Symmetric patterns of dislocations in Thomson's problem

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Determination of the classical ground-state arrangement of N charges on the surface of a sphere (Thomson's problem) is a challenging numerical task. For special values of N we have obtained, using the ring-removal method of Toomre, low-energy states in Thomson's problem that have icosahedral symmetry. Lines of dislocations run between the 12 disclinations which are induced by the spherical geometry into the near triangular lattice that forms on a local scale. [S0163-1829(99)02643-0]

Thomson's problem consists of finding the ground state of N Coulomb charges confined to move on the surface of a sphere. While this problem is simple to specify its solution is not. It has been studied by many authors; see Refs. 1–8 and references therein. On a local scale, charges are disposed like those on a triangular lattice and each charge has six nearest neighbors. On the other hand, Euler's theorem guarantees the existence of at least 12 fivefold disclinations (charges with only five nearest neighbors) on the sphere. More precisely, if v_i is the number of charges with i nearest neighbors, then

$$\sum_i (6-i)v_i = 12. \tag{1}$$

There exist methods to place the charges in configurations with just 12 disclinations, each of which is at the corners of an icosahedron, see Ref. 7. Those configurations are called icosadeltahedral and only exist when N is given by

$$N = 10(h^2 + hk + k^2) + 2, \tag{2}$$

with h and k integers.

It was suggested in Ref. 7 that these configurations might be the ground states of Thomson's problem. Further work showed, however, that configurations with dislocations (bound pairs of fivefold and sevenfold disclination) have less energy than icosadeltahedral configurations,[6,8] as lines of dislocations emanating from the disclinations act to screen the disclinations by reducing their strains fields.[9] However, we were unable to find any patterns of icosahedral symmetry containing dislocations.[6] It is the purpose of this Brief Report to show that such patterns can be found if one uses the ''ring-removal'' technique of Toomre.[10]

Each disclination in an icosadeltahedral configuration is surrounded by rings of $5n$ charges, where n is the order number of the ring. By removing the charges in one of these rings and then relaxing the energy of the system it is possible to obtain a configuration with five dislocations symmetrically disposed around the disclination. Removing several rings we can get lines of dislocations which act to screen the disclination as predicted by Dodgson and Moore.[9] One must be careful how one chooses the rings to be removed; if one removes consecutive rings the final configurations are not usually symmetric. In Fig. 1 we have plotted an icosadeltahedral configuration with $h=k=20$, i.e. 12 002 charges, after removing the third and seventh rings around each disclination. This type of initial configuration was used in conjunction with standard numerical procedures (mostly the conjugate gradient method) to minimize the interaction energy E of the Coulomb charges with each other.

It is possible to estimate the total number of rings n_r to be removed around each disclination (but not the actual ring numbers themselves, unfortunately) as follows. In Fig. 2 are shown examples of regions (which we shall refer to as facets) for icosadeltahedral configurations which naively one would expect to have three equal sides but which cannot achieve this because of the spherical geometry.

Let us denote by A and A' the length of the equal sides of the facets and B the remaining one. $A=A'<B$. These

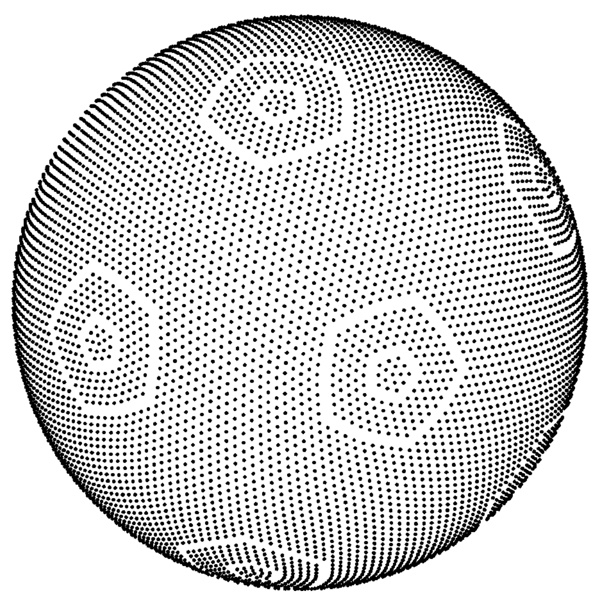
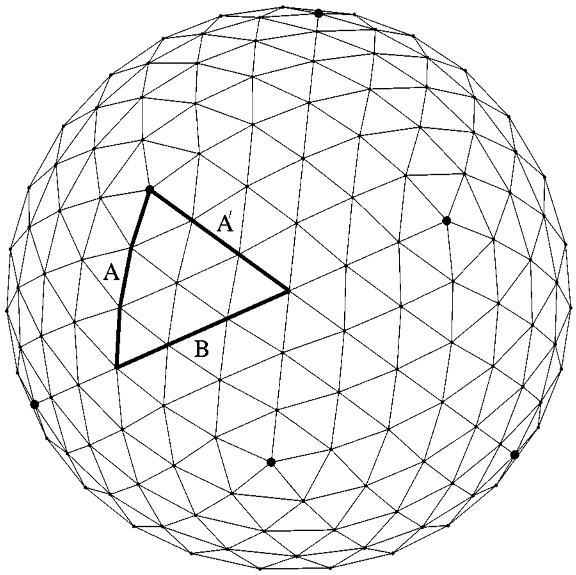


FIG. 1. Initial configuration with the third and seventh rings removed for an initial icosadeltahedral with 12 002 charges ($h=k=20$).



