	1.570796	1.570796
6	42	100	9.98528137	0	1.570796	1.570796
7	2161	100	14.45297741	0	1.256637	1.359080
8	183	100	19.67528786	0	1.251299	1.306527
9	280	100	25.75998653	0	1.207589	1.230959
10	440	100	32.71694946	0	1.134387	1.154480
11	501	100	40.59645051	0.013220	1.021708	1.107149
12	77	100	49.16525306	0	1.107149	1.107149
13	1288	100	58.85323061	0.008820	0.913103	0.997223
14	256	100	69.30636330	0	0.922687	0.971567
15	437	100*	80.67024411	0	0.859136	0.936506
16	293	72.7*	92.91165530	0	0.854098	0.911836
	394	27.3	92.92035396	0	0.874880	
17	679	100	106.05040483	0	0.874550	0.891694
18	501	100	120.08446745	0	0.829632	0.864927
19	9123	100	135.08946756	0.000135	0.783822	0.832381
20	662	100	150.88156833	0	0.804480	0.827827
21	3957	100	167.64162240	0.001406	0.773536	0.796089
22	547	96.9	185.28753615	0	0.755763	0.780863
	1377	3.1	185.30795160	0	0.746305	
23	440	100*	203.93019066	0	0.723982	0.762883

N	Average iterations	Frequency (percent)	Coulomb energy	Dipole moment	Coulomb angle (rad.)	Tammes angle (rad.)
24	445	100*	223.34707405	0	0.734178	0.762548
25	7515	100	243.81276030	0.001021	0.691333	0.726658
26	2283	100*	265.13332632	0.001919	0.677923	0.716191
27	673	100	287.30261503	0	0.697089	0.709958
28	529	100*	310.49154236	0	0.660149	0.685449
29	3144	100*	334.63443992	0	0.635147	0.675571
30	2442	100*	359.60394590	0	0.644763	0.673647
31	387	100	385.53083806	0.003205	0.634831	0.658160
32	239	97.5	412.26127465	0	0.652358	0.654066
	676	2.5	412.46839720	0	0.621525	
33	7829	100	440.20405745	0.004356	0.588174	0.633280
34	1582	100*	468.90485328	0	0.580730	0.624829
35	3796	80.6*	498.56987249	0.000419	0.577711	0.616418
	5335	19.3	498.57345404	0.001266	0.581227	
36	19189	100*	529.12240842	0.000049	0.579500	0.614174
37	1855	18.7	560.61888773	0	0.564307	0.598581
	3553	81.3*	560.62797306	0.000925	0.558252	
38	636	44.2	593.03850357	0.000001	0.580086	0.597786
	1114	55.8	593.04894354	0.001687	0.563323	
39	472	66.7	626.38900902	0	0.559429	0.583334
	5202	28.8*	626.44095841	0.000399	0.547982	
	4040	4.5	626.44096635	0.000371	0.547924	
40	751	66.9	660.67527883	0	0.557045	0.578722
	7632	22.9*	660.72530410	0.000004	0.551384	
	745	10.2	660.74121431	0.001465	0.545251	

N	Average iterations	Frequency (percent)	Coulomb energy	Dipole moment	Coulomb angle (rad.)	Tammes angle (rad.)
41	475	94.2	695.91674434	0	0.550264	0.571223
	1467	5.8*	695.97869944	0	0.545295	
42	481	97.3	732.07810754	0	0.545324	0.567343
	1748	1.5*	732.15182672	0	0.540498	
	4775	1.1*	732.19816736	0.003638	0.529379	
43	7192	100	769.19084646	0.000400	0.538723	0.557814
44	3598	100	807.17426309	0.000060	0.545548	0.557814
45	6731	100*	846.18840106	0	0.527214	0.544976
46	711	11.7*	886.16711364	0	0.519938	0.537244
	1367	45	886.17021602	0.001066	0.504669	
	1835	26.7*	886.17143242	0.001395	0.509081	
	1524	16*	886.17710517	0.001838	0.509578	
	12308	0.6	886.25028042	0	0.500098	
47	1473	54*	927.05927068	0.002483	0.502432	0.537244
	4236	32.5*	927.06226967	0.002536	0.487302	
	12172	9	927.07222457	0.004684	0.505445	
	2255	4.2*	927.08823351	0.000803	0.505048	
	2147	0.2*	927.14108835	0.001525	0.491380	
48	1158	100*	968.71345534	0	0.518182	0.536912
49	1118	100*	1011.55718265	0.001529	0.495439	0.519287
50	832	100	1055.18231473	0	0.501108	0.519287
51	1489	98.5*	1099.81929032	0	0.491578	0.511448
	1502	1.5	1099.94023114	0.002506	0.474308	

