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MINIMUM-ENERGY POINT CHARGE CONFIGURATIONS ON A CIRCULAR DISK

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Abstract: Stochastic global optimization methods are used to find configurations of n point charges on a circular disk such that the potential energy is minimized. Previously such optimal or conjecturally optimal configurations have been published for $n \leq 23$ and $n = 29, 30, 50$. In this work configurations for $n \leq 80$ are presented.
Keywords: point charge configurations, potential energy minimization.

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Contents

1 Introduction

The question what is the minimum-energy configuration of n equal point charges on a circular disk was raised in 1985 by A. A. Berezin [7]. To his surprise it appeared that in the optimal configuration not all the charges are located on the circle boundary when $n \geq 12$ (for proofs of this fact, see [28, 33, 43, 49]). In his opinion, the charges on a circular disk behaved differently from those in a conducting sphere, where all charges are on the surface in optimal configurations [16].

Berezin's conclusion "This may lead to some modification of usual theorems of electrostatic stability ... " [7] got many replies where this statement was refuted, although some of these replies based their argumentation on Earnshaw's theorem, which probably should not be used any more in scientific literature [4, 5].

MacGowan [32] pointed out that when Berezin's example is interpreted correctly as a thin three-dimensional disk, the charges actually are on the surface; now the charge in the center of the disk is necessarily on one of the two flat sides of the disk. If one wants to develop a theory of two-dimensional electrostatics, a different potential must be used [29, 32], for example that between infinitely long parallel charged lines, in which case the charges will lie on the circle boundary [16]. Berezin's original note was further criticized in [37].

In [15, 16] it was shown that a (non-optimal) configuration of 17 charges where two charges are placed in the interior of the circle has lower energy than the configuration with 16 charges evenly spaced on the circle boundary and one in the center of the circle. When the number of charges approaches infinity, the problem tends to the well-known problem of charge distribution over a conducting disk [38]. On a conducting circular disk of unit radius the charge density is proportional to $(1 - r^2)^{-1/2}$, where r is the distance from the center of the disk [41]. This is also the limit charge density, when a conducting ellipsoid is "flattened" to a thin circular disk [19].

1.1 Earlier Results

The first calculations to find the globally optimal, least energy configurations for $n > 12$ were performed in [35] ($n \leq 20$), [41] ($n \leq 17$, $n = 29, 30$), and [58] ($n \leq 23$, $n = 50$). Wille and Vennik [58] used a simulated annealing algorithm (see also [54, 56]) and failed to find the globally optimal configurations for $n = 16, 17, 18, 21, 22, 23$, c.f. [59], which partly reflects the difficulty of this problem when n grows. Munera [35] failed to find the optimal solutions for $n = 17, 19, 20$ and the energy for $n = 18$ was inaccurate.

Since [59] no more tables or figures of (conjecturally) optimal charge configurations have been published. In this work we will partially fill that gap in the literature by presenting a number of conjecturally optimal, or conjectural *ground-state*, configurations of up to 37 charges and the best configurations found of up to 80 charges. We expect the vast majority of these configurations to be optimal, too.

The optimization methods that we have used can be classified as probabilistic global optimization methods [47], which cannot *guarantee* that the best solutions found are globally optimal. We must keep in mind that the number of variables in many problem instances of this paper is relatively high, thus we cannot expect that the current deterministic global optimization methods can solve this problem completely.

It appears that when the number of charges is increased there are many local optima with high potential barriers between them. An outline for a catastrophe theoretical model relating different locally optimal configurations has been presented in [11].

1.2 Related Problems

A related problem of packing charges on the surface of a sphere (or equivalently, in the sphere [16]) has been studied for a longer time, and it is known as Thomson's problem [53]. It is interesting to note that Berezin [7], incorrectly, considered it probable that similar ejection of a charge into the center of the sphere will occur when n is large enough, c.f. [6, 9]. A system, where one test charge is placed in the center of the conducting ball and the rest of the charges on the surface, is not stable and a slightest perturbation will result in a configuration where all the charges are on the surface [42].

For Thomson's problem many extensive tables exist in the literature. The first computer search for stable configurations was performed in the 50's by H. Cohn [17]. A few configurations were discussed in [34]. More solutions were published in the 80's [3, 24, 35, 51], but the most extensive tables have appeared in the last few years [1, 20, 21, 22, 25, 52]. As so often when trying to find global optima in a difficult multi-modal optimization problem, several conjectured global optima have turned out to be only local optima, see for example [1] and [2, 23]. Some authors restrict the solutions, or sometimes just the initial solutions, to have certain symmetries [21, 35], in which case the optimization problem may be significantly easier. But if the globally optimal configuration does not have such a required symmetry, then it cannot be found by that kind of a method. Examples can be found comparing [35] and [50, 51]. Hardin, Sloane, and Smith are preparing a book on spherical codes

[27], and they maintain tables containing the best currently known solutions to Thomson's problem. The tables are available in the World Wide Web through Neil Sloane's home page [46].

It is possible to consider other than Coulombic potentials when searching for optimal configurations in a sphere or on a circular disk [8, 10, 12, 15, 16, 48]. Leech [31] showed that on the surface of the sphere the only configurations which are in equilibrium under all laws of repulsion forces are those that have a rotational symmetry about every diameter through particles of the system, see also [34].

Other related problems are those of packing circles in a circle [26] or on a sphere [18, 30, 39], also in higher dimensions [55]. Packing equal circles can be thought of as finding optimal configurations for sets of points with a repulsion force which increases very rapidly as the distance decreases, i.e. the shortest distance determines the potential energy of the system.

