Minimum perimeter rectangles that enclose congruent non-overlapping circles

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ABSTRACT

We use computational experiments to find the rectangles of minimum perimeter into which a given number, n, of non-overlapping congruent circles can be packed. No assumption is made on the shape of the rectangles. In many of the packings found, the circles form the usual regular square-grid or hexagonal patterns or their hybrids. However, for most values of n in the tested range $n \leq 5000$, e.g., for $n = 7, 13, 17, 21, 22, 26, 31, 37, 38, 41, 43, \ldots, 4997, 4998, 4999, 5000$, we prove that the optimum cannot possibly be achieved by such regular arrangements. Usually, the irregularities in the best packings found for such n are small, localized modifications to regular patterns; those irregularities are usually easy to predict. Yet for some such irregular n, the best packings found show substantial, extended irregularities which we did not anticipate. In the range we explored carefully, the optimal packings were substantially irregular only for n of the form $n = k(k + 1) + 1, k = 3, 4, 5, 6, 7$, i.e. for $n = 13, 21, 31, 43$, and 57. Also, we prove that the height-to-width ratio of rectangles of minimum perimeter containing packings of n congruent circles tends to 1 as $n \to \infty$.

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1. Introduction

Consider the task of finding the rectangular region of least perimeter that encloses a given number n of circular disks of equal diameter. The circles must not overlap with each other or extend outside the rectangle. The aspect ratio of the rectangle, i.e. the ratio of its height to width, is variable and subject to the perimeter-minimizing choice as well as the positions of the circles inside the rectangle.

Dense packings of circles in rectangles of a fixed shape, in particular, in squares, have been the subject of many investigations [3,5–7]; a comprehensive survey is given in [13], see also [12]. When the aspect ratio of the enclosing rectangle is fixed, the densest packing minimizes both the area and the perimeter of the rectangle. However, by allowing a variable aspect ratio, the two optima may differ for the same number of circles n. In 1970, Ruda relaxed the restriction of the fixed aspect ratio while trying to minimize the area, see [11]. He found the minimum-area packings of n congruent circles in the variably shaped rectangles for $n \leq 8$ and conjectured the minima for $9 \leq n \leq 12$. In [4], we extended Ruda's conjectures to $n \leq 5000$.

In this paper we switch our attention to minimizing the rectangle perimeter, while keeping the aspect ratio of the rectangle variable. We report the results of essentially the same computational procedure for finding the minimum-perimeter packings as the procedure used in [4] for finding the minimum-area packings. Even though the optima themselves are usually different, the structures of the set of optimal packings turn out to be very similar for the two minimization tasks.

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In either case for many n, the optimum pattern is regular, i.e. it is a square-grid pattern, or a hexagonal pattern, or a hybrid of these two patterns. One difference is that the occurrence of the non-regular patterns is more frequent in the minimum-perimeter case than in the minimum-area case: the smallest non-regular n for the minimum-perimeter criterion is $n = 7$ while that for the minimum-area criterion is $n = 49$ in [4]; for almost all n that are close to $n = 5000$ the minimum-perimeter packings are not regular while for the majority of n everywhere in the range $1 \leq n \leq 5000$, the regular packings still supply the minimum-area rectangles.

It appeared in [4], that if the minimum-area rectangular packing for a particular $n \leq 5000$ is not regular, then the minimum could be obtained by a small and easy-to-predict, localized modification to a regular pattern. In the case of the minimum perimeter, modifications of the same type apparently supply the optima for most numbers of circles n in the studied range $n \leq 5000$ for which the minimum-perimeter rectangular packing happens not to be regular. But not for all such numbers! For certain exceptional numbers of circles n, the packing pattern with the smallest perimeter we found is complex and/or requires extended modifications to a regular pattern.[1] A further surprise was that these exceptionally irregular packings, their patterns being complex and unpredictable, seem to occur quite predictably. In particular, in the range $n \leq 62$ which we explored carefully, our experiments detected such irregular packings only for n of the form $n = k(k+1)+1$, i.e. for $n = 13, 21, 31, 43$, and 57. The best packings for larger terms n of this sequence, i.e. for $n = 73, 91, \ldots$, are probably similarly irregular, although we could not test that as thoroughly as for the smaller terms because the computational resources needed for such a testing grow very rapidly with n.

Most of our findings are unproven conjectures, the outcome of computer experiments. We do not know why the exceptionally irregular values of n appear along the sequence $n = k(k+1)+1$ and only speculate by suggesting a possible reason. A few facts which we can prove are explicitly stated as being provable.

2. Computational method

To obtain the minimum-perimeter packing conjectures we use a variant of the computational technique employed in [4] for generating the minimum-area packing conjectures. The technique consists of two independent algorithms: the restricted search algorithm and the "compactor" simulation algorithm. We now review these procedures.

The restricted search algorithm operates on the assumption that the desired minimum is achieved on a set of configurations which is much smaller than the set of all possible configurations. The set is restricted to include only hexagonal patterns, square-grid patterns, their hybrids, and the patterns obtained by removing some circles from these patterns. For a given number of $n > 0$ circles, a configuration in the restricted set R_n is defined by 6 integers:

w, the number of circles in the longest row,

h, the number of rows arranged in a hexagonal alternating pattern,

h_-, those among the h hexagonally arranged rows that consist of $w - 1$ circles each; the rest $h - h_-$ rows consist of w circles each,

s, the number of rows, in addition to h rows, that are stacked in the square-grid pattern,

s_-, those among the s square-grid rows that consist of $w - 1$ circles each; the remaining $s - s_-$ rows consist of w circles each,

v, the number of "mono-vacancies" or holes.

