Global minimum for Thomson's problem of charges on a sphere

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Using numerical arguments, we find that for $N=306$ a tetrahedral configuration (T_h) and for $N=542$ a dihedral configuration (D_5) are likely the global energy minimum for Thomson's problem of minimizing the energy of N unit charges on the surface of a unit conducting sphere. These would be the largest N by far, outside of the icosadeltahedral series, for which a global minimum for Thomson's problem is known. We also note that the current theoretical understanding of Thomson's problem does not rule out a symmetric configuration as the global minima for $N=306$ and 542. We explicitly find that analogues of the tetrahedral and dihedral configurations for N larger than 306 and 542, respectively, are not global minima, thus helping to confirm the theory of Dodgson and Moore [Phys. Rev. B **55**, 3816 (1997)] that as N grows, dislocation defects can lower the lattice strain of symmetric configurations and concomitantly the energy. As well, making explicit previous work by ourselves and others, for $N<1000$ we give a full accounting of icosadeltahedral configurations which are not global minima and those which appear to be, and discuss how this listing and our results for the tetahedral and dihedral configurations may be used to refine theoretical understanding of Thomson's problem.

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What configuration of N unit charges on the (surface) of a unit conducting sphere minimizes the Coulombic energy $\Sigma_{i\neq j}1/r_{ij}$ [1]? Beyond physics, this question has utility in assembly of biological [2] and chemical structures [3,4], to benchmark optimization algorithms, and, as well, in mathematics Smale [5] has noted this question to be a *Hilbert problem* for the 21st Century. For $2\leqslant N\leqslant 100$, which was the original question asked by J.J. Thomson a century ago, and a bit beyond, there is agreement of all numerical [6–10] and theoretical [11] methods, suggesting that the global minimum configuration has been found. However, for larger N owing to an exponential growth in good local minima [7], finding global minima, general principles, or insights for minimization, or even methods or cases to test hypotheses, has proven extremely difficult. For $N=10(h^2+k^2+hk)+2$, highly symmetric icosadeltahedral configurations can be constructed. While it was initially thought that such configurations might be global minima [12], for large N adding defects to the icosadeltahedral lattice lowers the energy [13–17]. Here we note a tetrahedral configuration for $N=306$ and a dihedral configuration for $N=542$ which, based on numerical arguments, appear to be global minima. This is the largest such N by far, aside from the icosadeltahedral series, for which a global energy minimum configuration is known. Study of tetrahedral analogues larger than 306 and dihedral analogues larger than 542 helps confirm the theory [18] on defects lowering lattice strain and energy. As well, we note that the fact that lattice configurations fail to be global minima for $N>800$ may help explain why Mo_{154} anions self-assemble into a spherical superstructure with a nonlattice number of subunits [4].

For $N=78$, as originally suggested by Edmunson [11], the presumed global minimum configuration has tetrahedral (T_h) symmetry [Fig. 1(a)] [7–11]. We had previously suggested that an analogue of this configuration with 306 charges [Fig. 1(b), see below for the method of construction of this analogue] also might be a global minimum and we did limited numerical testing of this idea [12]. Now, here we have extensively checked numerically on over 1000 runs, and we have found no configuration of lower energy. [Numerically to look for nonlattice configurations with energies lower than the lattice configuration, we used random initial configurations followed by a local steepest-descent method. For $N=306$, we could not find a configuration in 1000 runs with an energy lower than the lattice energy, though for many other N considered in this paper including $N=1218$ and 4866, and smaller N with icosadeltahedral lattices (see Tables I and II and Fig. 2), configurations with energies lower than the lattice energy could be found in only 15 runs.] But 1000 runs is orders of magnitude less than the estimated [7] over 1.5 million local minima for $N=306$. As well, without analytic proof we could not be certain the tetrahedral configuration in Fig. 1(b) is the one of minimum energy for $N=306$. Current theoretical understanding of Thomson's problem [13,16–19], to be discussed below, does not exclude the possibility of a symmetric configuration as the global energy minimum for $N=306$. Of course, our configuration stands open to challenge.

