Possible Global Minimum Lattice Configurations for Thomson's Problem of Charges on a Sphere

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What configuration of N point charges on a conducting sphere minimizes the Coulombic energy? J. J. Thomson posed this question in 1904. For $N \leq 112$, numerical methods have found apparent global minimum-energy configurations; but the number of local minima appears to grow exponentially with N, making many such methods impractical. Here we describe a topological/numerical procedure that we believe gives the global energy minimum lattice configuration for N of the form $N = 10(m^2 + n^2 + mn) + 2$ (m, n positive integers). For those N with more than one lattice, we give a rule to choose the minimum one.   [S0031-9007(97)02835-4]

Given N unit point charges on the surface of a unit conducting sphere, what is the configuration of the charges for which the Coulombic energy $\sum_{i,j=1;j>i}^{N} 1/|\mathbf{r}_i - \mathbf{r}_j|$ is minimized? This question was originally asked by J. J. Thomson long ago [1] and has since been investigated by many authors [2–12]. Besides its interest as a physics and mathematical optimization problem, the question posed by Thomson is similar to problems in other fields such as the arrangement of the protein subunits of a protein coat of a spherical virus [13–15] and the arrangement of atoms in a spherical molecule [16]. Somewhat surprisingly, it turns out that the configuration of minimum energy for Thomson's problem is not the configuration which places the charges at the farthest distance from each other, or the configuration of greatest symmetry. For example, for eight charges, the configuration of minimum energy is not a cube, but a twisted noncubic rectangular parallelepiped [5]. For $2 \leq N \leq 100$ by means of extensive trials utilizing a number of methods, it appears that the minimum-energy configurations may have been found [1–12]. However, as the number of closely spaced local minima seems to grow tremendously with N [11],

for an arbitrarily large N it may be extremely difficult to find the global minimum configuration. Generalizing from topological properties of the apparent local minimum energy configurations for $N \leq 100$, we here describe a topological/numerical procedure to generate "lattice" configurations which we think are global minima for Thomson's problem for numbers of charges of the form $N = 10(m^2 + n^2 + mn) + 2$ with m and n integers > 0.

We can consider the charges on the sphere as vertices of a convex polytope. It had been noted that for $12 \leq N \leq 60$, $N = 72$, $N = 78$, $N = 100$ the minimum-energy configuration usually has 12 vertices with five nearest neighbors (pentamers) and $N - 12$ vertices with six nearest neighbors (hexamers) ([7,9], and references therein). We have confirmed this for the other $61 \leq N \leq 100$ (Table I, Refs. [7,9], and references therein). This observation can be appreciated from a topological point of view with reference to Euler's formula relating faces (F), vertices (V), and edges (E) of a convex polytope ($F + V = E + 2$). Indeed, if all the faces of our polytope are triangles and we consider the polytope to consist only of tetramers (vertices with four nearest neighbors) (V_4), pentamers (V_5),

TABLE I. Most apparent minimum-energy configurations for $12 \leq N \leq 100$ have 12 pentamers and $N - 12$ hexamers. Exceptions are given in the table. N is the number of charges. If the polytope contains Q quadrilateral faces, V_5 pentamers, V_4 tetramers, and V_7 heptamers, then it can be shown that $V_5 + 2V_4 - V_7 - 2Q = 12$ with all the rest of the vertices being hexamers (V_6). To decide if two vertices v and w are nearest neighbors we look at the triangles with vertices v, w, and x, where x ranges over all other vertices. If the angle at the vertex x is 90° or more (for any x) then v and w are not nearest neighbors. We join vertices determined to be nearest neighbors by an edge. The resulting polytopes have mainly triangular faces with an occasional quadrilateral face. (Especially for polytopes with quadrilateral faces, there can be some ambiguity in assignment of nearest neighbors. Another method for doing so with less ambiguity is given in Ref. [22].)