Physical experiments have been made with equal parallel cylindrical bar magnets on an air table [40], where the potential is slightly different, because instead of d^{-2} the repulsion force is proportional (to a considerable degree of accuracy) to

$$\frac{1}{d^2} - \frac{d}{(d^2+h^2)^{3/2}},$$

where h is the distance between the point poles of the supposedly rigid magnetic dipole and d is the distance between the magnets. As noted in [40], this problem was studied experimentally already in the last century by A. M. Mayer. Experiments with small charged conductive balls were made in [13].

2 The Optimization Methods Used in This Work

We denote a point charge configuration by $C = \{\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_n\}$, where the points are confined into the unit circle, i.e. $\|\mathbf{p}_i\| \le 1$. The energy function to be minimized is

$$E(C) = \sum_{1\le i<j\le n} \|\mathbf{p}_i - \mathbf{p}_j\|^{-1}. \tag{1}$$

This corresponds to minimizing the potential energy when there is a Coulombic repulsion force between each pair of equal point charges.

Because (1) is a nonlinear, nonconvex function, the problem of finding global optima can be very hard. A related more general problem of determining the ground states of atom clusters with artificial central-body forces is NP-hard [57].

All the optimization algorithms that we have used in this work select a suitable set of initial solutions and then apply a local optimization algorithm to each solution. The algorithms described below can be regarded as probabilistic global optimization algorithms and they differ only in the selection of the initial solutions. In all the computations we have used a truncated Newton method `TN/TNBC` [36] as a local optimizer.

2.1 Algorithm A1: Multistart with Initial Solutions from the Infinite Case

In the first approach we simply take random initial solutions and perform a local optimization run for each solution; then we take the best solution found. This is the multistart algorithm.

When the number of charges n tends to infinity (it is assumed that the total charge is constant), the limit density of charges when the potential energy is minimized is

$$f(r) = \frac{K}{2\pi\sqrt{1-r^2}}, \tag{2}$$

where K is the total charge on the disk and r is the distance from the center of the unit radius disk [41]. In the first approach we take the random initial solutions from the distribution defined by $f(r)$.

Even this simple approach was able to find most of the configurations in Section 3, including all of those in [59] that were not found in [58].

Using the results found with this approach we can further develop the selection of initial solutions. When selecting the initial solutions, the number of points near the disk boundary is crucial, because if a charge is caught on the boundary, a strictly descent [44] local optimization algorithm cannot push it back inside the circle. In our opinion the failures in [58] (c.f. [59]) were caused mainly by high potential barriers between solutions with different number of points on the circle boundary.

If we manage to estimate reasonably well the number of charges on the boundary in the optimal configuration, we can use an initial solution with that number of charges on the boundary, thus reducing the number of variables and speeding up the optimization process considerably.

2.2 Algorithm A2: Multistart with Heuristic Initial Solutions

In the second approach we take the best configuration of n charges found so far and assume that the number of charges on the circle boundary (denote this

1. Set $k := 0$, choose $N > 0$ and $0 < \gamma \leq 1$.
2. Let $k := k + 1$.
3. Add N random samples to previously sampled initial solutions.
4. Select γNk lowest-energy samples of all Nk samples; this is the *reduced sample.*
5. Apply local optimization from each sample in the reduced sample except if there exists another sample with higher function value at a distance which is less than or equal to the threshold r_k.
6. If the stopping condition is not satisfied, repeat from 2.

Figure 1: Multi-level single linkage algorithm.

by $\widetilde{n}_0$) is approximately the same as in the (possibly still unknown) optimal configuration.

Now we form the initial solutions first by putting b, $\widetilde{n}_0 - \delta \leq b \leq \widetilde{n}_0 + \delta$, charges evenly spaced on the disk boundary, where δ is an integer constant reflecting our confidence in the quality of the solutions found so far. Then we distribute the remaining charges according to (2), when the number of the charges on the boundary is taken into account. In the computations we used $\delta = 6$; in no case the best configuration found (see Section 3) had a greater deviation from $\widetilde{n}_0$ than 2.

2.3 Algorithm A3: Multi-level Single Linkage

One weakness of the multistart algorithm is that it repeatedly performs optimization runs with samples that are in the same region of attraction [44]. One way of overcoming this problem is to store the samples and start a new optimization run only if no better sample has been sampled in the neighborhood of the new sample. This idea has been developed into the *multi-level single linkage* algorithm [45], hereafter MLSL.

As the third optimization approach in this paper we have used the reduced sample version of MLSL. The algorithm is depicted in Figure 1. The threshold value r_k for deciding whether a sample is "near" another sample is gradually decreased during the optimization run as the number of samples is increased. Note that even if at one time a local optimization run is not started from a certain sample, this decision may be revoked later when the threshold value has become smaller. It is necessary to store the results of the local optimization runs so that no more than one optimization run is applied to a single initial solution.

When using standard Euclidean vector norm as the distance function between solutions, we can get very high distances between solutions that are essentially the same, obtained from each other by permuting the points and rotating or reflecting the configuration.

The key idea in our adaptation of MLSL is a special heuristic distance function that tries to compensate the difficulties caused by different orientations of the solutions and different permutations of the points. Let us first consider different permutations of the points. We take two configurations, denote these by S and T, and for each point of the configurations we find the nearest neighbor in the other configuration. We get the distance function

$$d(S,T) = \sum_{i=1}^{n} \min_j \|\mathbf{s}_i - \mathbf{t}_j\|^2 + \sum_{i=1}^{n} \min_j \|\mathbf{t}_i - \mathbf{s}_j\|^2 ,$$

which clearly equals 0 if S and T are obtained from each other by just permuting the points.

