Defect free global minima in Thomson's problem of charges on a sphere

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Given N unit points charges on the surface of a unit conducting sphere, what configuration of charges minimizes the Coulombic energy $\sum_{i>j=1}^{N} 1/r_{ij}$? Due to an exponential rise in good local minima, finding global minima for this problem, or even approaches to do so has proven extremely difficult. For $N = 10(h^2 + hk + k^2) + 2$ recent theoretical work based on elasticity theory, and subsequent numerical work has shown, that for $N \sim> 500$–1000 adding dislocation defects to a symmetric icosadeltahedral lattice lowers the energy. Here we show that in fact this approach holds for all N, and we give a complete or near complete catalogue of defect free global minima.

What configuration[1] of N unit point charges on (the surface of) a unit conducting sphere minimizes the Coulombic energy $\sum_{i>j=1}^{N} 1/r_{ij}$? Beyond physics, this questions has utility in understanding the assembly of biological[2] and chemical[3, 4] macromolecules, benchmarking optimization methods and, in mathematics, Smale[5] has noted the question to be a *Hilbert* problem for the 21st century. For $2 < N < 100$, the question originally posed by Thomson more than a century ago[1], there is agreement of numerical and theoretical work from numerous groups[6, 7, 8, 9, 10, 11, 12, 13, 14, 15] using a variety of methods so as to have strong confidence that the minimum energy configurations have been found. However, as N grows, due to exponential growth of good local minima[10], finding global minima has been extremely difficult. For $N = 10(h^2 + k^2 + hk) + 2$, with h and h integers $h \geq k \geq 0$, highly symmetric icosadeltahedral configurations can be constructed (see, e.g., Fig. 1). Initially it was thought that such configurations might be global minima[12], but as N grows Dodgson and Moore[16] using continuum elasticity theory[17] suggested that better energy minima could be found for $N >\sim 500 - 1000$ by adding dislocation defects to the icosadeltahedral lattice (Fig. 1). Indeed, this was found to be so[18, 19, 20, 21, 22]. In a full census of icosadeltahedral configurations we had recently found that defects lower the lattice energy for $N > 792$[23]. We also noted that the theory of Dodgson and Moore can also be applied to non-icosadeltahedral defect free configurations. For example, for $N = 78$ a tetrahedral (T_h) configuration (Fig. 1) is the global energy minimum[8], and a larger analogue also appears to be the global energy minimum for $N = 306$, see Refs. [12, 23], but for the next larger analogue for $N = 1278$ addition of dislocation defects lower the energy[23]. Here we show that the theory of Dodgson and Moore in fact applies for all N, and give a full or nearly full accounting of defect free configurations for Thomson's problem.

For each N with a presumed dislocation defect free global minimum[7, 8, 9, 10, 11, 14, 15, 24] we initially tried 100 trials as such to see if a configuration including dislocation defects with a lower energy could be found: For a given N we started the charges at random locations and minimized the energy with a standard local gradient descent method. If we found a configuration with no dislocation defects and a lower energy than the previously proposed configuration, we then tested another 1000 trials to see if a configuration with dislocation defects and lower energy could be found. One hundred or one thousand trials is hardly even a start to exploring the more than $1.14 \cdot 10^6$ predicted[10] local minima, for example, for $N = 300$. But as we see below, even this few trials yields crucial trends in minima for Thomson's problem. For some larger N, especially those with icosadeltahedral configurations, we have tried up to 1000 random trials. Clearly, more extensive trials for all N may give lower energy configurations.