N	V_5	V_6	V_7	V_4	Q
13	10	2		1	
18	8	8		2	
21	10	10		1	
33	15	17	1		1
53	16	37			2
59	14	43	2		
70	20	50			4
71	16	55			2
73	16	57			2
79	15	63	1		1
83	14	67	2		

hexamers (V_6), and heptamers (V_7), then

$$V_5 + 2V_4 - V_7 = 12, \qquad (1)$$

with all the rest of the vertices being hexamers [17]. From Table I we see that in general the apparent minimum-energy configuration has exactly 12 pentamers and $N - 12$ hexamers. Many of the exceptions occur for numbers of charges such as 33, 70, 71, and 73 which are very close to $N = 32$ and $N = 72$, which have extremely stable supposed global minimum configurations (see below).

For

$$N = 10(m^2 + n^2 + mn) + 2, \qquad (2)$$

with m and n positive integers and $m \geq n$, a particularly symmetric icosahedral lattice configuration can be formed with exactly 12 pentamers (and no tetramers or heptamers) with the vertices of the pentamers at the vertices of an icosahedron (Fig. 1). The procedure for generating the lattices is given in Fig. 1. For $N = 32$ ($m = 1$, $n = 1$) and $N = 72$ ($m = 2$, $n = 1$) this procedure generates the previously known apparent minimum-energy configurations. The next lattice numbers are $N = 122$ ($m = 2$, $n = 2$) and $N = 132$ ($m = 3$, $n = 1$). It has been noted that for $70 \leq N \leq 112$ the number of local minima increases as $0.382 \exp(0.0497N)$ [11]. In accordance with this we used a conjugate gradient [18] starting from 200 and 300 random configurations for $N = 122$ and 132, respectively, and did not find an energy lower than the lattice energy for either value of N. We also ran from some configurations slightly perturbed from the lattice loading. Without an analytical proof we cannot be sure that the lattice

configurations are the ones of minimum energy for $N = 122$ and $N = 132$. We believe that the lattice configurations are the ones of minimum energy for $N = \{122, 132\}$, and in general we believe that the lattice configurations are the ones of minimum energy for N of the form of Eq. (2). (However, if the ratio of m to n is too large, then the lattice configuration may not be the one of minimum energy. See below.) For potential energies of the form $\{1/r^\alpha | \alpha = 2, 3\}$ (where r is the Euclidean distance between charges) we have found that lattice configurations also appear to be the minimum-energy configurations, with the exact location of the charges depending on the potential (E. L. A. et al., unpublished data). For $N \leq 312$, a number of groups using various methods have also found icosahedral lattices to be minimum-energy configurations [6,7,9,19–22].