Using a genetic algorithm, Morris, Deaven, and Ho [9] confirmed previously found [10] presumed global minima for $N\leqslant 112$ and gave their likely global minima for $N\leqslant 200$. Fitting the energy of these minima for $N\leqslant 200$ to the function $E=N^2/2(1+aN^{-1/2}+bN^{-3/2})$ (see [9] and references.

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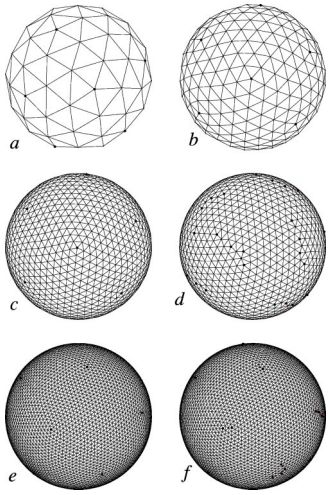

FIG. 1. Tetrahedral configurations. For (a) $N=78$ ($E=2662.046\,47$), (b) $N=306$ ($E=43\,862.569\,78$), the symmetric tetrahedral lattice configuration appears to be the global energy minimum, while for $N=1218$ (c) ($E=718\,284.037\,47$), (d) ($E=718\,281.631\,10$), and $N=4886$ (e) ($E=11\,651\,484.512\,95$), (f) ($E=11\,651\,440.241\,77$), addition of defects to the lattice produces a configuration of lower energy. For $N=1218$ and 4886, we give the lowest energy configuration we have found, though we cannot be certain this is a global energy minima. Fivefold-coordinated charges (points) (pentamers) are indicated by large dots, and sevenfold-coordinated charges (septamers) are indicated by small dots. The rest of the charges are sixfold coordinated (hexamers).

therein for an explanation of why this function was used) for $N>100$, they found particularly deep minima with respect to this function for icosadeltahedral configurations for $N=122$, 132, and 192 and for dihedral D_5 configurations for $N=137$, 182, and 187 and D_2 configuration for $N=146$. By our numerical testing as well, these dihedral configurations appear to be global minima, though we have no analytic proof and numerically we are orders of magnitude short [7] to even sample a majority of local minima. We next looked at the higher split analogues of these dihedral configurations with $4N-6$ charges. (See below for the method of construction of such analogues.) The next larger dihedral analogues for $N=146$, 182, and 187, which are $N=578$, 722, and 742, respectively, are found not to be global minima after only a few runs (Altschuler and Pérez-Garrido data not shown). However, the next larger dihedral (D_5) analogue of $N=137$, which is $N=542$, after over 1000 runs appears possibly to be a global minimum. As for the tetrahedral configuration for $N=306$, we have no analytic proof of this proposition and, given the huge number of local minima for an N this large [7], our numerical runs only begin to address the question. Conversely, we easily found that the next analogue of $N=137$, which is $N=2162$, is explicitly not a global energy minimum. See Fig. 3 for dihedral configurations for $N=137$, 542, and 2162.

Euler's theorem asserts that when a (convex) polyhedron is constructed by joining points on a sphere, the number of faces (F) plus the number of vertices (V) is equal to the number of edges (E)$+2$; $F+V=E+2$. For $N>12$, this has the result that in addition to the sixfold-coordinated points of a planar two-dimensional lattice (hexamers), there must be at least 12 points of fivefold-coordination (pentamers). The tetrahedral configurations for $N=78$ and 306, dihedral configurations for $N=137$ and 542, and icosadeltahedral configurations for $N=10(h^2+k^2+hk)+2$ have exactly 12 pentamers and the rest hexamers [see, e.g., Figs. 1(a)–1(c) and 1(e), Figs. 2(a) and 2(b), and Figs. 3(a)–3(c)]. Larger analogues (*split* configurations) of the tetrahedral configuration for $N=78$ (for $N=306, 1218, 4886$) and for the dihedral configuration for $N=137$ [$(N=542, 2162)$] [Figs. 1(a), 1(c), and 1(e), and Figs. 3(b) and 3(c)] are made as follows: in addition to the N charges preexisting, place one charge at the center of each of the $3N-6$ edges. (If all the charges were sixfold-coordinated hexamers, there would be $3N$ edges; six must be subtracted from this to take into account the 12 fivefold-coordinated pentamers.) Then relax to the final position by a local gradient method. The resulting configuration has $N+(3N-6)=4N-6$ charges. [See Figs. 1(b), 1(c), and 1(e)]. Some icosadeltahedral configurations can be made (*split*) as