The numbers must be non-negative and must satisfy the following additional restrictions:

$w > 0, h + s > 0, s_- \leq s, s_- < s + h, h \neq 1, v \leq \min\{w, h + s\} - 1$,

if h is even, $h = 2k$, then h_- can take on only two values $h_- = 0$ or $h_- = k$,

if h is odd, $h = 2k + 1$, then h_- can take on only three values $h_- = 0$ or $h_- = k$ or $h = k + 1$.

Finally, the total number of circles must equal n,

$$w(h + s) - h_- - s_- - v = n. \tag{1}$$

A "general case" example is shown in Fig. 2.1. As further examples, we now identify the 6-tuples (w, h, h_-, s, s_-, v) for some configurations presented in the following sections. In each example that follows, the unmentioned parameters of the tuple are equal zero.

In Fig. 5.1:

configuration "1 circle" has $w = s = 1$;

configuration "2 circles" has $w = 2, s = 1$; it can also be identified as having $w = 1, s = 2$;

configuration "4 circles" has $w = s = 2$;

configuration "6 circles" has $w = 3, s = 2$; it can also be identified as having $w = 2, s = 3$;

configuration "9 circles" has $w = s = 3$;

configuration "11 circles" has $w = 4, h = 3, h_- = 1$;

configuration "12 circles" has $w = 4, s = 3$; it can also be identified as having $w = 3, s = 4$;

configuration "15 circles" has $w = 4, h = 3, h_- = 1, s = 1$;

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[1] We now realize that similar exceptions might also exist in the case of minimizing the area. See the footnote in Section 6 for an example.
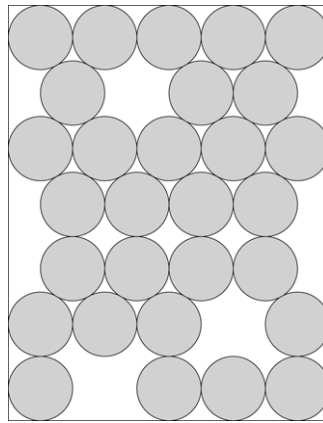
Fig. 2.1. A configuration in the restricted set R_n for $n = 29$ circles; here $w = 5, h = 5, h_- = 2, s = 2, s_- = 1$, and $v = 3$, so that $29 = w(h + s) - h_- - s_- - v$.

configuration "19 circles" has $w = 5, h = 3, h_- = 1, s = 1$.
In Fig. 3.1:
    configuration a has $w = h = 3, h_- = 2$;
    configuration b has $w = 2, h = 3, h_- = 1, s = 1$;
    configuration c has $w = h = 3, h_- = 1, v = 1$.
In Fig. 3.2:
    configuration a has $w = 4, h = 5, h_- = 2, v = 1$;
    configuration c has $w = 5, h = 6, h_- = 3, v = 1$.
In Fig. 5.2:
    configuration a has $w = 13, h = 16, h_- = 8$;
    configuration b has $w = 29, h = 7, h_- = 3$.
Given the values of w, h, h_-, and s, and that of the common radius of the circles r, the height H, width W, and perimeter P of the enclosing rectangle can be found from

$$H/r = 2s + \begin{cases} 2 + (h - 1)\sqrt{3} & \text{if } h > 0 \\ 0 & \text{if } h = 0 \end{cases} \tag{2}$$

$$W/r = 2w + \begin{cases} 1 & \text{if } h > 0 \text{ and } \quad h_- = 0 \\ 0 & \text{if } h = 0 \text{ or } \quad h_- > 0 \end{cases} \tag{3}$$

$$P = 2(W + H). \tag{4}$$

Note that this ratio P/r is a number of the form $x + y\sqrt{3}$, where the non-negative integers x and y are obvious functions of w, h, h_- and s.

Sometimes several different patterns correspond to a given tuple w, h, h_-, s, s_-, v; those may differ in the ways the s or s_- rows are attached or the v holes are selected. Since the shape and the perimeter of the enclosing rectangle do not change among these variations, the minimization procedure treats them all as the same packing.

An important fact is that for each $n > 0$, there are only a finite number of 6-tuples w, h, h_-, s, s_-, v, that satisfy the restrictions above. For a given value of n, our procedure lists all such 6-tuples, and for each of them computes P/r, and selects the configurations that correspond to the minimum value of P/r. By presenting the values P/r in the form $x + y\sqrt{3}$ with integers x and y, only comparisons among integers are involved and the selection of the minimum is exact.

The reader should be reminded that we do not claim that our restricted search procedure produces the global optimum for packing n circles in a rectangle. In fact, we include some configurations which are clearly non-optimal, for example, those with $v > 0$. The usefulness of the given definition of the sets R_n should become apparent when we compare below the restricted search algorithm outcomes with those of the "compactor" simulation algorithm.

The "compactor" simulation works as follow (see also [10]). It begins by generating a random starting configuration with n circles lying inside a (large) rectangle without circle–circle overlaps. The starting configuration is feasible but is usually rather sparse. Then the computer imitates a "compactor" with each side of the rectangle pressing against the circles, so that the circles are being forced towards each other until they "jam". Possible circle–circle or circle–boundary conflicts are resolved using a simulation of hard collisions so that no overlaps or boundary-penetrating circles occur during the process.

The simulation for a particular n is repeated many times, with different starting circle configurations. If the final perimeter value in a run is smaller than the record achieved thus far, it replaces the current record. Eventually in this process, the record stops improving up to the level of accuracy allowed by the double precision accuracy of the computer. The resulting packing now becomes a candidate for the optimal packing for this value of n.