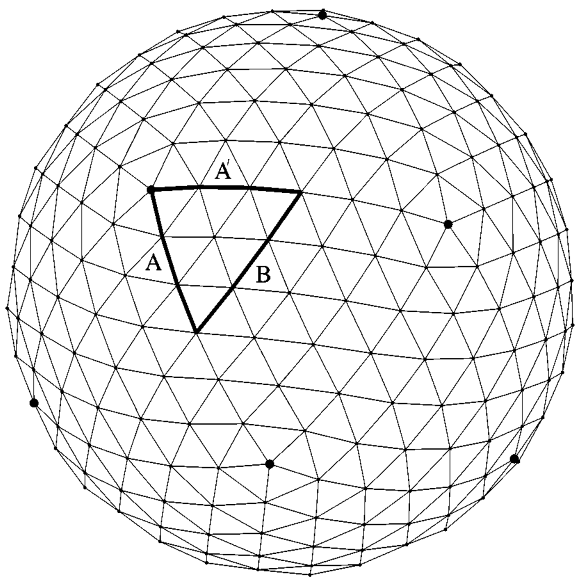


FIG. 2. Icosadeltahedral configurations for low number of particles. Disclinations are represented by solids dots. Each line links two nearest-neighbors particles. Thicker lines indicate a region (facet) which would be equilateral but for the spherical geometry, for the cases $h=k=3$ (figure at the top) and $h=6$, $k=0$ (figure at the bottom).

lengths can be calculated by simple geometric arguments. For the case $h=k$ one has

$$A=R\tan^{-1}\left(\frac{\alpha/2}{\cos\frac{2\pi}{10}}\right), \tag{3}$$

and

$$B=R\cos^{-1}(1-0.690\,983\sin^2 A/R), \tag{4}$$

where R is the radius of the sphere and α is the angle between two neighboring disclinations, where

$$\alpha=2\tan^{-1}\left(\frac{\sqrt{5}-1}{2}\right). \tag{5}$$

TABLE I. This table shows the smallest value of h at which the number of rings to be removed should be increased by one and n_r, the total number of rings to be removed for particle numbers $N=30h^2+2$, $(h=k)$ in the original icosadeltahedral state.

$h=k$	N	n_r
5	752	1
15	6752	2
24	17 282	3
34	34 682	4
43	55 472	5
52	81 122	6
62	115 322	7
71	151 232	8

For $h>k=0$, A is given by

$$A=\frac{R\alpha}{2}. \tag{6}$$

One should note that the above is only exact for h even. When h is odd, A is slightly larger but since the difference tends to zero as h increases we shall not take it into account.

To triangulate each facet one subdivides A and B into D_A and D_B segments, respectively. In Fig. 2 D_A and D_B are both equal to 3, but this need not be the case for larger values of N. To find the number of rings to take out, n_r, one requires that A/D_A be as close as possible to B/D_B, since then the spacing between charges will be most uniform, thereby minimizing the strain field energy caused by the spherical geometry. The difference between D_A and D_B is then the number of rings to remove, n_r. With this in mind we obtain the following expression for n_r:

$$n_r=\mathrm{Round}\left[\left(1-\frac{A}{B}\right)D_B\right], \tag{7}$$

where the function Round$[x]$ gives the closest integer to x. D_B is related to the number of particles N by the relation

$$D_B=\sqrt{\frac{N-2}{p}}, \tag{8}$$

TABLE II. This table shows the smallest value of h at which the number of rings to be removed should be increased by one and n_r, the total number of rings to be removed, for particle numbers $N=10h^2+2$, $(k=0)$ in the original icosadeltahedral state.

h, $(k=0)$	N	n_r
5	1002	1
13	6762	2
22	19 362	3
30	36 002	4
38	57 762	5
47	88 362	6
55	121 002	7
64	163 842	8