TABLE I. Energy of icosadeltahedral configurations with $N<400$. An asterisk indicates a configuration of lower energy, though not necessarily the global minimum. For each N, here and in Table II, we tried 15 runs—random initial configurations followed by a local gradient descent—to find a configuration with an energy lower than that of the icosadeltahedral lattice. For $N=42$, 92, and 162, the best known configuration has exactly 12 pentamers (and thus no dislocation defects), but does not have icosadeltahedral symmetry. We note that the split larger analogue of the global minimum configuration for $N=42$ is not the global minimum configuration for $N=162$, and neither are the split larger analogues of the $N=92$ and 162 global minima (data not shown).

Charges			Energy
12	h=1	k=0	49.1652530580000
32	h=1	k=1	412.261274651000
42	h=2	k=0	732.256241038000
	*Nonicosadeltahedral		732.078107551000
72	h=2	k=1	2255.00119099000
92	h=3	k=0	3745.61873908500
	*Nonicosadeltahedral		3745.29163624500
122	h=2	k=2	6698.37449926100
132	h=3	k=1	7875.04534281600
162	h=4	k=0	11984.5514338730
	*Nonicosadeltahedral		11984.0503358310
192	h=3	k=2	16963.3383864710
212	h=4	k=1	20768.0530859690
252	h=5	k=0	29544.2821928610
	*Nonicosadeltahedral		29543.5286475291
272	h=3	k=3	34515.1932926880
282	h=4	k=2	37147.2944184740
312	h=5	k=1	45629.3627238190
362	h=6	k=0	61720.0233978130
	*w/defects		61719.3090545160
372	h=4	k=3	65230.0271225660
392	h=5	k=2	72546.2583708950

TABLE II. Energy of icosadeltahedral configurations with $N > 400$. An asterisk indicates a configuration of lower energy, though not necessarily the global minimum. Thus, for $N < 792$ we also cannot be certain that the symmetric icosadeltahedral configurations are the global minima.

Charges			Energy
432	h=6	k=1	88354.2293807250
	*w/defects		88354.1906652260
482	h=4	k=4	110318.139920155
492	h=7	k=0	115006.982258289
	*h=5	k=3	115005.255889700
522	h=6	k=2	129655.833007858
572	h=7	k=1	156037.879346228
	*w/defects		156037.316647696
612	h=5	k=4	178910.494981768
642	h=8	k=0	197100.363816212
	*w/defects		197098.637958037
672	h=7	k=2	216171.432658341
732	h=8	k=1	256975.527362500
	*w/defects		256974.262894426
752	h=5	k=5	271362.588212841
762	h=6	k=4	278704.548700071
792	h=7	k=3	301321.818305597
812	h=9	k=0	316895.372099956
	*w/defects		316892.668538128
842	h=8	k=2	340988.383415978
	*w/defects		340987.675098937
912	h=9	k=1	400662.383224662
	h=6	k=5	400660.132041002
	*w/defects		400659.747279004
932	h=7	k=4	418596.898209635
	*w/defects		418595.636527970
972	h=8	k=3	455654.618623736
	*w/defects		455653.441695822
1082	h=6	k=6	565703.908873765
	*w/defects		565703.766602964

analogues of smaller ones [see, e.g., $N=1242$ in Fig. 2(b), a larger analogue of $N=312$ in Fig. 2(a)]. A method for making icosadeltahedral configurations *de novo* has been discussed previously [12].