The main advantage of the "compactor" simulation vs. the restricted search is that in the simulation no assumption is made about the resulting packing pattern. The circles are "free to choose" any final configuration as long as it is "jammed". This advantage comes at a price: the simulation time needed in multiple attempts to achieve a good candidate packing for a particular n is typically several orders of magnitude longer than the time needed on the same computer to deliver the minimum in set R_n by the restricted search procedure. For example, it may take a fraction of a second to find the minimum perimeter packing of 15 circles by the search in R_{15} and it may take days with thousands of attempts to produce the same answer by simulation.

3. Results: Regular and semi-regular optimal packings

Table 3.1 lists the packings of n equal circles in rectangles of the smallest found perimeter for each n in the range $1 \le n \le 62$, except $n = 13, 21, 31, 43,$ and 57. A somewhat arbitrary bound $n = 62$ was set so that the "compactor" simulation was performed for each $n \le 62$ but only for a few isolated values $n > 62$ since the simulation slows down significantly for larger n. On the other hand, the minimum perimeter packings in R_n were produced by the restricted search procedure for each $n \le 5000$.

All packings presented in Table 3.1 can be split into two sets. The first set consists of either perfectly hexagonal packings or perfectly square-grid packings or their hybrids. We will call these *regular* packings. A regular packing of n circles is characterized in Table 3.1 by the parameters $n, w, h, h_-,$ and s, as defined in Section 2. Note that the parameters s_- and v which are also defined in Section 2 are not present in Table 3.1. These s_- and v equal 0 for each regular packing.

Table 3.1
Packings of n circles in rectangles of the smallest found perimeter for all n in the range $1 \le n \le 62$, except $n = 13, 21, 31, 43,$ and 57

n	w	h	h−	s	δ	n	w	h	h−	s	δ	n	w	h	h−	s	δ
1	1	0	0	1	0	*22	5	5	2	0	δ_2	*41	6	7	0	0	δ_2
2	2	0	0	1	0	23	5	5	2	0	0	42	6	7	0	0	0
3	2	2	1	0	0	24	5	3	1	2	0	44	6	8	4	0	0
4	2	0	0	2	0	25	5	5	0	0	0	*45	7	7	3	0	δ_3
5	2	3	1	0	0	*26	5	6	3	0	δ_2	46	7	7	3	0	0
6	3	0	0	2	0	27	5	6	3	0	0	47	7	5	2	2	0
*7	3	3	1	0	δ_1	28	5	5	2	1	0	48	6	8	0	0	0
8	3	3	1	0	0		6	5	2	0	0	49	7	7	0	0	0
9	3	0	0	3	0	29	5	3	1	3	0	50	6	9	4	0	0
10	3	4	2	0	0		6	3	1	2	0	*51	7	8	4	0	δ_3
11	3	3	1	1	0	30	5	6	0	0	0	52	7	8	4	0	0
	4	3	1	0	0	32	5	7	3	0	0	53	7	7	3	1	0
12	4	0	0	3	0	33	6	6	3	0	0		8	7	3	0	0
14	4	4	2	0	0	34	6	5	2	1	0	54	6	9	0	0	0
15	4	3	1	1	0	35	5	7	0	0	0	*55	7	8	0	0	δ_3
16	4	0	0	4	0	36	6	6	0	0	0	56	7	8	0	0	0
*17	4	5	2	0	δ_2	**37	6	7	3	0	δ_1	*58	7	9	4	0	δ_4
18	4	5	2	0	0	*38	6	7	3	0	δ_3	59	7	9	4	0	0
19	4	3	1	2	0	39	6	7	3	0	0	60	8	8	4	0	0
	5	3	1	1	0	40	6	5	2	2	0	61	8	7	3	1	0
20	4	5	0	0	0		7	5	2	1	0	*62	7	9	0	0	δ_3

The packing patterns are described with parameters $w, h, h_-, s,$ and δ_i and with star markings as explained in the text.

For example, Table 3.1 lists two conjectured minimum-perimeter packings of $n = 11$ circles: one with $w = 3, h = 3, h_- = 1,$ and $s = 1$, and the other with $w = 4, h = 3, h_- = 1,$ and $s = 0$. The latter is perfectly hexagonal as seen in Fig. 5.1 (configuration "11 circles"). The former is a hybrid of hexagonal and square-grid packings. A similar hybrid is also the only conjectured minimum-perimeter packing of $n = 15$ circles which is listed in Table 3.1. It has parameters $w = 4, h = 3, h_- = 1,$ and $s = 1$ and it is shown in Fig. 5.1 (configuration "15 circles").

Given the parameters of a regular packing, one easily determines the shape and the perimeter of the rectangle that encloses the circles using formulas (2), (3) and (4). The perimeter for each conjectured minimum-perimeter packings of 11 circles is $20 + 4\sqrt{3}$ and for that of 15 circles $24 + 4\sqrt{3}$ in units equal to the common circle radius.

It will be convenient to define the shape of a rectangle by the ratio L/S where

$$L = \max\{H, W\}, \quad S = \min\{H, W\}, \tag{5}$$

so that

$$L/S \ge 1. \tag{6}$$

In these three examples, we have, respectively $L/S = (4 + 2\sqrt{3})/6 = 1.2440169\ldots$, for the first packing of 11 circles in Table 3.1;
$L/S = 8/(2 + 2\sqrt{3}) = 1.4541016,\ldots$, for the second packing of 11 circles in Table 3.1;
$L/S = 8/(4 + 2\sqrt{3}) = 1.0717968,\ldots$, for the packing of 15 circles.

Similar simple calculations can be done for all the other regular packings.

