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LETTER TO THE EDITOR

# 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 configurations 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 1985–1986 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 $r^{-n}$, $n \to \infty$. 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

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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 $\{\boldsymbol{r}_i,\ 1 \leqslant i \leqslant N\}$ completely specifies the position of $N$ points on the surface of a unit sphere. The (dimensionless) Coulomb energy is:

$$E(N) = \sum_{i=1}^{N} \sum_{j>i}^{N} \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} \tag{1}$$

and therefore the Coulomb force acting on the $i$th point is

$$\boldsymbol{F}_i = \sum_{j=1}^{N} \frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^3} \qquad (i \neq j). \tag{2}$$

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

$$E_i = \sum_{j=1, j\neq i}^{N} \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} \qquad E(N) = \frac{1}{2} \sum_{i=1}^{N} E_i. \tag{3}$$

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: $\boldsymbol{r}_i \to \boldsymbol{r}_i' = (\boldsymbol{r}_i + \gamma \boldsymbol{F}_i)/|\boldsymbol{r}_i + \gamma \boldsymbol{F}_i|$, with $\gamma$ chosen to maximize convergence, was used on this problem by Claxton [13]. It turns out that if $\gamma \to \infty$ the update formula becomes simply $\boldsymbol{r}_i \to \boldsymbol{r}_i' = \boldsymbol{F}_i/|\boldsymbol{F}_i|$, which is an over-relaxed update step with good convergence. If this step is so large that $\{\boldsymbol{r}_i'\}$ has a higher energy than $\{\boldsymbol{r}_i\}$ then the $\gamma$ 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 'centre of charge', or dipole moment $d(N) = |\Sigma_{i=1}^{N} \boldsymbol{r}_i|$ 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.

**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 |
| 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 |

**Table 1.** (continued)

| N | Average iterations | Frequency (percent) | Coulomb energy | Dipole moment | Coulomb angle (rad.) | Tammes angle (rad.) |
|---|---|---|---|---|---|---|
| 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 | |
| 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 |

**Table 1.** (continued)

| N | Average iterations | Frequency (percent) | Coulomb energy | Dipole moment | Coulomb angle (rad.) | Tammes angle (rad.) |
|---|---|---|---|---|---|---|
| 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 | |
| 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 | |

**Table 1.** (continued)

| N | Average iterations | Frequency (percent) | Coulomb energy | Dipole moment | Coulomb angle (rad.) | Tammes angle (rad.) |
|---|---|---|---|---|---|---|
| 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 | |
| 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 | |

**Table 1.** (continued)

| N | Average iterations | Frequency (percent) | Coulomb energy | Dipole moment | Coulomb angle (rad.) | Tammes angle (rad.) |
|---|---|---|---|---|---|---|
| 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 | |
| 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 | |

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 $\approx 0.433\,762$, this split of the solutions is due to dynamic sysmmetry 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 (3)), the angular separations $\cos^{-1}(\boldsymbol{r}_i \cdot \boldsymbol{r}_j)$, 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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