N	Average iterations	Frequency (percent)	Coulomb energy	Dipole moment	Coulomb angle (rad.)	Tammes angle (rad.)
52	954	56.8*	1145.41896432	0.000457	0.482930	0.509055
	1118	27.1*	1145.42198063	0	0.485412	
	1342	9.9*	1145.43570898	0.000720	0.484667	
	4490	6.2*	1145.43759698	0.002189	0.480119	
53	7813	68.2	1191.92229042	0.000279	0.473629	0.499761
	1052	31.8*	1191.93158471	0.000293	0.471423	
54	1825	80.4*	1239.36147473	0.000138	0.471755	0.496935
	2125	3.9*	1239.36525530	0	0.475519	
	3861	8*	1239.37119227	0.000371	0.474284	
	1371	7.6*	1239.37320071	0	0.478224	
55	1052	31.1*	1287.77272078	0.000392	0.464521	0.493271
	1598	19.4*	1287.77702746	0.000114	0.461470	
	2337	15.8	1287.77726081	0.000118	0.470319	
	2937	12.4*	1287.78870934	0.000025	0.466465	
	1488	20.1*	1287.78905724	0.000191	0.464988	
	2844	1.2*	1287.80015929	0.000552	0.467767	
56	1896	10.3*	1337.09494528	0	0.465704	0.485048
	1951	48.7*	1337.09534827	0.000174	0.464409	
	2789	40.9*	1337.09872742	0.000275	0.465149	
57	2499	89.9*	1387.38322925	0	0.466045	0.480759
	2547	2.6	1387.42008235	0.000753	0.453765	
	3735	2.7*	1387.43037248	0.000285	0.453468	
	1882	4.4*	1387.43113006	0.000273	0.452877	
	1286	0.4*	1387.47189278	0.000870	0.452564	

N	Average iterations	Frequency (percent)	Coulomb energy	Dipole moment	Coulomb angle (rad.)	Tammes angle (rad.)
58	1372	25.5*	1438.61825064	0	0.456495	0.480759
	2611	18.9*	1438.62550858	0.000058	0.455361	
	2337	5.7*	1438.62628995	0	0.454155	
	2920	26.4*	1438.62722515	0.000308	0.456654	
	6352	5.1*	1438.63370800	0.000002	0.454608	
	1597	18.2*	1438.63810500	0.000198	0.452373	
	2470	0.2*	1438.64735982	0.001029	0.453854	
59	1992	27.7*	1490.77333528	0.000154	0.456757	0.474241
	2609	61.4*	1490.77438608	0.000623	0.456849	
	6143	3.3*	1490.78475584	0.000245	0.457361	
	1645	7.6*	1490.79077309	0.000608	0.453876	
60	937	24.8*	1543.83040098	0	0.453046	0.474241
	977	70.4*	1543.83509960	0.000130	0.452967	
	2026	3.6*	1543.84153514	0.000177	0.452851	
	1258	0.6	1543.86465762	0.000018	0.447471	
	6581	0.5*	1543.96947231	0	0.451689	
61	1953	63.6*	1597.94183020	0.001092	0.443168	0.464456
	1132	10.4*	1597.95155534	0.000648	0.442475	
	8210	13.6*	1597.95512785	0.001364	0.444070	
	2825	9.7*	1597.97036059	0.000634	0.445656	
	3051	2.7*	1597.98080362	0.001003	0.437863	

N	Average iterations	Frequency (percent)	Coulomb energy	Dipole moment	Coulomb angle (rad.)	Tammes angle (rad.)
62	1223	27.4*	1652.90940990	0	0.451689	0.461411
	3138	62*	1652.92859368	0.001117	0.444936	
	1538	10.6*	1652.94201427	0.000513	0.446840	
63	2135	99.8*	1708.87968150	0	0.440812	0.457888
	964	0.2	1709.00838502	0	0.434249	
64	2444	84*	1765.80257793	0	0.434936	0.457888
	2323	3.8	1765.81619775	0	0.435611	
	3001	8.9*	1765.82032129	0.000254	0.430896	
	1107	1.2	1765.87533511	0	0.434467	
	2021	0.8*	1765.89790410	0.000152	0.427295	
	1644	1.3*	1765.91167428	0	0.439880	
65	4579	93.8*	1823.66796027	0.000400	0.428072	0.454333
	6515	1.6*	1823.69459614	0	0.434582	
	2269	4.6*	1823.71802820	0.001283	0.423836	

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