All entries n that correspond to regular packings are not marked by stars in the table. Now consider the other set of the packings, those with entries n that are marked by stars in the table. The smallest example is $n = 7$. The smallest perimeter rectangle that we could find (using the simulated "compactor" procedure) is that for configuration d in Fig. 3.1. Because this configuration does not fit the description in Section 2 of a possible pattern in R_7, the restricted search procedure cannot find the packing d. Instead, the best in R_7 happen to be the configurations a, b, and c. Having among them different aspect ratios of the enclosing rectangle, the configurations a, b, and c are of the same perimeter $P/r = 16 + 4\sqrt{3} = 22.928293\ldots$. Out of these three, the c requires the smallest number of circles to be moved and the smallest readjustment of the boundary to obtain the d. We move circles labeled in Fig. 3.1 as A, B, and C to turn the c into the d.
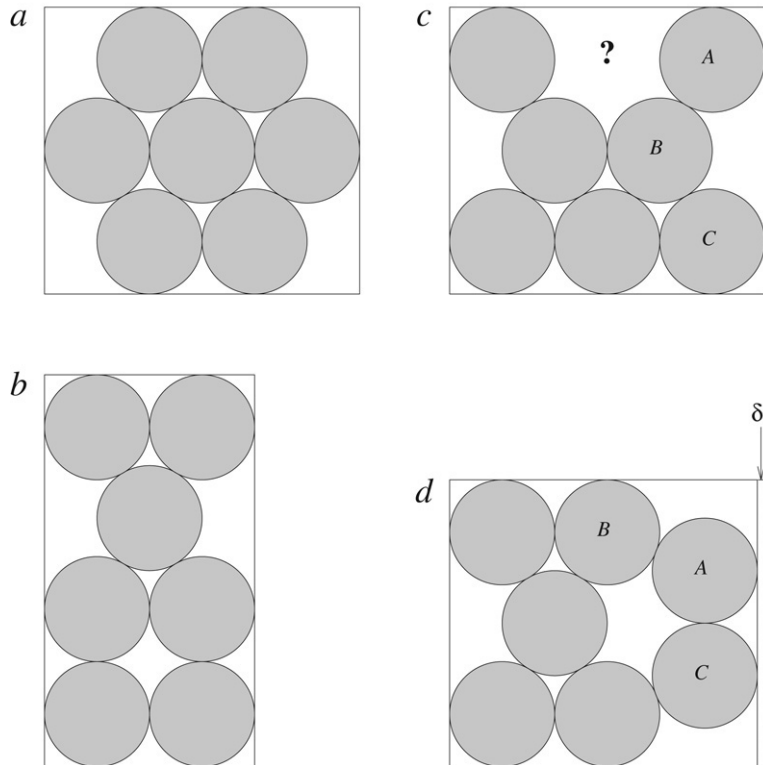

Fig. 3.1. Packings of 7 equal circles in the smallest perimeter rectangle: (a) among the hexagonal configurations, (b) among the hybrid configurations, (c) among the regular-with-holes configurations, (d) among all configurations tested. The perimeters of the rectangles of the packings a, b, and c are the same and are larger than the perimeter of the packing d.

For the entry $n = 7$, Table 3.1 lists parameters $w = 3$, $h = 3$, and $h_- = 1$ and those are of the configuration c. Also the entry is marked with one star which represents one mono-vacancy in the pattern c. The implied convention here is that this entry represents the configuration d because d, while not being describable in the terms of the table, can be obtained by a simple and standard transformation from c. (Note that the configuration c can be defined in several ways depending on the position of the hole; the resulting different configurations are not distinguished by the restricted search procedure or in the table.) As c is turned into d, the width of the rectangle decreases by the value $\delta = \delta_1$ where

$$\delta_1 = 2 - \sqrt{2\sqrt{3}}. \tag{7}$$

The smallest found perimeter for the 7 circles thus becomes

$$P^{opt}/r = P/r - 2\delta, \tag{8}$$

which is $22.650743\ldots$ here.

The δ will be called the *improvement* parameter. The equality $\delta = 0$ together with the absence of star markings distinguishes a regular packing entry in Table 3.1. On the other hand, the entries with $\delta = \delta_i > 0$, $i = 1, 2, 3$ or 4, in Table 3.1 correspond to packings that are not regular. The number of stars that marks the n for such an entry equals the number of mono-vacancies v in the packing according to the definition of class R_n in Section 2.

Figs. 3.2–3.4 show six other non-regular packings. Those are labeled b and d in each figure. Their regular-with-holes precursors, as found by the restricted search procedure, are the configurations which are labeled a and c in each figure. Note
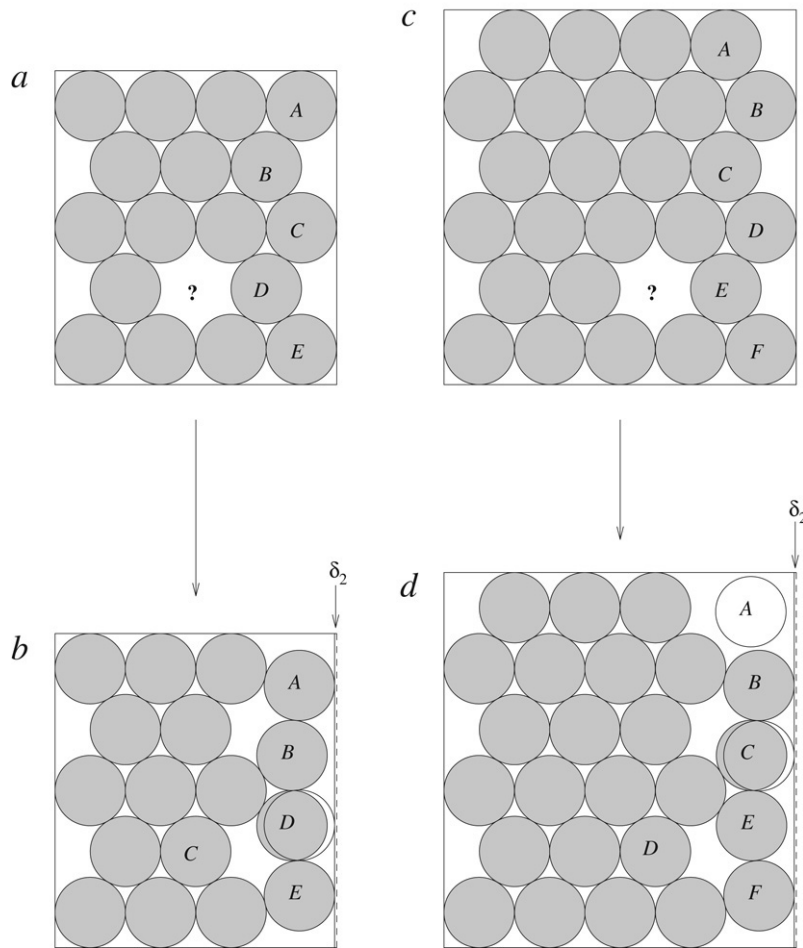
Fig. 3.2. Packings of 17 (*a* and *b*) and 26 (*c* and *d*) equal circles in rectangles. Packings *a* and *c* are the best in R_{17} and R_{26}, respectively. Packings *b* and *d* are the best we could find for their number of circles. Alternative equivalent positions of circles *D* in packing *b* and *C* in packing *d* are shown.