Now two initial solutions (samples) S and T with the same number b of points on the circle boundary are compared by calculating the b rotations of S that make the boundary points coincide with those of T. Then we calculate the reflection of S, and after another n rotations we select the smallest distance between T and the rotations and reflections of S. Clearly, this approach gives distance 0 whenever S is a (possibly reflected) rotation of T. If S and T have different number of points on the circle boundary, they are considered having infinite mutual distance and thus the distance function partitions the solution space into disjoint subsets infinitely far from each other.

Unfortunately, with our heuristic distance function the critical distance r_k of [45] cannot be used. As the critical distance r between two solutions S and T we have used

$$r = c\left(\frac{\log p}{p}\right)^{\frac{1}{u}} ,$$

where u is the number of variables and a suitable value for the constant c is determined experimentally. The number of sampled initial solutions in the solution space partition containing S and T is denoted by p – we keep a separate critical distance for each partition. If S and T are in different partitions, then they are considered having infinite mutual distance and the value of r does not matter. Our method can be seen as if we were running an MLSL algorithm on each solution space partition in parallel, giving the computing resources to the most promising samples.

Table 1: Energies of the configurations.

n	E	n	E	n	E
12	59.575675	35	672.34218	58	2008.0682
13	71.807362	36	715.06832	59	2083.0334
14	85.347290	37	759.34275	60	2159.3584
15	100.22096	38	804.92000	61	2237.1926
16	116.45200	39	851.91130	62	2316.2518
17	133.81652	40	900.11872	63	2396.9504
18	152.47790	41	949.85158	64	2478.9810
19	172.49482	42	1000.8254	65	2562.5685
20	193.62980	43	1053.3045	66	2647.4781
21	216.17911	44	1107.0794	67	2733.9499
22	240.12168	45	1162.3304	68	2821.6862
23	265.20104	46	1218.9808	69	2910.8539
24	291.72783	47	1277.0070	70	3001.4558
25	319.66551	48	1336.3752	71	3093.5796
26	348.77089	49	1397.2009	72	3187.0854
27	379.35332	50	1459.5821	73	3281.8499
28	411.34431	51	1523.2092	74	3378.1982
29	444.54775	52	1588.2065	75	3475.8612
30	479.07957	53	1654.6578	76	3575.2077
31	514.91713	54	1722.6842	77	3675.7938
32	552.26974	55	1791.9737	78	3777.8992
33	590.80630	56	1862.6497	79	3881.4275
34	630.83438	57	1934.7385	80	3986.2335

The problem of determining a suitable stopping criterion is a very hard problem in global optimization. We have simply limited the number of samples and the number of local optimization runs; the algorithm stops when either of these limits are reached.

3 Results

The lowest-energy configurations of 12 to 80 charges found during this research are depicted in Figures 2 through 7.

The energies of the configurations are tabulated in Table 1, where E is the energy of the configuration. The best previously published energies for configurations with $n \leq 23$, $n = 29, 30$ [35, 41, 58, 59] coincide with the values in our table. In [58] a figure of a configuration of 50 charges was shown, but