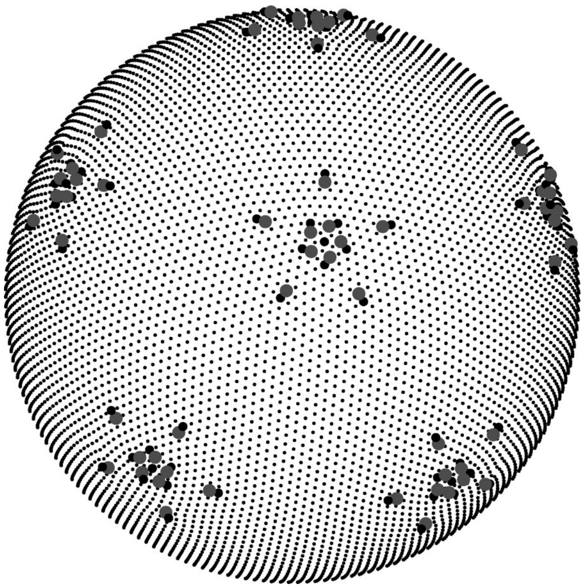


FIG. 3. 11 342 charges after relaxation ($h=k=20$, 12 002 charges minus the second and ninth rings, hence minus 660 charges) Largest spots correspond to seven-fold disclinations, medium spots represent five-fold disclinations and smallest spots are normal six-fold coordinated charges. $E_i=-1.105\,589\,42$.

for the case $h=k$, $p=30$ while for $h>k=0$, $p=40$. Thus, within this approximation, one is able to estimate out how many rings to remove for given h and k. In Tables I and II we show for both cases the value of N at which n_r changes its value. These estimates of N are consistent with our observations on systems with up to 16 000 particles. We have not studied the general case $h>k>0$ as it is difficult to identify the facets to triangulate.

We next describe how we are going to report our values for this energy. Using Ewald sums one can calculate the energy for charges on an infinite-plane triangular lattice[11] and deduce that for the sphere with unit radius and for unit charges[1]

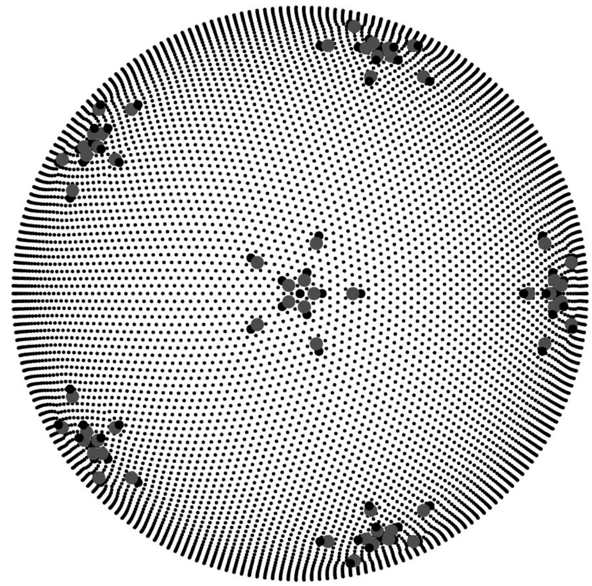


FIG. 5. 15 152 charges after relaxation ($h=k=23$, 15 872 charges minus the third and ninth rings, hence minus 720 charges). $E_i=-1.105\,619\,17$.

$$2E=N^2-1.106\,103\,3\ldots N^{3/2}+\cdots, \tag{9}$$

as $N\to\infty$. It is useful, therefore, to study E_i given by

$$E_i=\frac{2E-N^2}{N^{3/2}}, \tag{10}$$

which will approach $-1.106\,103\,3\ldots$ as $N\to\infty$. We will refer to E_i as the ''energy'' of the system.

We examine first configurations with $h=k$. For them the final configurations obtained after energy relaxation following ring removal have dislocations on the lines between the disclinations as envisaged in Ref. 6. Figure 3 is an example of a configuration with ($h=k=20$, 12 002 charges) minus

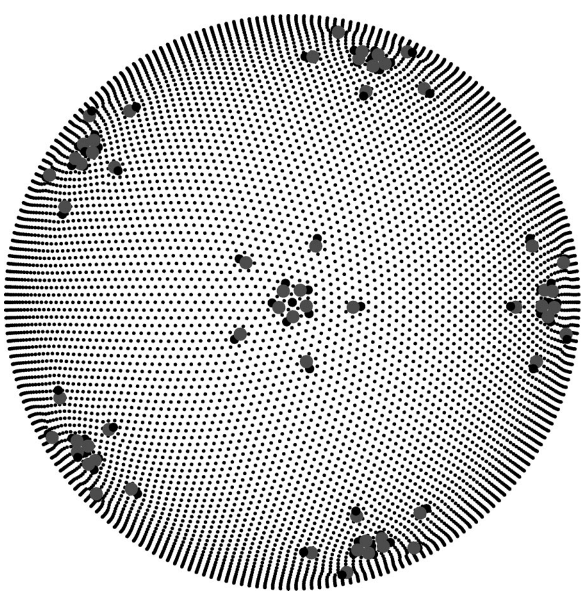


FIG. 4. 15 152 charges after relaxation ($h=k=23$, 15 872 charges minus the second and tenth rings, hence minus 720 charges). $E_i=-1.105\,623\,21$.