The question arises as to the configuration of minimum energy for those N which can be obtained by substituting more than one pair of m and n into Eq. (2). For example, for $N = 912$, two icosahedral lattice configurations can be constructed: one with $m = 6$ and $n = 5$, and another with $m = 9$ and $n = 1$. Now, for $N = 42$ and $N = 92$ which would correspond to ($m = 2$, $n = 0$) and ($m = 3$, $n = 0$), respectively, in Eq. (2) it is known that the minimum-energy configuration is *not* the lattice configuration. We have shown that for $N = 162$ ($m = 4$, $n = 0$) the lattice configuration is also not the minimum-energy configuration (E. L. A. et al., unpublished data, [19–21]). In general we think that for $N = 10m^2 + 2$ [except for the very special case of $N = 12$ ($m = 1, n = 0$)] the lattice configuration is not the minimum-energy configuration. From the result that the cases of Eq. (2) with $n = 0$ appear not to be global minima, we hypothesized that for those N that can be obtained by substituting more than one pair of m and n into Eq. (2), the lattice configuration with a smaller ratio of m to n has lower energy than the configuration with a larger ratio, which might more closely resemble a configuration with $n = 0$ ($m/n = \infty$) (Table II, Fig. 2). For example, for $N = 912$ the lattice configuration with $m = 6$, $n = 5$ has a lower energy than the lattice configuration with $m = 9$, $n = 1$ (Fig. 2). As well, we have verified this hypothesis for the other four examples of such N which are less than 2500 (Table II). A smaller ratio of m to n may lower the energy by permitting more twisting of the high-energy pentamers with respect to each other than for a larger ratio of m to n. Given that N of the form of Eq. (2) with $n = 0$ the lattice configurations are not local minima, it may be that for a sufficiently large ratio of m to n the lattice configuration is not the global energy minimum configuration. (Icosahedral lattice configurations have been discussed in relation to the Tammes problem—maximization of the minimum distance between N points on the surface of a unit sphere [23]. However, it has been shown that in many cases including $N = 72$ an icosahedral lattice and other configurations of high symmetry are not necessarily the best ones for the Tammes problem [24,25].) We note the trend toward
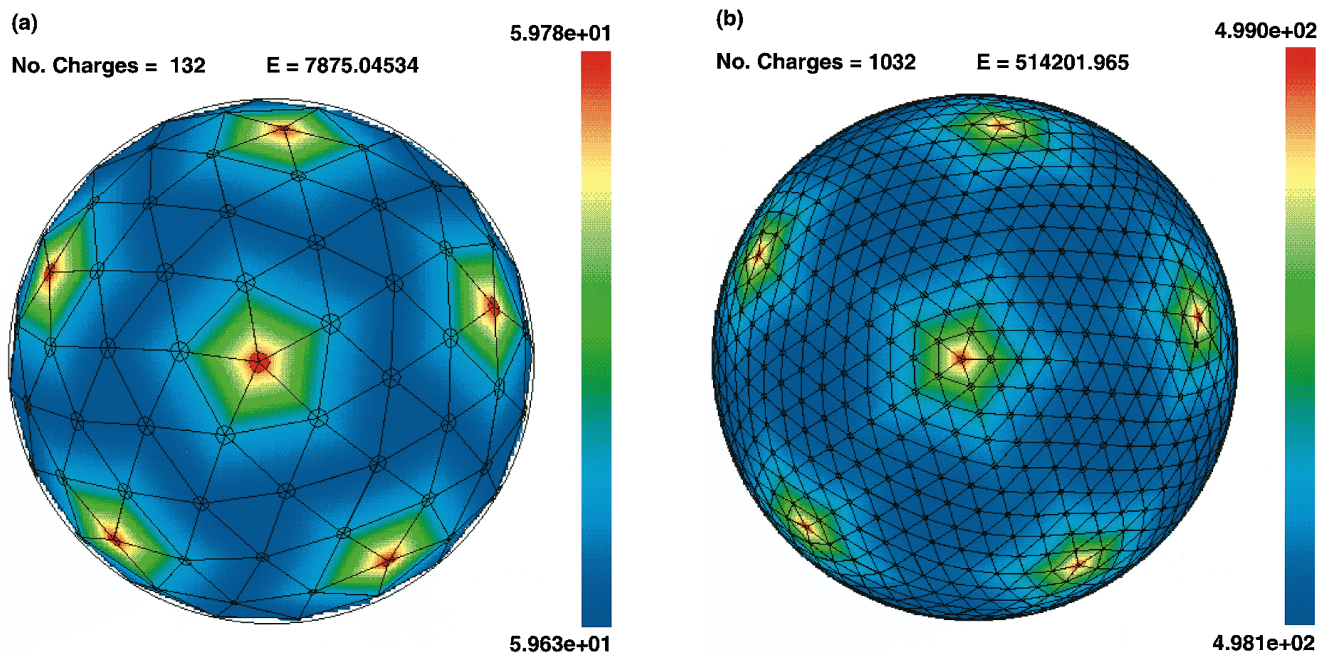
FIG. 1(color). Lattice configurations for 132 (a) and 1032 (b) charges. To go from one vertex of a pentamer to another vertex of a pentamer for 132 charges (a) one goes up three edges and over one edge, while for 1032 charges one goes up nine edges and over two edges. Vertices of hexamers are indicated by a small black circle, vertices of pentamers by a small red circle, and edges by black lines. The other points on the sphere are colored as follows: The potential energy $\sum_{j=1;j\neq i}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$ (self-energy term omitted) is computed at the locations $\mathbf{r}_i$ of each of the charges. The potential at other points is estimated using a linear finite element triangular function. The color scale is shown at the right with blue being the lower potential and red being the higher potential. To obtain lattice configurations we begin by placing points on the faces of an icosahedron. Essentially, we want to place $(N - 12)/20$ points on each of the 20 faces of the icosahedron, taking care not to double count points on the edge between two faces. The other 12 points are the vertices of the icosahedron. For example, if one joins any three of the vertices of the pentamers in (a) there are $(132 - 12)/20 = 6$ points contained within each resulting equilateral triangle. Specifically, we identify one face of an icosahedron with an equilateral triangle in the complex plane having vertices at $[0, (m + n\eta), (m\eta + n\eta^2)]$ with $\eta = \exp(\pi i/3)$. Points are placed on this first triangle by including all points from the lattice $k + l\eta$ (k, l integers) which are contained in or on the boundary of the triangle. Points on the other faces of the icosahedron can be obtained by 180° rotation about the midpoint of the edge common to two triangles. We project the points from the icosahedron radially out to a circumscribed unit sphere. We then use a conjugate gradient minimization [18] using $E = \sum_{i,j=1;j>i}^{N} 1/|\mathbf{r}_i - \mathbf{r}_j|$ to obtain the final location of the charges.

