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 $\Sigma_{i>j=1}^{N} 1/r_{ij}$? 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 $N \gtrsim 500-1000$ 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.

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What configuration of N unit point charges on (the surface of) a unit conducting sphere minimizes the Coulombic energy $\Sigma_{i>j=1}^{N} 1/r_{ij}$–? a question originally asked by more than a century ago by Thomson, for $2<N<100$ [1]. Beyond physics, this question 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 twenty-first century. For $2<N<100$ there is agreement of numerical and theoretical work from numerous groups [6–15] 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 k integers $h \geqslant k \geqslant 0$, highly symmetric icosadeltahedral configurations can be constructed (see, e.g., Fig. 1 in Ref. [16]). Initially it was thought that such configurations might be global minima [12], but as N grows Dodgson and Moore [17] using continuum elasticity theory [18] suggested that better energy minima could be found for $N \gtrsim 500-1000$ by adding dislocation defects to the icosadeltahedral lattice (Fig. 1 in Ref. [16]). Indeed, this was found to be so [19–23]. In a full census of icosadeltahedral configurations we had recently found that defects lower the lattice energy for $N>792$ [16]. We also noted that the approach of Dodgson and Moore can also be applied to nonicosadeltahedral defect free configurations. For example, for $N=78$ a tetrahedral (T_h) configuration (Fig. 1 in [16]) is the global energy minimum [8], and a larger analogue also appears to be the global energy minimum for $N=306$ (see Refs. [12,16]), but for the next larger analogue for $N=1278$ addition of dislocation defects lower the energy [16]. Here we show that the approach 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 [7–11,14,15,24] 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 Fig. 1 and Table I. For $N=12-200$ our search of random configurations confirmed previously obtained global minima [7–11,14,15,24] (see Ref. [24] for energies and coordinates, except for $N=38$ and 46

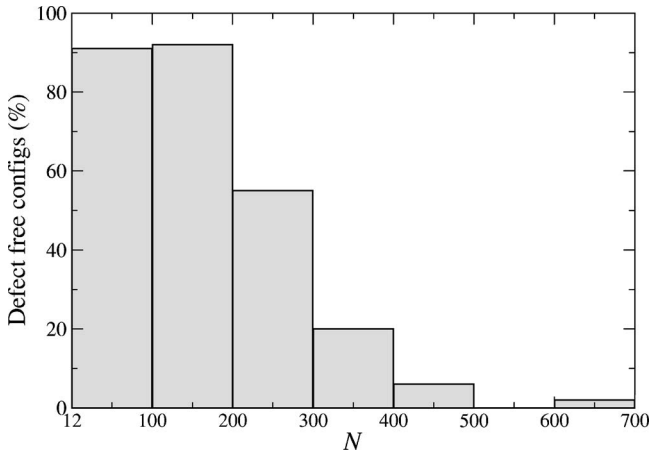

FIG. 1. Significantly decreased percentage of N with presumed defect free global minima for increasing N.

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TABLE I. $N \leqslant 632$ 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	

see [10,11]). For $N=12-100$, there are 81 defect free global minima (91%). For $N=101-200$, in 92 cases the presumed global minimum is defect free. For $N=201-300$ we found 55 instances for which the presumed global energy minimum had no dislocation defects. For twelve of these (see Table II) 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]). For 214, 215, and 227 charges (see Table III) the previously presumed global energy minimum had no dislocation defects, but we found a configuration with dislocation defects with a lower energy. For $N=301-400$ we found twenty instances where the presumed global energy configuration had no dislocation defects—all previously known (see Ref. [24] for energies and coordinates). Of these twenty there is one case—$N=327$ (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 $400<N\leqslant 632$ we find only eight examples (see Table I) 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 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 [16], 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 $N\leqslant 632$, 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 [12,16,25].