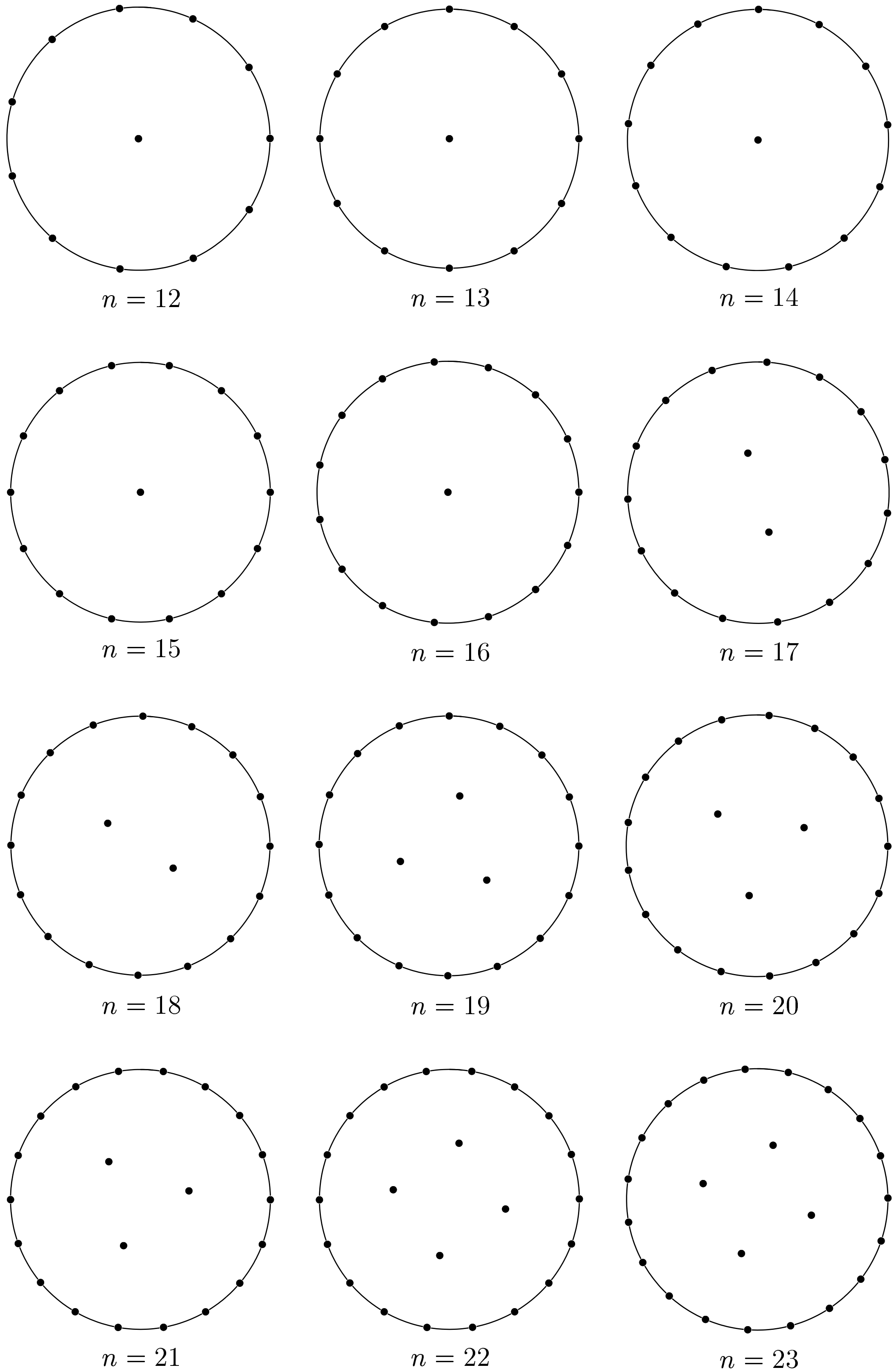

Figure 2: Configurations of 12 to 23 charges.

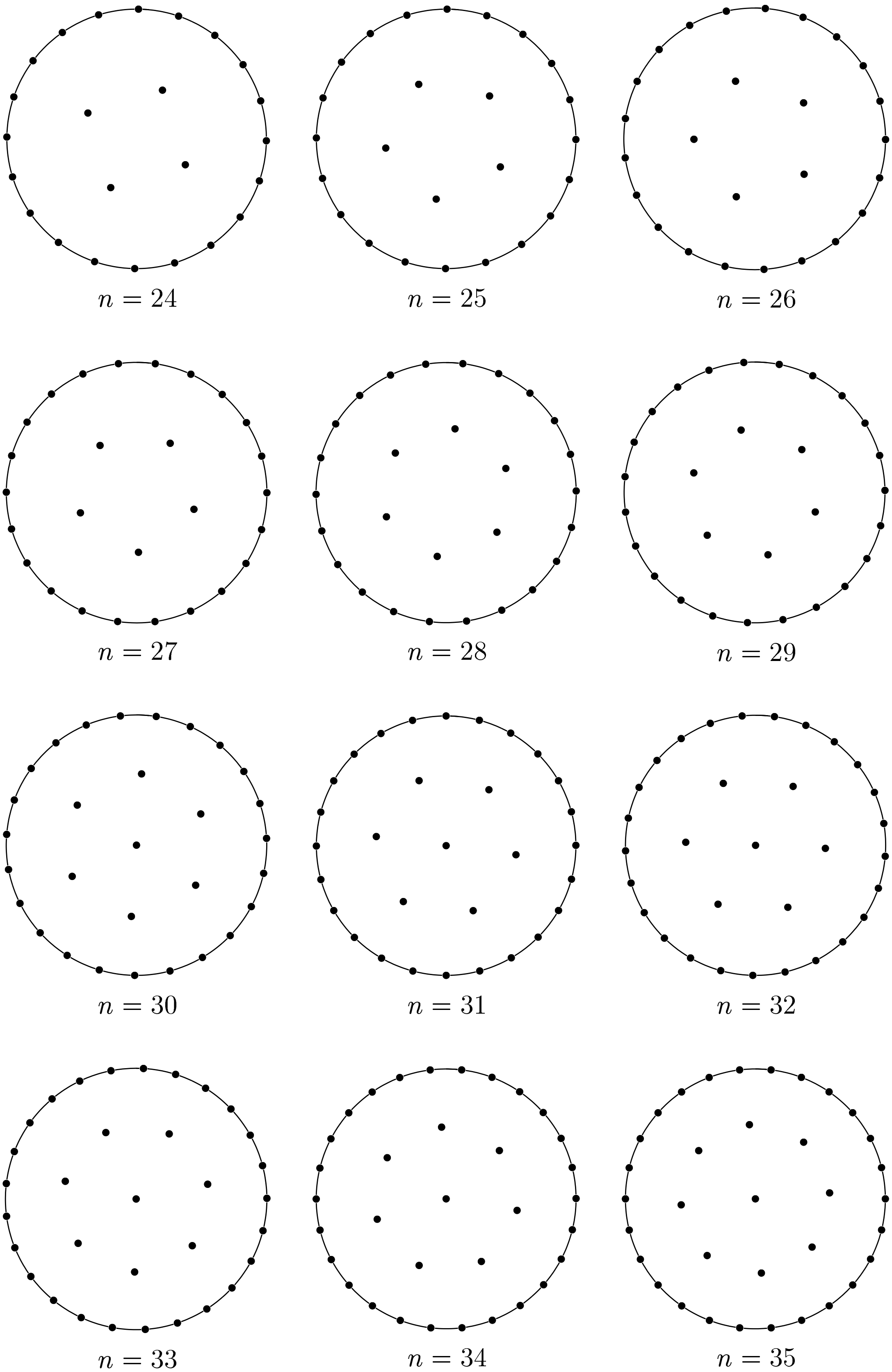

Figure 3: Configurations of 24 to 35 charges.