smaller energy spacing between the pairs of states in Table II is consistent with the bunching of local minima closer to the global minimum described in Ref. [22]. Our values of the energy for $N = 122, 132, \ldots, 912, \ldots$ agree well with empirical formulas [8,19] for the energy of the

TABLE II. For $N < 2500$ when two lattice configurations have the same number of charges, the configuration with a smaller ratio of m to n has a lower energy. The construction of the lattices, see Fig. 1.

N	m	n	Energy
912	6	5	400 660.1320
	9	1	400 662.3832
1332	9	4	860 260.5582
	11	1	860 264.5477
1472	7	7	1 052 197.474
	11	2	1 052 200.022
2172	9	8	2 302 877.842
	13	3	2 302 880.777
2472	11	7	2 987 501.183
	14	3	2 987 505.566

minimum-energy configuration for a given N. Though, not surprisingly, the energies of the lattice configurations are somewhat lower than predicted as the lattices are such good configurations.

[Using algebraic number theory [26] it can be shown that those N for which more than one icosahedral lattice can be constructed are of the form $N = 10k^2 3^j p_1^{m_1} p_2^{m_2} \ldots p_n^{m_n} + 2$ where k is an integer >0 with no prime factors $\equiv 1$ mod 6; j is an integer ≥ 0; $p_1, \ldots, p_n$ are distinct prime numbers $\equiv 1$ mod 6; $m_1, \ldots, m_n$ are integers ≥ 0; and at least one of n or m_1 is ≥ 2. The number of icosahedral lattices which can be constructed for such an N is equal to $0.5(m_1 + 1)(m_2 + 1) \cdots (m_n + 1)$, rounding up if this expression is not an integer. For example, for $N = 912$, $k = 1, j = 0, n = 2, p_1 = 7, m_1 = 1, p_2 = 13, m_2 = 1$, and the number of icosahedral lattices is two.]