Our results are summarized in Table I: For $N = 12$–200 our search of random configurations confirmed previously found global minima[7, 8, 9, 10, 11, 14, 15, 24] (See Ref. [24] for energies and coordinates, except for $N = 38$ and 46 see [10, 11].): For $N = 12$–100, there are 81 defect free global minima (91%). For $N = 101$–200, 92 N have defect free presumed global minima. For $N = 201$–300 we found 55 N for which the presumed global energy minimum had no dislocation defects. Of these (see Table II) 12 are N for which the previously presumed global minimum[24] also had no dislocation defects but our configuration has a lower energy. (Contact A.P.G. for coordinates for N listed in Table II; for other N see Ref. [24]). There are also three N–see Table III-for which a previously presumed global energy minimum had no dislocation defects, but we found a configuration with dislocation defects with a lower energy. For example, for $N = 214$ a defect free configuration had been thought to be the global minimum with energy 21170.0694327506[24], but we found a configuration that has defects with energy 21170.0688491490. For $N = 301$–400 20 N have presumed global energy minimum configurations with no dislocation defects–all previously known (see Ref. [24] for

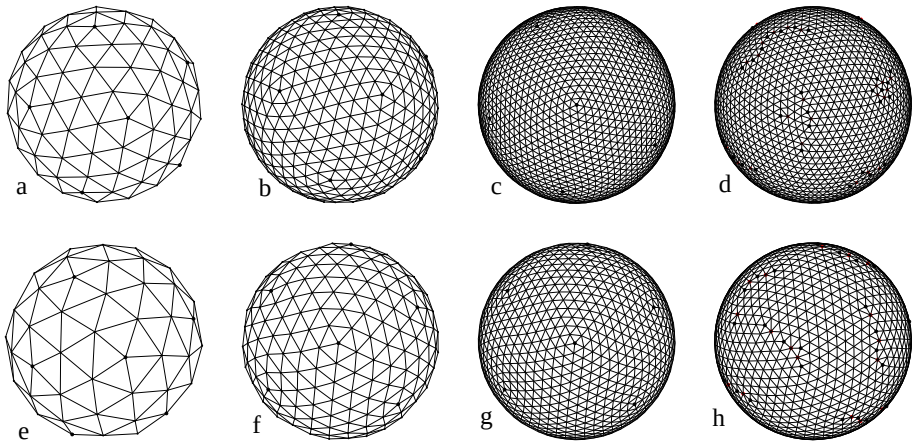

FIG. 1: Defect free global energy minimum configurations. Fivefold coordinated charges (pentamers) are indicated by large black dots, and sevenfold coordinated c harges (septamers) are indicated by small red dots. The rest of the charges are sixfold coordinated (hexamers). a) $N = 132$ (a (3,1) icosadeltahedral configuration) $E = 7875.0453428$. For construction of icosadeltahedral configurations see [12]. b) $N = 522$ (a (6,2) icosadeltahedral configuration $\equiv 4\times132-6$), E =129655.8330078. c) $N = 2082$ (a (12,4) icosadeltahedral configuration $\equiv= 4\times522$-6) $E = 2114888.07077971$ d) $N = 2082$ (defects) $E = 2114878.739395074$. e) Tetrahedral (T_h) configuration for $N = 78$ E =2662.04647456. f) T_h configuration for $N = 306$ E = 43862.56978081. g) T_h configuration for $N = 1278$ has a higher energy 718284.03746827, than for a configuration h) with dislocation defects 718281.63109628, though we cannot be certain this is the configuration of minimum energy.

energies and coordinates). For $N = 301$–400 we found one N–see Table III– for which we found a configuration with dislocation defects with lower energy than the previously presumed global energy minimum with no defects. For $400 < N \leq 632$ we find only eight N for which the presumed global minimum has no dislocation defects and of these eight, the largest four are icosadeltahedral configurations (N =482, 492, 612, 632). We did not find any new configurations with no dislocation defects with lower energy than previously presumed global minima, but we did find sixteen instances–see Table III–of cases for which the presumed global minimum had no dislocation but a configuration with lower energy that includes dislocation defects. These sixteen included, interestingly, two instances–672 and 762–in which the presumed global minimum had icosadeltahedral symmetry[23], and also $N = 542$ for which a configuration with high dihedral (D_5) symmetry had been the presumed global minimum.