Conversely to the cases of $N=78$ and 306 and $N=137$ and 542 for the larger analogues we have studied ($N=1218$, 4886, and 2162), we find that adding dislocation defects to the lattice produces a configuration with lower energy [Figs. 1(c)–1(f) and Figs. 3(c) and 3(d)]. Similarly, for $N>792$ icosadeltahedral configurations with dislocation defects, additional fivefold-coordinated points and then necessarily also sevenfold-coordinated points (septamers) have lower energy than symmetric lattice configurations, while for smaller N the symmetric lattice configurations appear to be global minima (see Tables I and II and Fig. 2 for an example), though further numerical testing may show that some such configurations are not global minima.

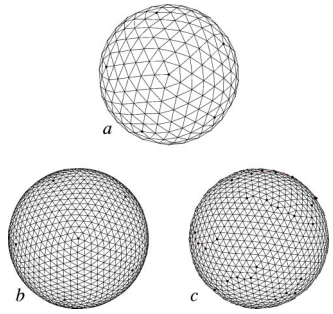

FIG. 2. Icosadeltahedral configurations. For (a) $N=312$ ($E=45629.36272$) the symmetric icosadeltahedral configuration appears to be a global energy minimum, while for $N=1242$ (b) ($E=747107.43183$), (c) ($E=747106.46027$), addition of defects produces a configuration of lower energy (though not necessarily the global energy minimum). As in Fig. 1, fivefold-coordinated charges (points) (pentamers) are indicated by large dots, and sevenfold-coordinated charges (septamers) are indicated by small dots. The rest of the charges are sixfold-coordinated hexamers.

These numerical results on the N at which tetrahedral, dihedral, and icosadeltahedral configurations fail to be global energy minima are in remarkable concordance with a theory given by Dodgson and Moore [13] originally for icosadeltahedral configurations: Using continuum elasticity theory [18], they studied the energy cost of a pair of pentamers, compared with a pure hexagonal lattice, and suggested that dislocation defects—extra fivefold-coordinated points, with (necessarily) paired sevenfold-coordinated points—would lower lattice strain and energy for N in the $\approx 500-1000$ range. Similar reasoning should apply to the tetrahedral configurations in the $N=78$ series and dihedral configurations in the $N=137$ series. Our results given here are strong confirmation of Dodgson and Moore's theory [13].

The fact that apparently for $N>792$ all symmetric tetrahedral, dihedral, or icosadeltahedral lattices are not global

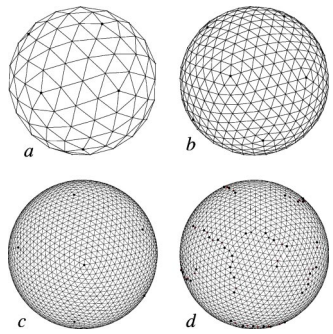

FIG. 3. Dihedral configurations. For (a) $N=137$ ($E=8499.534\,49$), (b) $N=542$ ($E=139\,913.694\,61$), the symmetric dihedral lattice configuration appears to be the global energy minimum, while for $N=2162$ (c) ($E=2\,281\,595.051\,27$), (d) ($E=2\,281\,587.487\,35$), addition of defects to the lattice produces a configuration of lower energy. We give the lowest energy configuration we have found, though we cannot be certain this is a global energy minima. Fivefold-coordinated charges (points) (pentamers) are indicated by large dots, and sevenfold-coordinated charges (septamers) are indicated by small dots. The rest of the charges are sixfold-coordinated (hexamers).

minima, along with the exponential growth in good local minima, may help explain why the number of Mo_{154} anions which self-assemble into a spherical superstructure [4] is a nonlattice number 1165, rather than, for example, 1172, the closest icosadeltahedral lattice, or the tetrahedral lattice at 1218, while for small N, self-assembly often produces a symmetric lattice configuration [2,3].