that the best found packings of $n = 17$ and $n = 26$ circles shown in the diagrams *b* and *d* in Fig. 3.2 are obtained from the best packings found by the restricted search procedure and shown, respectively, in the diagrams *a* and *c* in this figure, using improvement parameter $\delta = \delta_2$ where

$$\delta_2 = 2 - 0.5\sqrt{3} - 3^{1/4}(2\sqrt{3} - 1)/(2\sqrt{4 - \sqrt{3}}). \tag{9}$$

Also note that there are several equivalent ways of the improvement resulting in the same value of $\delta = \delta_2$. For example, circle *D* in Fig. 3.2*b*, can occupy an alternative position in which *D* contacts the right side of the rectangle instead of the unlabeled circle to its left while remaining in contact with circles *B* and *E*. This position is also shown in the figure. A similar equivalent re-positioning of circle *C* is shown in Fig. 3.2*d*.

The best found packing of $n = 38$ circles shown in Fig. 3.3*b* is obtained from the best packing found by the restricted search procedure and shown in Fig. 3.3*a* using improvement parameter $\delta = \delta_3$. The best found packing of $n = 58$ circles shown in Fig. 3.4*b* is obtained from the best packing found by the restricted search procedure and shown in Fig. 3.4*a* using improvement parameter $\delta = \delta_4$. The values of δ_i are given in Table 3.2. In the packing *a* shown in Fig. 3.4 and in all the previously discussed packing diagrams, the distances in circle–circle or circle–boundary pairs are zero whenever the circles in each pair are apparently in contact with each other. The packing *b* in Fig. 3.4 gives an exception to this rule: the distance between the circles *C* and *J* and that between the circles *G* and *K* is 0.05323824 . . . of the common circle radius, perhaps too small to be discerned as positive from the diagram.

Note that the δ-improvement of the configuration sometimes releases certain circles from the contacts with their neighbors. The released circles become the so-called *rattlers*. In Fig. 3.2, circle *A* becomes a rattler during the δ_2-conversion of the configuration *c* into the configuration *d*. In Fig. 3.3, circle *D* becomes a rattler during the δ_1-conversion of the configuration *c* into the configuration *d*. Rattlers are represented by unshaded circles in the packing diagrams.

In all the examples in Table 3.1, the δ-improvement of the configuration is localized: not counting the circles possibly used for covering the holes, all the circles involved in the change are located by the boundary on one side. During the change
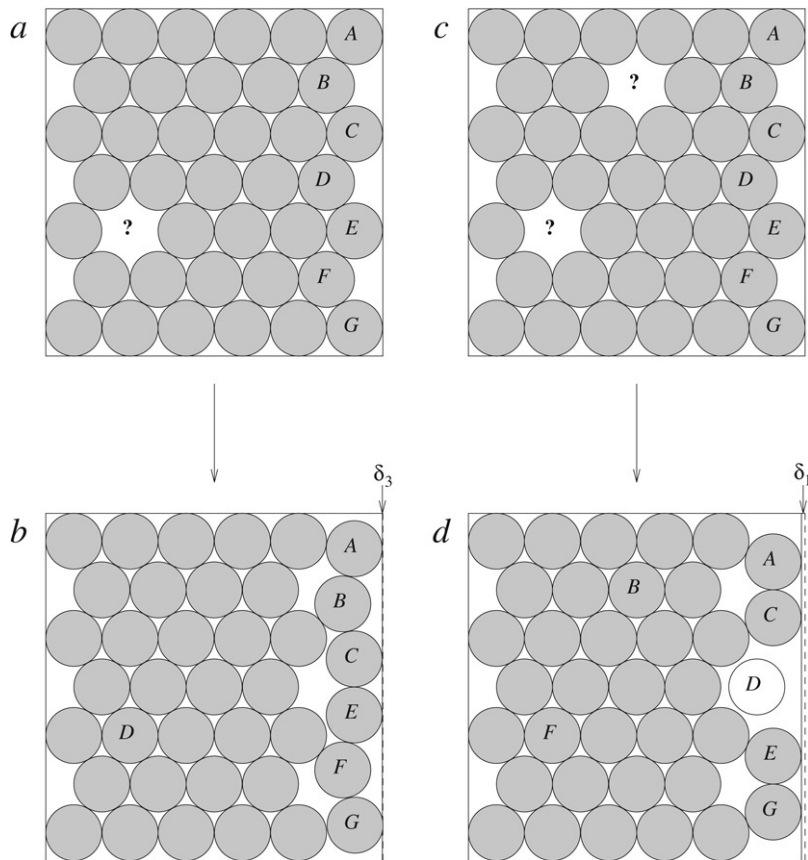
Fig. 3.3. Packings of 38 (*a* and *b*) and 37 (*c* and *d*) equal circles in rectangles. Packings *a* and *c* are the best in R_{38} and R_{37}, respectively. Packings *b* and *d* are the best we could find for their number of circles.