Results for $N = 10(h^2 + hk + k^2) + 2$ are summarized in Table IV. For $N > 632$ no icosadeltahedral configuration is a global minimum, and for $N \leq 632$ whether or not an icosadeltahedral configuration is a global minimum depends on the ratio of h to k, with smaller ratios protecting global minima by decreasing energy by rotation of vertices of the pentamers with respect to each other[12, 23, 25].

For any N for which a defect free configuration appears to be a global minimum we have split this N to see if for the next larger analogue the defect free configuration still remains an apparent global energy minimum. Configurations are split by putting a new charge midway between each of the $3N - 6$ pairs of charges–for a total of $4N - 6$ charges–and then using a local gradient descent method.

TABLE I: $N \leq 632$ with apparent global minimum energy configurations with no dislocation defects.

12	14–17	19–20	22–32
34–58	60–70	72–78	80–82
84–108	110–122	124–125	127–139
141–148	150–168	170–171	173–178
180–200	202–210	212–213	217–226
228–229	232	234–236	239–242
244	246	252	255–258
260	262	264	266
269–270	272–273	276	279
282–283	288–289	292–293	300
302	304	306	312
316–317	322	324	328
348	352	357	361
372	382	387	390
392	397	400	402
412	462	477	482
492	612	632	

We continue to split the configuration until we found a larger analogue for which the defect free configuration is not a global minimum. For example, for $N = 78$ it was appreciated some time ago that a tetrahedral (T_h) configuration was the global energy minimum[8]. We suggested that for the next larger analogue, $N = 306$, the tetrahedral defect free configuration was also a global energy minimum[12] and this appears to be the case[23, 24]. But for the next larger analogue at $N = 1278$ the tetrahedral configuration has a higher energy than one with dislocation defects. Besides $N = 78$ and 306 (78, 306), we have found the following cases in which a split configuration itself also appears to be a global energy minimum: (15, 54), (19, 70), (25, 94), (32, 122, 482), (72, 282) and (77, 302).

As mentioned above, we had previously thought[23]

TABLE II: New apparent global minimum energy configurations with no dislocation defects.

N	Ref. [24]	This work
206	19586.024651029	19586.023817485
218	21985.328738558	21985.276740701
219	22191.574733521	22191.485474828
229	24307.641707488	24307.607278979
234	25401.953728147	25401.933332294
235	25623.795960898	25623.763144220
236	25846.579605445	25846.500563170
241	26975.230903304	26975.204068314
246	28128.062826837	28128.056910358
258	30994.404751420	30994.290832296
264	32480.027262398	32480.025885504
269	33744.825254911	33744.824929632

TABLE III: Configurations with defects (this work) for N with previously presumed[24] global minima with no dislocation defects. Contact A.P.G. for energies and coordinates. Our data will be added to that in Ref. [24].

214	215	227	327
417	447	472	512
516	518	532	534
537	538	542	548
672	722	762	777

that (137, 542) was a split pair of likely global minima with high dihedral D_5 symmetry. However, the more trials tested for this paper found that for $N = 542$ a configuration with dislocation defects had a lower energy than the D_5, no dislocation defect, analogue of $N = 137$. Though in the intermediate and somewhat indeterminate range of the theory of Dodgson and Moore[16] –$N \sim$ 500–1000–clearly for N as small as 542 with a high dihedral, but not icosahedral symmetry, adding dislocation defects lowers the energy. Also, the global energy minimum for $N = 522$ is not the icosadeltahedral configuration [24], and thus (132, 522) is not a pair of split global minima. However, the currently presumed global energy minimum for 522 [24], while possessing dislocation defects, has twelve defect pairs of a pentamer and a septamer arranged rather symmetrically and concordantly with the twelve obligatory pentamers (disclinations). Thus for $N = 522$, in the intermediate range for Dodgson and Moore's theory, we see the addition of defects but in a controlled way.