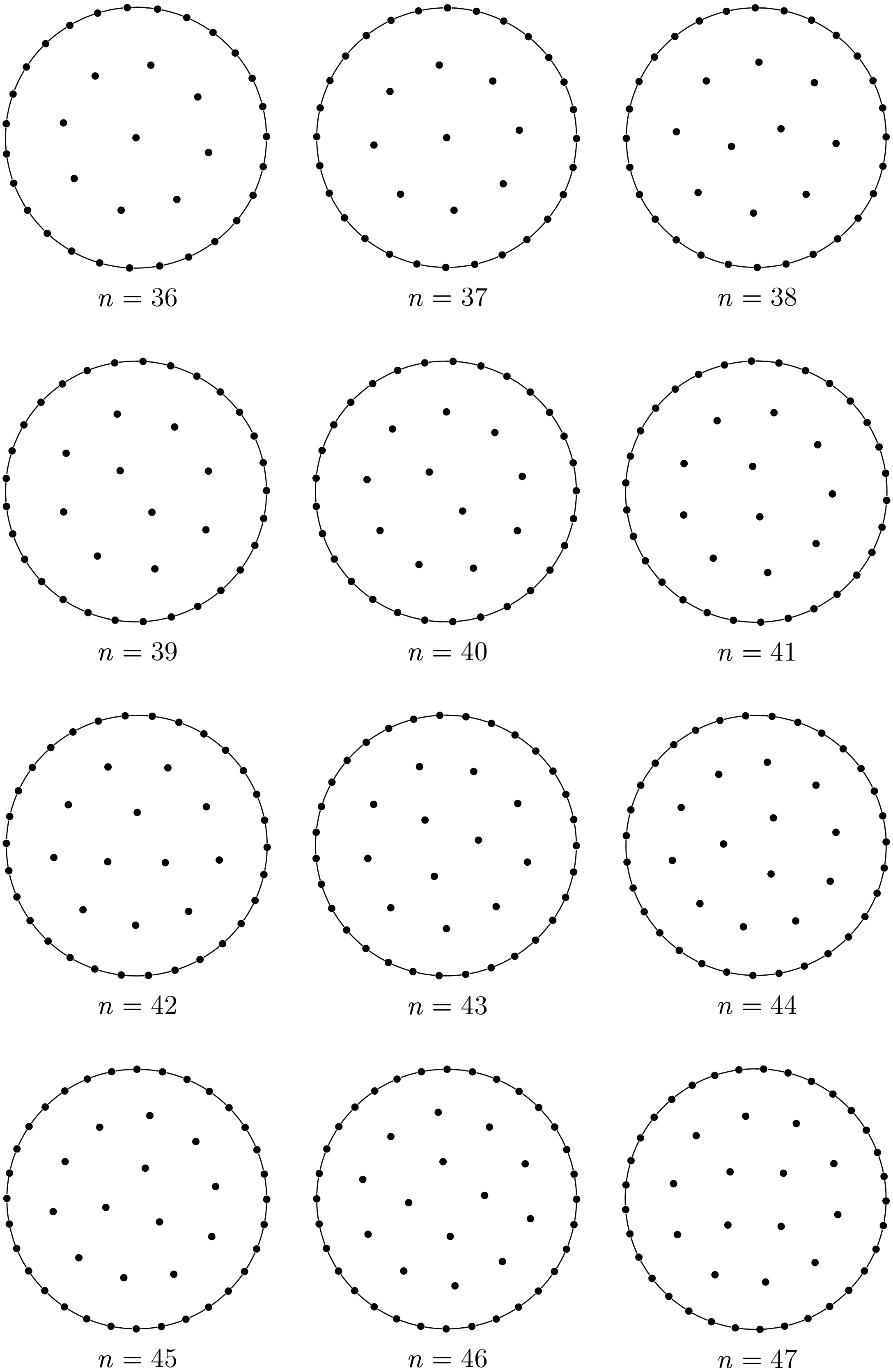

Figure 4: Configurations of 36 to 47 charges.