For icosadeltahedral configurations for $N \leqslant 792$, whether or not a lattice configuration is a potential global minimum depends not only on the magnitude of N, but also apparently on the details of the lattice itself. All lattice N are listed in Tables I and II. As can be seen for $N=42$, 92, 162, 252, 362, 432, 492, 572, 642, and 732, the icosahedral lattice configuration is manifestly not the global minimum, while for the other N, the lattice configuration appears to be so.

In an icosadeltahedral lattice $N=10(h^2+k^2+hk)+2$, to go from the center of one pentamer to the center of an adjacent pentamer, one moves h steps along one basis vector for the lattice, and then k steps in the other. We noted previously [12] (also discussed in Ref. [19]) that the energy in an icosadeltahedral lattice configuration with a large ratio of h to k ($h \geqslant k$) may be increased due to the vertices of the pentamers being closely aligned (or perfectly aligned in a lattice with $k=0$). It has previously been noted that as N grows, the icosadeltahedral lattice configuration may not be the global minimum [13–17], though we have not seen any explicit published accounting of the N for which the lattice fails to be a global minimum. This is given in Tables I and II (in addition to the rule that for $N>792$, the lattice is not the global minimum). A clear pattern emerges: for an icosadeltahedral configuration with $k=0$, besides the extremely exceptional case of $N=12$, the icosadeltahedral lattice configuration is not the global minimum. For the four small $N=42$, 92, 162, and 252, the apparent global minimum configuration has exactly 12 pentamers, and no dislocation defects, but arranged in a nonicosadeltahedral configuration, likely lowering the energy cost of having the vertices of pentamers aligned. For N larger than 252 in the $k=0$ series, the apparent global minimum incorporates dislocation defects. For $N=432$ and higher for lattices with $k=1$, the lattice is also not the global minimum, in accordance with the notion stated above that the energy of the lattice is increased by relative alignment of the vertices of the pentamers. The data in Tables I and II may be useful in refining theoretical predictions for global energy minima: The current general theory [13,18] correctly predicts that for $N>1000$, icosadeltahedral and tetrahedral configurations will not be global minima, but it does not yet account for various cases for $N<1000$. As well, for $k=0$ other theoretical work [17,19] predicts dislocations lowering the energy for $N>300$, and remarkably the first instance of this is found for $N=362$ (see Table I).

For tetrahedral or dihedral lattices, we have not yet been able to find an obvious rule or principle to predict for which N the lattice configuration is a global minimum. Indeed, while all groups using a variety of different methods find the T_h configuration to be a global minimum for $N=78$ [10], and we have found similarly for $N=306$, there are a number of $N<100$ for which T_h configurations are not the global minima [10,11], and also we have found that the next analogue of the global minimum for $N=100$ which has T (though not T_h) symmetry, namely $N=394$, is not a global minimum (E.L.A. and A.P.G. data not shown). And we see no obvious difference between the $N=78$ lattice and the others to explain why not only for $N=78$ but also for the next higher analogue the lattice appears to be the global minimum. Similarly, we have found no obvious reason why the next D_2 analogue of 146–578—or the next D_5 analogues of 182 and 187, namely 722 and 742, are not global minima, but the next D_5 analogue of 137–542 appears to also be a global minimum. The theory of Dodgson and Moore [13] does not predict *a priori* that defects would lower a lattice energy for an N of 306 and 542, as it does for the next analogues 1218 and 2162. Perhaps whatever the still unknown reasons are that explain the good minimum for the T_h lattice for $N=78$ and the D_5 lattice for $N=137$ also permit the $N=306$ and 542 analogues to be global minima. The delineation of specific instances of icosadeltahedral, tetrahedral, and dihedral configurations for $N<1000$ that appear to be global minima, and those that are not global minima, should be of help in further refining theoretical models.

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