Table I shows a remarkably strong confirmation that the theory of Dodgson and Moore[16] can be applied to general N. Not only do dislocation defect free configurations become ever vanishingly rare for $N > 400$, but for $N < 400$–the more so for smaller N–the global energy minima typically have no dislocation defects. Indeed, for $12 \leq N \leq 100$ in quite a number of cases special circumstances account for presumed global energy minima with dislocation defects: For example, for $N = 13$ it was *proven* many years ago[27] that there are no configurations without dislocation defects. For $N = 18$ the global minimum configuration has one charge at each pole and four rings of four charges each, staggered with respect to each other–dihedral D_{4d} symmetry[28]. For N =33, and 79 there seems to be no way to add one charge, and for N = 71 to subtract one charge, to the deep global minima for the symmetric configurations of N = 32, 72 and 78 and have a good minimum with no dislocation defects.

Two important questions remain: (1) For the N for which now a defect free configuration is the presumed global minimum (Table I), are these configurations the true global minima? Given the exponential rise in good local minima with N[10], we cannot be certain without an amount of numerical testing that exceeds current computational ability, that further numerical work may find that some of these configurations are not global minima. As discussed below, we would expect such instances where defect free configurations fail to be global minima to occur in the $\sim 100 < N < 500$ range. (2) Are there defect free global energy minimum configurations we have not yet found, either for N not listed in Table I, or even new lower energy defect free configurations for N in Table I? Dodgson and Moore[16] considered the energy cost of a pair of pentamers in an icosadeltahedral lattice and noted that for $N \sim$ 500–1000 adding dislocation defects would lower the energy of the overall configuration. Numerical work rapidly confirmed this theory[19, 20, 21, 22, 23], and in this work we find that even over 500 there are at most only two icosadeltahedral configurations that still are possibly global energy minima–though further searches on these N may also find these not to be global energy minima. We noted previously[23] that the theory of Dodgson and Moore could be applied similarly to a pair of pentamers in a highly symmetric, e.g., tetrahedral, but not icosadeltahedral lattice, and similarly (Ref. [23] and work above) finds that for $N < 500$ the symmetric defect free configuration appears to be a global energy minimum, but not for $N > 500$. Here we have pointed out that even for general N for a configuration that is dislocation defect free, but not necessarily highly symmetric, still one can use the theory of Dodgson and Moore and consider the energy cost of a pair of pentamers. As the energy cost of a pair of vertices will not be lower for a non-symmetric configuration than for a symmetric configuration–as in a non-symmetric configuration the cost must be borne of the pair of pentamers with their vertices most closely aligned–the range of 500–1000 will again be an absolute upper limit of where defect free configurations will remain global minima. Indeed, our numerical work is consistent with the lower range as we have found only six possible defect free configurations between 400 and 500.

So by the theory of Dodgson and Moore we don't expect any defect free global energy minima for $N > 1000$, and likely few even in in the $N \sim$500–1000 range. Thus, numerical searches to finalize the catalogue of defect free global energy minima should be focused on the $\sim$100–500 range (for $N \leq 100$ there has been sufficient numerical and theoretical work[6, 7, 8, 9, 10, 11, 12, 13, 14, 15] as to make finding new defect free global energy minimum configurations unlikely). In particular, we haven't studied closely yet those N for which the currently proposed[24]

TABLE IV: Energy of icosadeltahedral configurations. An * indicates a non-icosadeltahedral configuration (with or without defects) of lower energy, though not necessarily the global minimum.