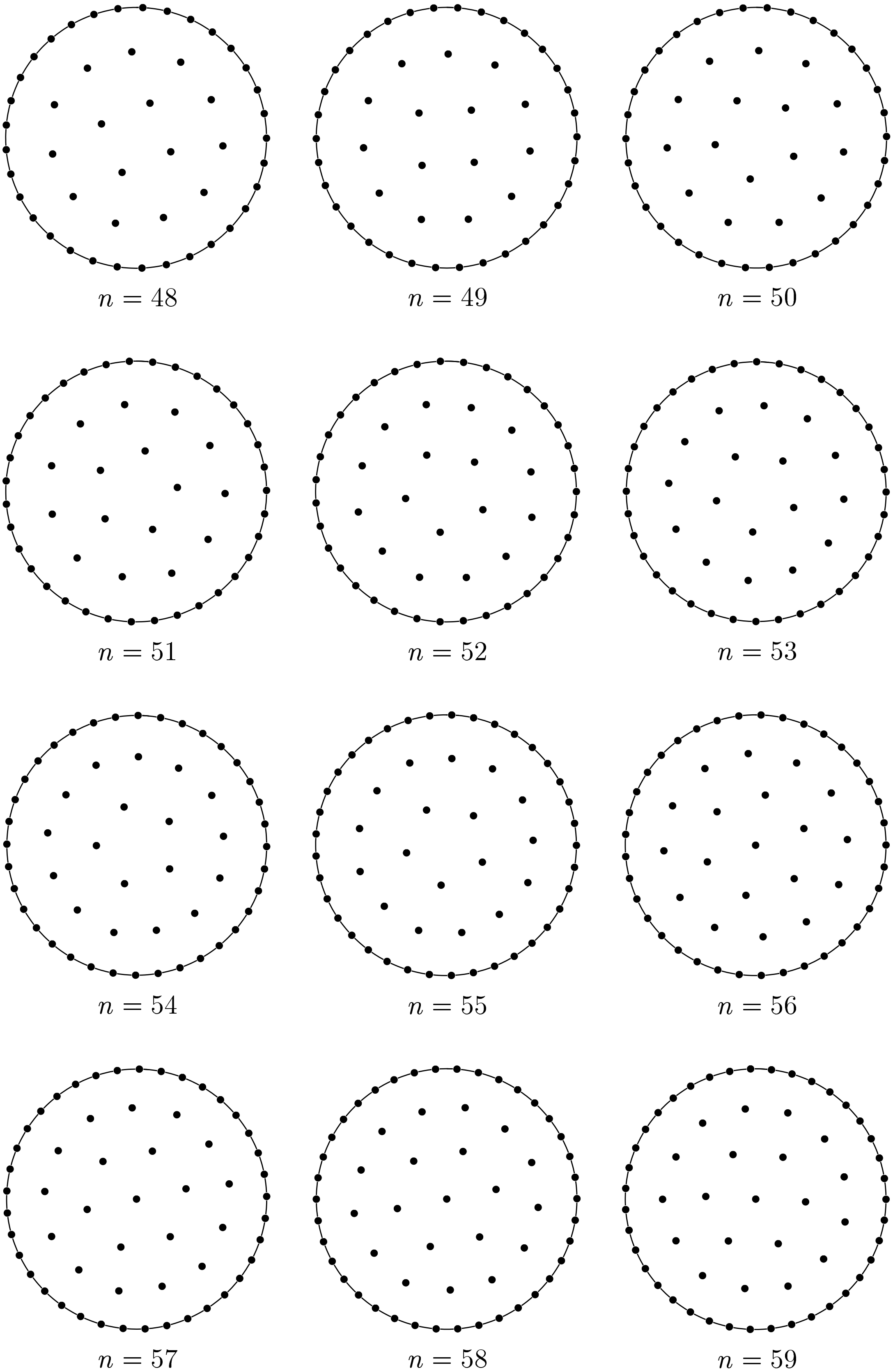

Figure 5: Configurations of 48 to 59 charges.

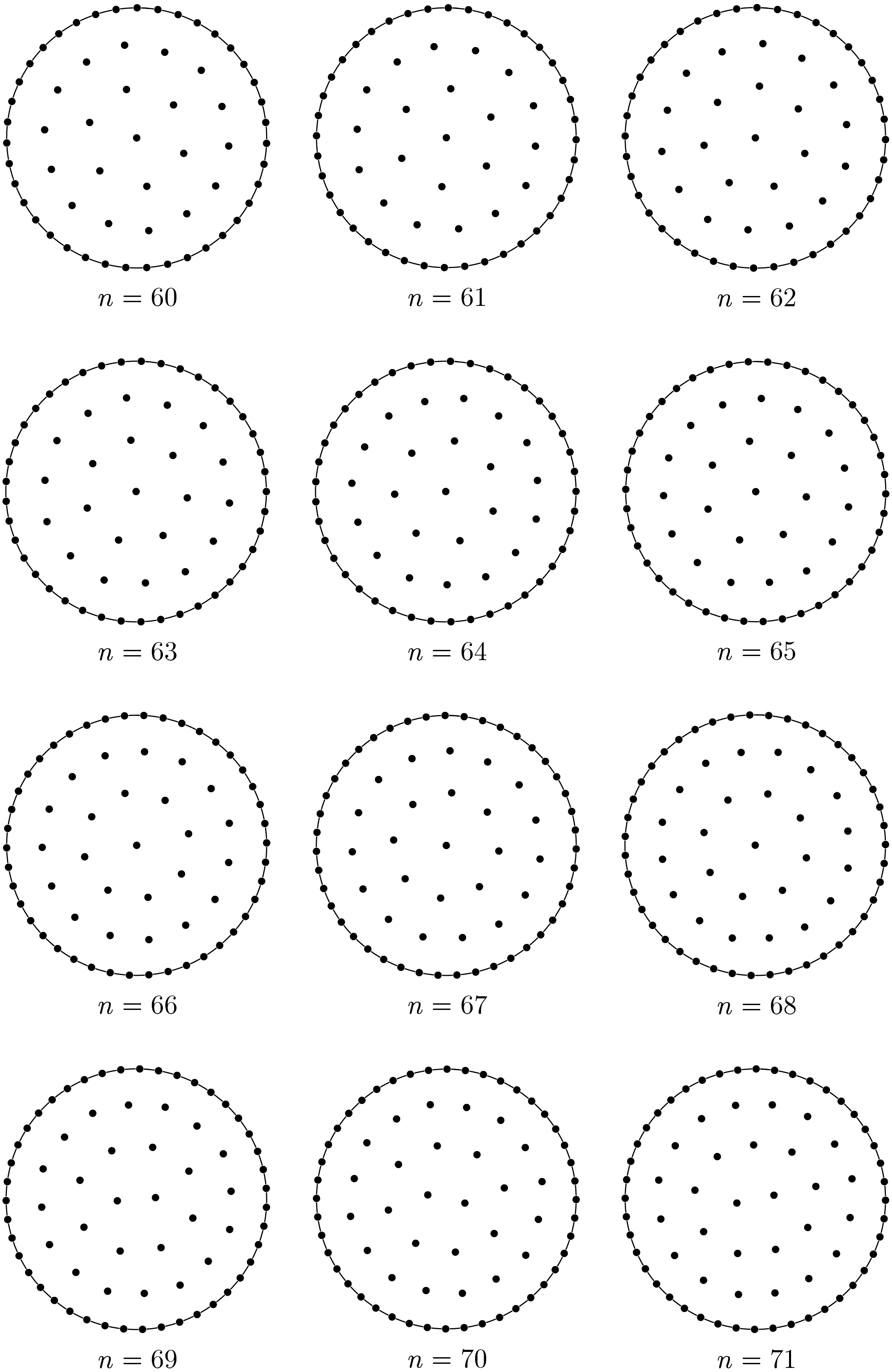

Figure 6: Configurations of 60 to 71 charges.