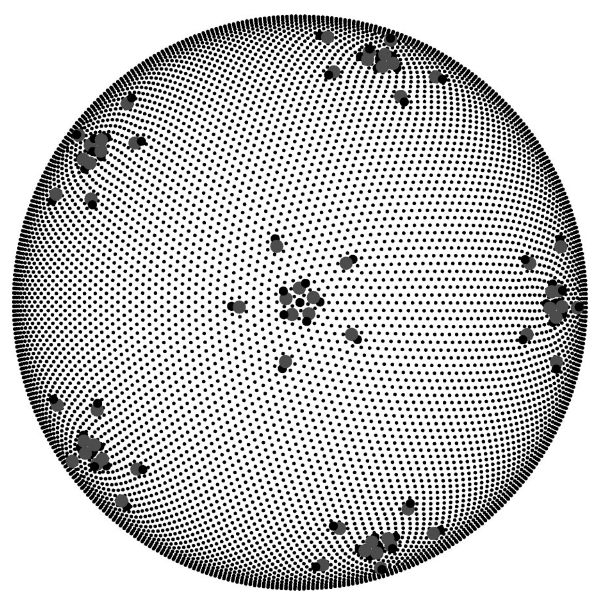


FIG. 6. 15 282 charges after relaxation ($h=40$, $k=0$, 16 002 charges minus the second and tenth rings, hence minus 720 charges). $E_i=-1.105\,610\,47$.

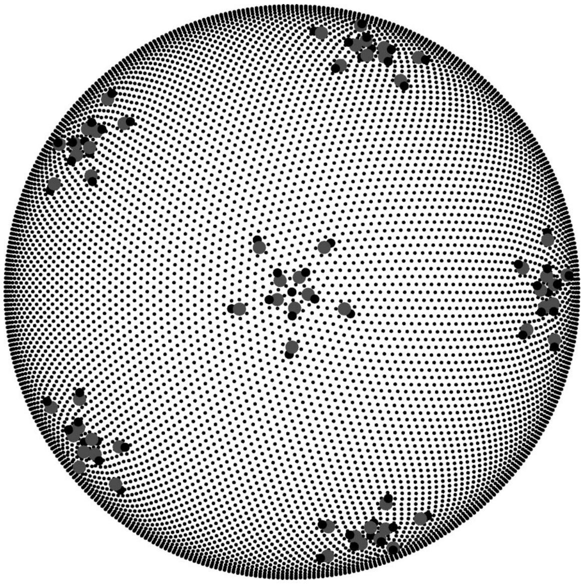


FIG. 7. 15 282 charges after relaxation ($h=40$, $k=0$, 16 002 charges minus third and ninth rings, hence minus 720 charges). $E_i=-1.105\,611\,47$.

the second and ninth rings, which means the removing of 660 charges, around each disclination so containing 11 342 charges. The largest spots correspond to sevenfold disclinations, the medium spots represent fivefold disclinations, and the smallest spots are normal sixfold coordinated charges. The final energy obtained is $E_i=-1.105\,589\,4$. In Figs. 4 and 5 we have plotted ($h=k=23$, 15 872 charges) minus the second and tenth rings in the former and minus the third and ninth rings in the latter. In both cases 720 charges are removed so the system contains 15 152 charges. The final energies obtained after relaxation is $E_i=-1.105\,623\,1$ and $E_i=-1.105\,619\,17$, respectively. Dislocations obtained by removing the second ring are bent forming pentagonal ''buttons''[10] as in Figs. 3 and 4. Figure 5 is very similar to the kind of pattern which was suggested in Ref. 6.

When $h\neq k$, the dislocations obtained after removing rings are not on the lines between disclinations but between these lines. The resulting patterns are therefore of lower symmetry. In any of these three cases, dislocations place themselves onto a line rotated an angle θ from the line between disclinations given by

$$\cos\theta=\frac{(h+k)(1+\cos 2\pi/5)}{\sqrt{(h^2+k^2+2hk\cos 2\pi/5)(2+2\cos 2\pi/5)}}. \tag{11}$$

In Figs. 6 and 7 we study ($h=40$, $k=0$, 16 002 charges) minus the second and tenth rings in the former and minus the third and ninth rings in the latter, hence minus 720 charges so we have a system with 15 282 charges.

In conclusion, we have demonstrated that for certain values of N there are low-energy arrangements of the charges that have full icosahedral symmetry. For these special values of N Thomson's problem seems to reduce to the much simpler task of finding which rings when removed minimize the energy. Unfortunately there is no known way of proving that that they are the global ground-state configurations.

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