Table 3.2
Improvement parameters δ_i

i	δ_i	Defined or used in
1	0.13879028…	Eq. (7), Figs. 3.1*d*, 3.3*d*
2	0.05728065…	Eq. (9), Figs. 3.2*b*, 3.2*d*, 4.5*b*
3	0.01935364…	Figs. 3.3*b*, 4.3*b*, 4.4*b*, 3.4*d*
4	0.00403953…	Fig. 3.4*b*

the width of the rectangle decreases by δ while the height stays unchanged. The obtained packings, though non-regular, are close to their regular-with-holes precursors. We will call such non-regular packings *semi-regular*. All the non-regular packings listed by their regular-with-holes representations in Table 3.1 are semi-regular.

We skipped several values of n in Table 3.1. The best found packings obtained for the skipped n show more irregularity than the semi-regular packings do. These excluded from Table 3.1 packings will be called *irregular*. An irregular packing is defined by negation: it is a packing that cannot be generated by the described above simple adjustment where the circles that move are limited to those covering the holes and to those located at a side column of a regular-with-holes packing.

We conclude this section with the following observation. If among the best packings in R_n delivered by the restricted search there is at least one with holes, or if a non-regular packing of n circles is known with a smaller perimeter than of those best in R_n, then the packing of n circles in a rectangle of the minimum perimeter *provably* cannot have a regular pattern. That is, it cannot be purely hexagonal or purely square-grid or a hybrid pattern. Thus, the optimum packings for each star-marked semi-regular n in Table 3.1 cannot possibly be regular. We will see in the following section that the optimum packings for the irregular n, those skipped in Table 3.1, cannot be regular either: for each skipped n we will present a packing which is better than the record best in R_n.

4. Results: Irregular optimal packings

The smallest skipped entry in Table 3.1 is $n = 13$. Fig. 4.1*a* presents the only existing best in R_{13} packing as found by the restricted search procedure. The packing has $w = 3$, $h = 5$, $h_- = 2$. Its perimeter is $P/r = 16 + 8\sqrt{3} = 29.856406\ldots$. Since
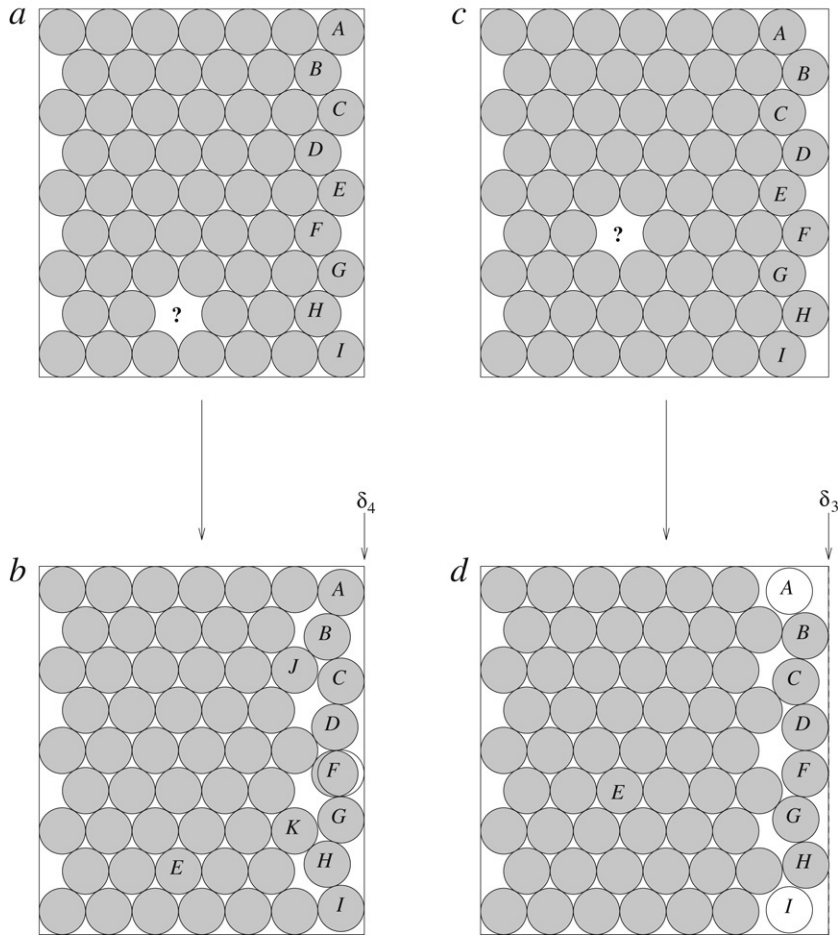
Fig. 3.4. Packings of 58 (*a* and *b*) and 62 (*c* and *d*) equal circles in rectangles. Packings *a* and *c* are the best in R_{58} and R_{62}, respectively. Packings *b* and *d* are the best we could find for their number of circles. A positive gap exists between circles *C* and *J* and also between circles *G* and *K* in packing *b*. An alternative equivalent position of circle *F* is shown in packing *b*.
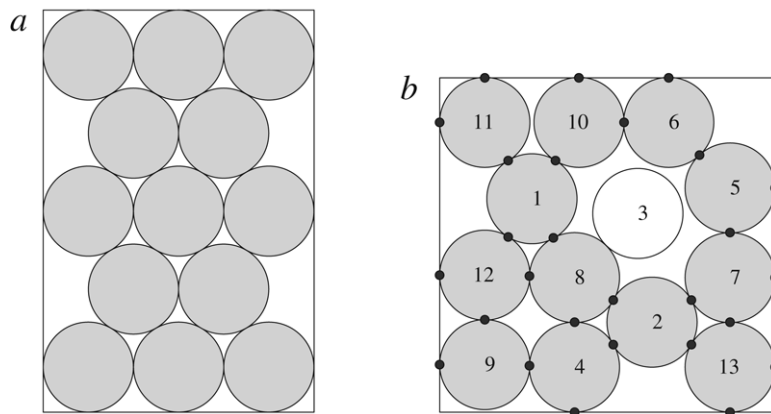