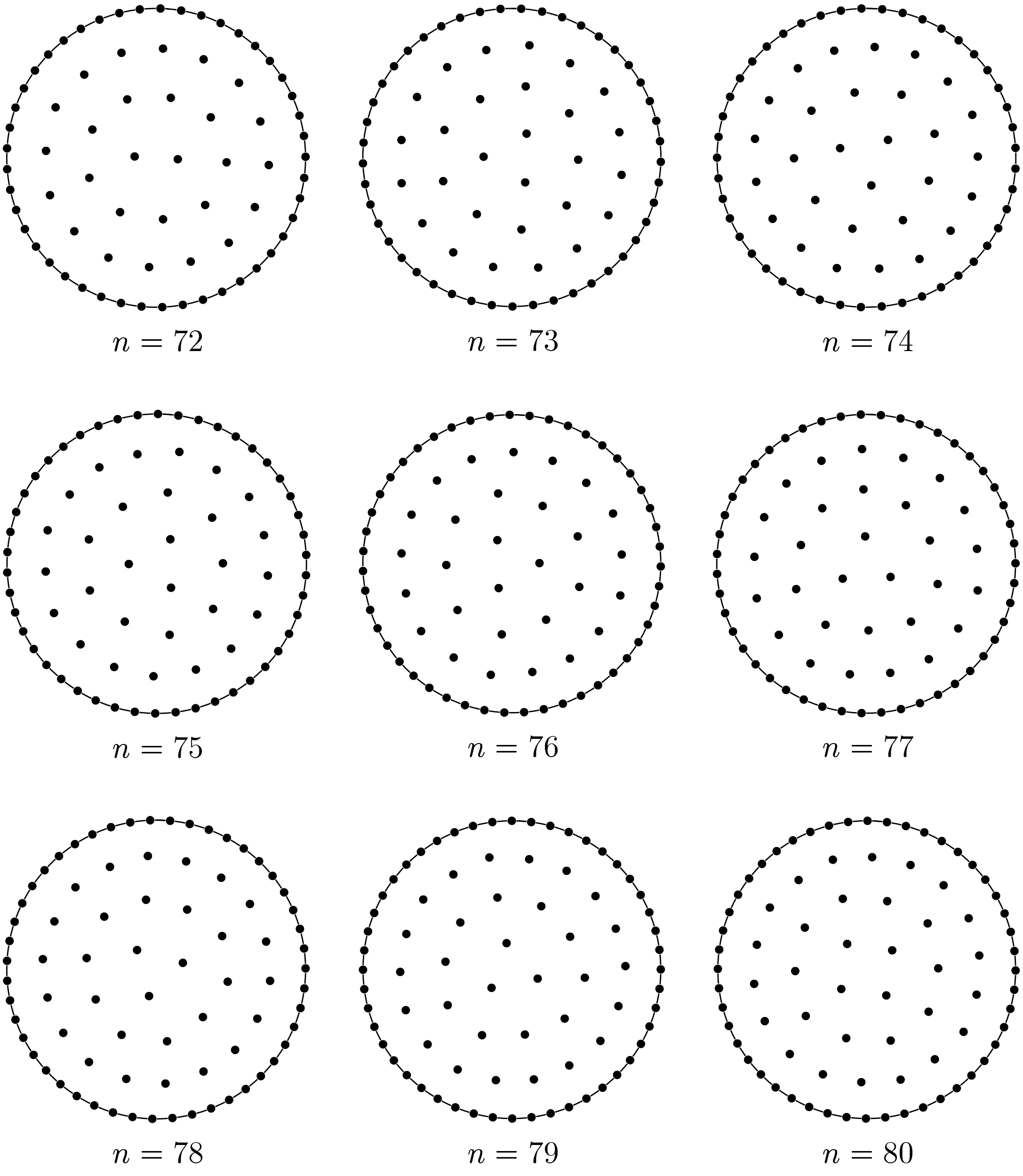

Figure 7: Configurations of 72 to 80 charges.

the energy was not given. By visual inspection the configuration looks similar to the one in Figure 5. No results have been previously published for other values of n.

Many of the configurations seem to have some kind of symmetries. However, since the optimization process can provide the coordinates of the points only with limited accuracy, the symmetries cannot be determined directly from the numerical results.

It would be very interesting to see how our MLSL approach works when the charges are confined in a sphere instead of a circular disk, but unfortunately the heuristic initial solutions and distance function cannot be easily extended to the case of a sphere.

When comparing the optimization algorithms of this paper we note that the multistart algorithm with heuristic initial solutions worked so well that it found all the configurations in Figures 2 through 7 except the configuration of 55 charges, which was found only by MLSL. However, fewer local optimization runs were needed when using MLSL, so it is clear that MLSL with a heuristic distance function is better when only a limited number of optimization runs can be performed. Our initial approach using multistart with initial solutions from the infinite case is clearly inferior to both of the more advanced approaches, but it is needed to provide an estimate for the number of charges on the disk boundary in the optimal case.