In Tables II–IV besides the raw energy—a quantity essential in searching for global minima—we also give the scaled energy $E'=(2E-N^2)/N^{3/2}$. E' is discussed more fully below. Here we note that E' is a measure of the uniformity of the configuration of the charges on the sphere, with a completely uniform configuration having $E'=-1.106\,103\,3$ [21,22,26–30]. As we can see—Fig. 2 and Tables II–IV—E' approaches $-1.106\,103\,3$ from above, though not completely monotonically. Also, for $N<500$ the presumed global energy minimum configurations that are defect free have especially low values of E'.

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 re-

TABLE II. Apparent global minimum energy configurations with no dislocation defects. $E'=(2E-N^2)/N^{3/2}$. See the text for an explanation and the significance of this scaling of the energy.

N	Energy (E) (Ref. [24])	Energy (E) (This work)	E'
206	19586.024651029	19586.023817485	−1.103933663
218	21985.328738558	21985.276740701	−1.103989748
219	22191.574733521	22191.485474828	−1.104021900
229	24307.641707488	24307.607278979	−1.103995680
234	25401.953728147	25401.933332294	−1.104098449
235	25623.795960898	25623.763144220	−1.104092693
236	25846.579605445	25846.500563170	−1.104123035
241	26975.230903304	26975.204068314	−1.104044842
246	28128.062826837	28128.056910358	−1.104066790
258	30994.404751420	30994.290832296	−1.104081763
264	32480.027262398	32480.025885504	−1.104081328
269	33744.825254911	33744.824929632	−1.104131775

TABLE III. Energy for configuration with defects (this work) for N with previously presumed [24] global minima with no dislocation defects. $E'=(2E-N^2)/N^{3/2}$ as in Table II. See the text for a discussion of E'.

N	Energy (E) for defect free [24]	Energy (E) for defective configurations (This work)	E'
214	21170.069432751	21170.068849149	−1.103915366
215	21372.407908194	21372.383791511	−1.103952947
227	23876.617954192	23876.576893749	−1.104016366
327	50199.780194689	50199.727656985	−1.104234429
417	82242.788173100	82242.565312557	−1.104339257
447	94686.088509962	94685.998909658	−1.104369695
472	105729.677538754	105729.521012745	−1.104392881
512	124674.465316290	124674.447998328	−1.104431758
516	126655.491595460	126655.452290185	−1.104410970
518	127652.666638557	127651.791961925	−1.104409748
532	134736.191769060	134735.828044478	−1.104452315
534	135763.659976040	135763.573407289	−1.104453456
537	137313.143595556	137312.971147939	−1.104388654
538	137830.955705555	137830.857655437	−1.104454394
542	139913.694700577	139913.598742969	−1.104496185
548	143068.145703381	143068.030518469	−1.104423970
672	216171.432658306	216171.227524558	−1.104551687
722	249928.040141904	249927.180548066	−1.104610220
762	278704.548699996	278704.428077126	−1.104619969
777	289902.659696523	289902.132123204	−1.104626867

mains an apparent global energy minimum. Configurations are split by putting a 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. 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 [16,24]. 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 [16] 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 for highly symmetric configurations from prior work [17]—$N\sim 500$ to 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 12 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 [17], we see the addition of defects but in a controlled way.

Table I shows a remarkably strong confirmation that the approach of Dodgson and Moore [17] 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 $12\leqslant N\leqslant 100$ 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 [31] 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 [32]. 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: (i) 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

TABLE IV. Energy of icosadeltahedral configurations. An asterik indicates a nonicosadeltahedral configuration (with or without defects) of lower energy, though not necessarily the global minimum. $E'=(2E-N^2)/N^{3/2}$. See the text for a discussion of E'.