Fig. 4.1. Packings of 13 equal circles in rectangles: (*a*) with the smallest perimeter of the enclosing rectangle among the set R_{13}, (*b*) with the smallest perimeter of the enclosing rectangle we could find.

there is no hole in the packing, the case $n = 13$ would have qualified as a regular one and would have been listed as such with its parameters *w*, *h*, and h_- in Table 3.1 were it not for the "compactor" simulation. Unexpectedly for us, the "compactor" produced a better packing! That packing with the perimeter $P^{opt}/r = 29.851847510\ldots$ which is smaller than the perimeter of the packing *a* in Fig. 4.1 by at least 0.004 is the packing *b* shown in the same figure. The pattern of the packing *b* in Fig. 4.1
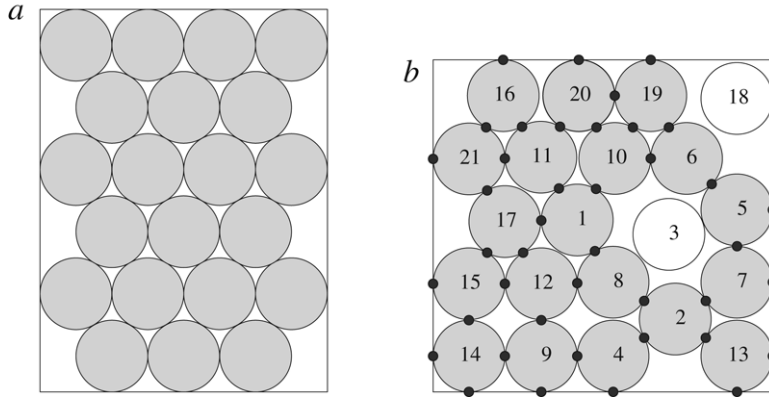
Fig. 4.2. Packings of 21 equal circles in rectangles: (*a*) with the smallest perimeter of the enclosing rectangle among the set R_{21}, (*b*) with the smallest perimeter of the enclosing rectangle we could find.
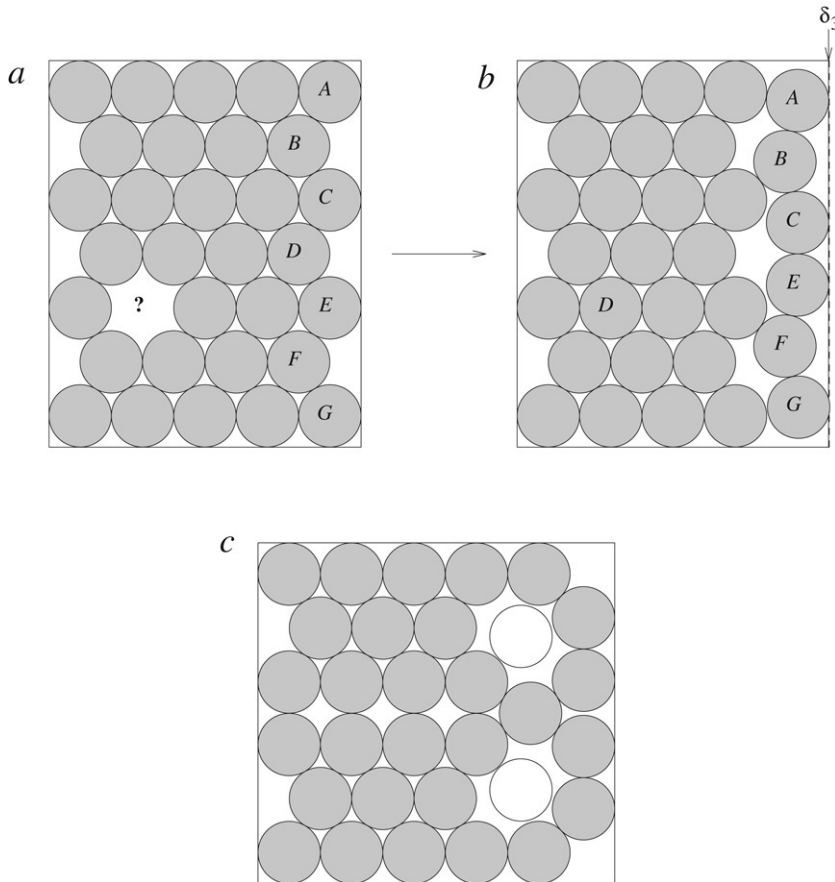

Fig. 4.3. Packings of 31 equal circles in rectangles: (*a*) with the smallest perimeter of the enclosing rectangle among the set R_{31}, (*b*) δ_3-improved packing *a*, (*c*) with the smallest perimeter of the enclosing rectangle we could find.

is truly irregular and non-obvious, unlike the straight-forward pattern of the packing *a*. Even the existence of the packing *b* should not be taken for granted. By contrast the existence of the packing *a* in Fig. 4.1 can be easily proven by construction and so can the existence of all the other regular and semi-regular packings discussed above.