N	h, k	Energy
12	h= 1 k= 0	49.165253058
32	h= 1 k= 1	412.261274651
42	h= 2 k= 0	732.256241038
	*Non–icosadeltahedral	732.078107551
72	h= 2 k= 1	2255.00119099
92	h= 3 k= 0	3745.618739085
	*Non–icosadeltahedral	3745.291636245
122	h= 2 k= 2	6698.374499261
132	h= 3 k= 1	7875.045342816
162	h= 4 k= 0	11984.551433873
	*Non–icosadeltahedral	11984.050335831
192	h= 3 k= 2	16963.338386471
212	h= 4 k= 1	20768.053085969
252	h= 5 k= 0	29544.282192861
	*Non–icosadeltahedral	29543.528647529
272	h= 3 k= 3	34515.193292688
282	h= 4 k= 2	37147.294418474
312	h= 5 k= 1	45629.362723819
362	h= 6 k= 0	61720.023397813
	* w/defects	61719.309054516[a]
372	h= 4 k= 3	65230.027122566
392	h= 5 k= 2	72546.258370895
432	h= 6 k= 1	88354.229380725
	* w/defects	88354.190665226[a]
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
	* w/defects	129655.326253464[b]
572	h= 7 k= 1	156037.879346228
	* w/defects	156037.222417655[b]
612	h= 5 k= 4	178910.494981768
632	h= 6 k= 3	190937.233325601
642	h= 8 k= 0	197100.363816212
	* w/defects	197098.532524683[b]
672	h= 7 k= 2	216171.432658341
	* w/defects	216171.227524558[c]
732	h= 8 k= 1	256975.527362500
	* w/defects	256973.838562012[b]
752	h= 5 k= 5	271362.588212841
	* w/defects	271361.125880198[b]
762	h= 6 k= 4	278704.548699996
	* w/defects	278704.428077126[c]
792	h= 7 k= 3	301321.818305597
	* w/defects	301320.370436992[b]

[a]Ref. [23]
[b]Ref. [24]
[c]This work

global minimum includes dislocation defects. For these N more numerical trials could find better minima that have no dislocation defects.

For another reason we think that if new defect free global energy minimum energy configurations are to be found one must look for $N < 500$. Using the method of Ewald sums[20, 21, 26], one finds that the energy of N charges on a unit sphere in the theoretically impossible (by Euler's theorem), but approximately useful, construct of a perfect triangular (hexagonal) lattice for $N \to \infty$ is

$$E = \frac{1}{2}\left(N^2 - 1.1061033N^{3/2}\right) \qquad (1)$$

where the term order $N^{3/2}$ is the energy of N charges uniformly distributed on a sphere and embedded in a uniform neutralizing background[26] and the term $N^2/2$ accounts for the lack of a uniform neutralizing background in Thomson's problem. Eq. (1) has been also obtained using other techniques by a number of authors[29, 30, 31]. As N grows large, in accordance with equation (1), $E' = (2E - N^2)/N^{3/2}$ approaches -1.11061033. Previous numerical calculations for $N \leq 200$ yielded a value -1.1046 for the constant coefficient of the $N^{3/2}$ term[31, 32], though this is clearly seen to be exceeded for $N >\sim 600$ (Fig. 2). Furthermore, a configuration with $N = 15152$ and $E' = -1.10562321$ has been found[20]. E' is plotted in Fig. 2. We see that for $N < 500$ the defect free energy configurations stand out as having particularly low relative scaled energies, while for $N > 500$ the defect free configurations are not particularly good compared with other presumed global energy minimum configurations. Thus, for $N > 500$ even for the currently presumed defect free global energy minimum configurations there seems no added benefit compared to configurations with defects, and thus we doubt that for other N in this range defect free configurations will be global minima.

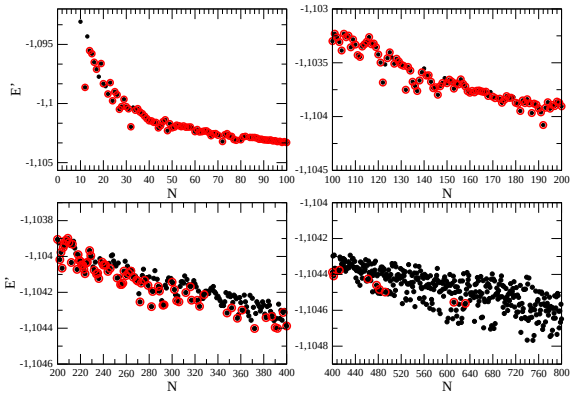

FIG. 2: $E' = (2E - N^2)/N^{3/2}$ *vs.* N. E' is defined using Eq. (1). Energies are plotted with black dots and are encircled in red if the associated presumed global minimum energy configuration has no dislocation defects.

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