As mentioned, many examples of apparent minimum-energy configurations which do not have exactly 12 pentamers—$N = \{33, 70, 71, 73\}$—have numbers of charges close to the apparent lattice global energy minimum configurations for $N = 32$ and $N = 72$. This may result because the lattice configurations are so symmetric that it
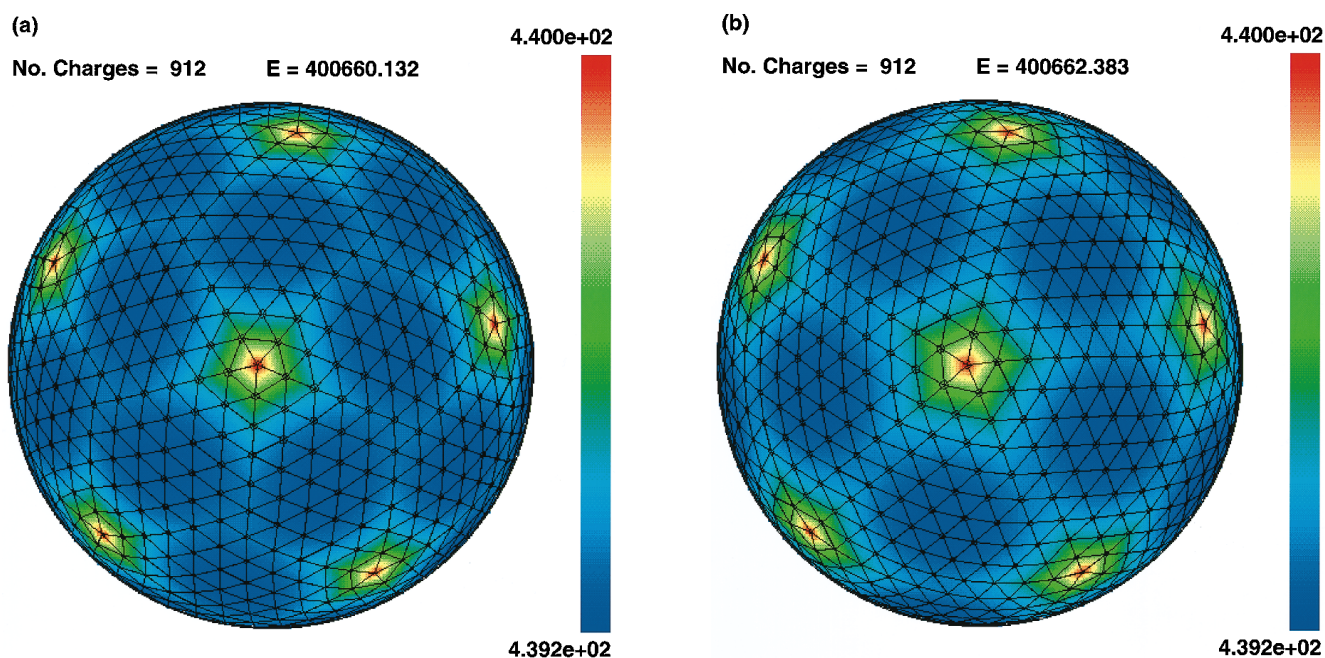
FIG. 2(color). Lattice configurations for $N = 912$: (a) $m = 6$, $n = 5$, (b) $m = 9$, $n = 1$. The configuration in (a) has a smaller ratio of m to n than the configuration in (b) and also a lower energy. For construction of the lattices, see Fig. 1.

would be difficult to add or subtract one or two charges and still have a good minimum with exactly 12 pentamers. (For $N = 13$ there exists no configuration of charges with 12 pentamers and 1 hexamer [27].)

There may be other families of solutions besides the icosahedral lattices. For example, the apparent minimum-energy configuration for $N = 78$ has a T_4 (tetrahedral) symmetry [9]. We have constructed an analog of this T_4 solution for $N = 78$ with $N = 306$ (E. L. A. *et al.*, unpublished data) which we suspect is the minimum energy configuration for $N = 306$; however, the number of random trials necessary to get confidence that this T_4 configuration for $N = 306$ is the global minimum seems prohibitive. Perhaps, similar to $N = \{33, 70, 71, 73\}$, the reason that the apparent global minimum configuration for $N = 79$ does not have exactly 12 pentamers may be because it is difficult to add one charge to the very symmetric T_4 configuration for $N = 78$ and still obtain a good minimum with exactly 12 pentamers. Recently, very good low-energy configurations have been found for $N = \{137, 146\}$ [19].

For $N = 10(m^2 + n^2 + mn) + 2$ with m, n positive integers we have given a method for generating configurations which we think are global minima for Thomson's problem, and tested these configurations extensively for $N = 122$ and 132. We have hypothesized that in cases in which more than one pair of m and n give a lattice configuration with the same N the configuration with the smaller ratio of m to n have a lower energy and verified this hypothesis for the five such $N < 2500$. Given that for $n = 0$ the icosahedral lattices are not the minimum-energy configurations, there is an interesting open question as to whether the lattices remain minimum-energy configurations as the ratio of m to n grows large. The topological

patterns and symmetries manifest in the lattice configurations for Thomson's problem also appear in a diverse array of other physical and biological systems [13–16]. These configurations may be useful for benchmarking optimization methods.

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