If the plane is filled with point charges with constant charge density, hexagonal lattice is the lowest-energy configuration [14]. However, when the charges are confined to a bounded area, the shape of the area determines the structure of the optimal configurations. It has been supposed that the optimal configurations on a circular disk consist of charges arranged in concentric rings, charges spaced evenly on each ring [41, 58]. Approximately, this seems to be the case in the configurations of this work, too. This observation can be used to construct special initial solutions consisting of a few concentric rings of charges [41, 59]. We have deliberately avoided this structure in the initial solutions, since it is not known how well this structure is preserved when n is increased.

It is interesting to find out which configurations in Figures 2 through 7 are in equilibrium under *any* law of repulsion. To do this we prove a theorem analogous to that in [31]. By "law of repulsion" we mean a repulsive force between two points that only depends on the distance between the points, i.e. the magnitude of the force between $\mathbf{p}_i$ and $\mathbf{p}_j$ is $v(\|\mathbf{p}_i - \mathbf{p}_j\|)$, where $v(d)$ is any function such that $v(d) \geq 0$ for all $d \geq 0$.

Theorem 1 *The configurations of $n \geq 2$ points on a circular disk that are in equilibrium under any law of repulsion are exactly*

1. *n points evenly spaced on the disk boundary, and*
2. *$n-1$ points evenly spaced on the disk boundary and one point in the center of the disk. In this case we require $n > 2$.*

Proof: A configuration is in equilibrium if and only if each of the points is in equilibrium, i.e. the resultant of the repulsive forces on the point is zero, or the point is on the circle boundary and the resultant is perpendicular to the tangent of the disk boundary at that point.

Assume for the rest of the proof that we have a configuration that is in equilibrium under any law of repulsion and thus all points are in equilibrium whatever the repulsion law may be.

The first part of the proof will show that there can be at most one point in the interior of the disk and if it exists, it must be located in the center of the disk. Let us assume that there is a point $\mathbf{p}$ not on the disk boundary. Now all the other points must be on one or more concentric circles centered in $\mathbf{p}$, we call these circles *shells*.

We can take the shell s with the greatest radius r around $\mathbf{p}$. This shell must clearly contain at least two points, because otherwise $\mathbf{p}$ would not be in equilibrium (take a potential function $v(d) = 1$, if $d = r$ and $v(d) = 0$ otherwise). Furthermore, if we take any 180° arc of the shell, it must contain at least one point. Now, suppose there were another shell around $\mathbf{p}$ apart from s, denote this shell by s'. This shell s' contains by definition at least one point $\mathbf{p}'$, see Figure 8. As noted before, there must be at least one point on the 180° arc of s directly across $\mathbf{p}'$ (shown bold in Figure 8). It follows that $\mathbf{p}'$ must have a shell s'' with radius r'' such that $r'' > r$, and because all the points are confined in s, there must be an empty arc greater than 180° on s''; thus $\mathbf{p}'$ is not in equilibrium under all repulsion laws.

Hence if there is a point $\mathbf{p}$ in the interior of the disk, then there must be at least 2 other points and they all must lie on a single circle whose center coincides with $\mathbf{p}$. Furthermore, this circle must coincide with the disk boundary, otherwise the points on it could not be in equilibrium under Coulombic repulsion force.

As the second step we show that the points on the disk boundary must be evenly spaced. As shown before, there must be at least two points on the boundary. We take two points on the boundary with the smallest mutual distance, let them be $\mathbf{b}_1$ and $\mathbf{b}_2$. Now if there is a point in the center of the

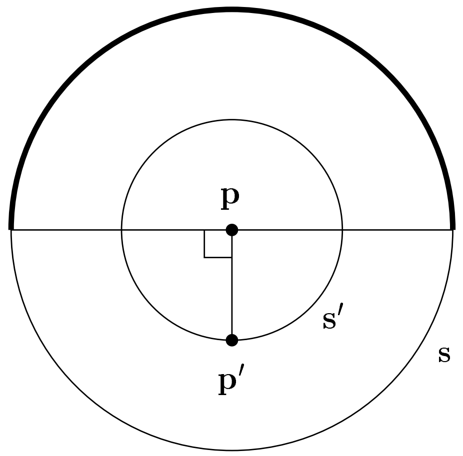

Figure 8: First part of proof.

disk, it cannot contribute any tangential force to the points on the boundary, so there must be a point $\mathbf{b}_3$ located on the boundary on the other side of $\mathbf{b}_2$ such that $\|\mathbf{b}_1 - \mathbf{b}_2\| = \|\mathbf{b}_2 - \mathbf{b}_3\|$. If such $\mathbf{b}_3$ does not exist, then $\mathbf{b}_2$ is not in equilibrium under repulsion force that varies according to $v(d) = 1$ when $d = \|\mathbf{b}_1 - \mathbf{b}_2\|$ and $v(d) = 0$ otherwise. Similarly we can infer the existence of $\mathbf{b}_4, \mathbf{b}_5, \ldots$ until $\mathbf{b}_i = \mathbf{b}_1$ for some i.

We have now shown that no such configuration that is in equilibrium under all repulsion laws exists except possibly the two types mentioned in Theorem 1. By symmetry considerations it is clear that all those configurations are in equilibrium under any potential that depends only on the distance between points. □

Using the theorem we find out that the best configurations of $n \leq 16$ charges are equilibrium configurations under any law of repulsion. They are also locally optimal circle packings, but of them only the configurations of up to 6 charges, all of type 1 in Theorem 1, are at the same time globally optimal circle packings (see [26] and its references). When $n = 6$ there exists another globally optimal packing of circles that is not a globally optimal charge configuration. We conjecture that the optimal circle packings and charge configurations are different for all $n > 6$.

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