N	h,k	Energy and (E')
12	$h=1$ $k=0$	49.165253058(−1.098637319)
32	$h=1$ $k=1$	412.261274651(−1.101967660)
42	$h=2$ $k=0$	732.256241038(−1.100284016)
	*Nonicosadeltahedral	732.078107551(−1.101592902)
72	$h=2$ $k=1$	2255.00119099(−1.103213648)
92	$h=3$ $k=0$	3745.618739085(−1.102364191)
	*Nonicosadeltahedral	3745.291636245(−1.103105557)
122	$h=2$ $k=2$	6698.374499261(−1.103683423)
132	$h=3$ $k=1$	7875.045342816(−1.103750768)
162	$h=4$ $k=0$	11984.551433873(−1.103288899)
	*Nonicosadeltahedral	11984.050335831(−1.103774949)
192	$h=3$ $k=2$	16963.338386471(−1.104078402)
212	$h=4$ $k=1$	20768.053085969(−1.104033530)
252	$h=5$ $k=0$	29544.282192861(−1.103755157)
	*Nonicosadeltahedral	29543.528647529(−1.104131894)
272	$h=3$ $k=3$	34515.193292688(−1.104253413)
282	$h=4$ $k=2$	37147.294418474(−1.104279760)
312	$h=5$ $k=1$	45629.362723819(−1.104201427)
362	$h=6$ $k=0$	61720.023397813(−1.104019113)
	*With defects	61719.309054516[a](−1.104226544)
372	$h=4$ $k=3$	65230.027122566(−1.104401774)
392	$h=5$ $k=2$	72546.258370895(−1.104401217)
432	$h=6$ $k=1$	88354.229380725(−1.104309518)
	*With defects	88354.190665226[a](−1.104318141)
482	$h=4$ $k=4$	110318.139920155(−1.104483525)
492	$h=7$ $k=0$	115006.982258289(−1.104182025)
	$h=5$ $k=3$	115005.255889700(−1.104498410)
522	$h=6$ $k=2$	129655.833007858(−1.104477761)
	*With defects	129655.326253464[b](−1.104562742)
572	$h=7$ $k=1$	156037.879346228(−1.104383422)
	*With defects	156037.222417655[b](−1.104479462)
612	$h=5$ $k=4$	178910.494981768(−1.104554921)
632	$h=6$ $k=3$	190937.233325601(−1.104561653)
642	$h=8$ $k=0$	197100.363816212(−1.104289432)
	*With defects	197098.532524683[b](−1.104514589)
672	$h=7$ $k=2$	216171.432658341(−1.104528136)
	*With defects	216171.227524558[c](−1.104551687)
732	$h=8$ $k=1$	256975.527362500(−1.104436225)
	*With defects	256973.838562012[b](−1.104606771)
752	$h=5$ $k=5$	271362.588212841(−1.104598730)
	*With defects	271361.125880198[b](−1.104740553)
762	$h=6$ $k=4$	278704.548699996(−1.104608500)
	*With defects	278704.428077126[c](−1.104619969)
792	$h=7$ $k=3$	301321.818305597(−1.104604201)
	*With defects	301320.370436992[b](−1.104734120)

[a]Reference [16].
[b]Reference [24].
[c]This work.

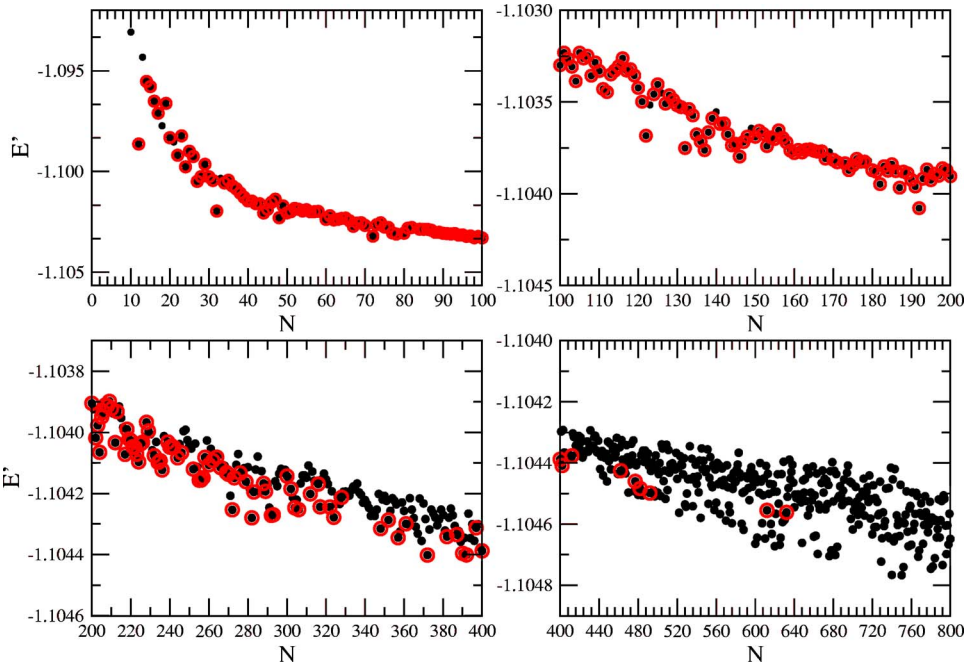

FIG. 2. (Color online) $E'=(2E-N^2)/N^{3/2}$ vs N. E' is defined using Eq. (1). Energies are plotted with black dots and are encircled in grey (red online) if the associated presumed global minimum energy configuration has no dislocation defects.

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. (ii) Are there defect free global energy minimum configurations we have not yet found, either for N not listed in Table I, or even lower energy defect free configurations for N in Table I? Dodgson and Moore [17] 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 prediction [16,20–23], 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 [16] that the approach 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. [16] 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 and verified that even for general N for a configuration that is dislocation defect free, but not necessarily highly symmetric, still one can consider the energy cost of a pair of pentamers. As the energy cost of a pair of vertices will not be lower for a nonsymmetric configuration than for a symmetric configuration—as in a nonsymmetric 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. As we can see from Fig. 1 and Table I that for $N \approx 250-300$ defect free global minima become increasingly scarce. This data may help guide future theoretical work on Thomson's problem.

Analysis by another group [23,25] discussed that adding defects produces configurations as N grows with lower energies than defect free configurations. They made exact quantitative predictions only for icosadeltahedral N for $k=0-N=10h^2+2$, that the global minimum configuration with defects for this series will appear for $N > 300$. As we have discussed previously [16], this prediction is remarkably accurate with the first such configuration appearing for $N=362$. It is interesting that $\approx N$ is also in the region of the N we have found where for general N configurations with defects become the norm for presumed global minima.

Thus, we do not expect any defect free global energy minima for $N > 1000$, and likely few even in the $N \sim 500-1000$ range. So, numerical searches to finalize the catalogue of defect free global energy minima should be focused on the $\sim 100-500$ range (for $N \leqslant 100$ there have been sufficient numerical and theoretical work [6–15] 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] 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 [21,22,26], 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

$$E = \frac{1}{2}(N^2 - 1.106\,103\,3N^{3/2}), \tag{1}$$

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. Equation (1) has been also obtained using other techniques by a number of authors [27–29]. As N grows large, in accordance with Eq. (1), $E'=(2E-N^2)/N^{3/2}$ approaches $-1.106\,103\,3$. Previous numerical calculations for $N\leqslant 200$ yielded a value -1.1046 for the constant coefficient of the $N^{3/2}$ term [29,33], though this is clearly seen to be exceeded for $N\gtrsim 600$ (Fig. 2). Furthermore, a configuration with $N=151\,52$ and $E'=-1.105\,623\,21$ has been found [21]. 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 to be 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.

Two very recent papers have looked analytically at the Thomson problem for large N [30,34]. The results we give here (Fig. 2) provide support for the first of these [30] which suggests that for asymptotically large N, E converges to $1.106\,103\,3$ with the charges approaching the crystalline state. The other paper [34] predicts a phase transition for some large N to a different final state.

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