The small black dots in the packing diagram *b* indicate the so-called *bonds* or contact points in circle–circle or circle–boundary pairs. A bond indicates the distance being exactly zero between the pair, while the absence of a bond in a spot of an apparent contact indicates the distance being positive, i.e. no contact. For example, there is no contact between circle 9 and the bottom boundary in the packing *b*. (The 13 circles are arbitrarily assigned distinct labels 1 to 13 in Fig. 4.1*b* to
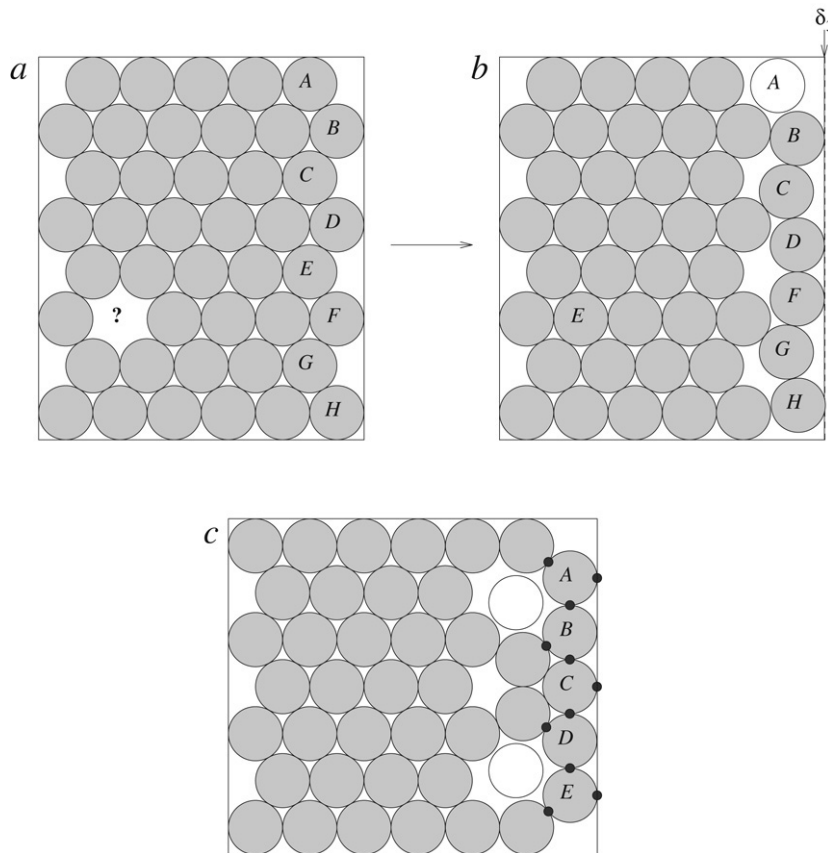
Fig. 4.4. Packings of 43 equal circles in rectangles: (*a*) with the smallest perimeter of the enclosing rectangle among the set R_{43}, (*b*) δ_3-improved packing *a*, (*c*) with the smallest perimeter of the enclosing rectangle we could find. The black dots indicate bonds of the labeled circles in the packing *c*.

facilitate their referencing.) No bond indication is needed in the diagram of the packing *a* in Fig. 4.1 nor in any other regular packing diagram because the points of apparent contacts are always the true contacts in such packings. In semi-regular packings such non-contacts do occur, for example the one between circles *C* and *J* in Fig. 3.4*b*.

With the explicit indication of the bonds, it is *provably* possible to construct the packing in Fig. 4.1*b* and this construction is *provably* unique, so the positions of all circles, except the rattler, and the rectangle dimensions are uniquely defined. The computed horizontal width and vertical heights of the packing in units equal the circle radius *r* are

$$W/r = 5.463267269314\ldots \qquad H/r = 5.462656485780\ldots$$

which implies the perimeter value given above and $L/S = 1.000111810716\ldots$ so the rectangle is almost a square to within about 0.01%.

Note that when in [4] we minimized the area of the rectangle we were unable to find packings better than, in the present paper terminology, either regular or semi-regular. The case $n = 13$ is a violation of such structure for the case of minimizing the perimeter. Suspicious of other such violations, we ran many more tries of the "compactor" simulation for $n = 14, 15, 16, 17, 18, 19$ and 20. No violation was detected. All these cases seem to be either regular or semi-regular as presented in Table 3.1. But for $n = 21$ we encountered another gross violation of regularity.

The case of $n = 21$ is similar to that of $n = 13$. Here again, the restricted search procedure delivers the best in R_{21} packing (shown in Fig. 4.2*a*) with $w = 4$, $h = 6$, $h_- = 3$ and perimeter $P/r = 20 + 10\sqrt{3} = 37.3205081\ldots$. The packing is regular and looks very different from the best packing found by the simulation (shown in Fig. 4.2*b*), the latter with the perimeter $P^{\mathrm{opt}}/r = 37.309294229\ldots$ which is smaller than the perimeter of the packing shown in Fig. 4.2*a* by at least 0.01. Same as in the case of $n = 13$, the best found packing for $n = 21$ exhibits a rather irregular structure, which makes the existence of the packing non-obvious. With the bonds shown in Fig. 4.2*a*, it is possible to *prove* the existence of the packing by construction and it is possible to *provably* uniquely determine the position of the circles, except the rattlers, the width, height and the L/S ratio of the rectangle:

$$W/r = 7.433745175630\ldots \qquad H/r = 7.220901938764\ldots \qquad L/S = 1.029475990489\ldots.$$

The patterns of both irregular best found packings, while being dissimilar to all the other conjectured optimum packings considered thus far, show some similarity between themselves. This similarity is emphasized by the circle labeling. Labels
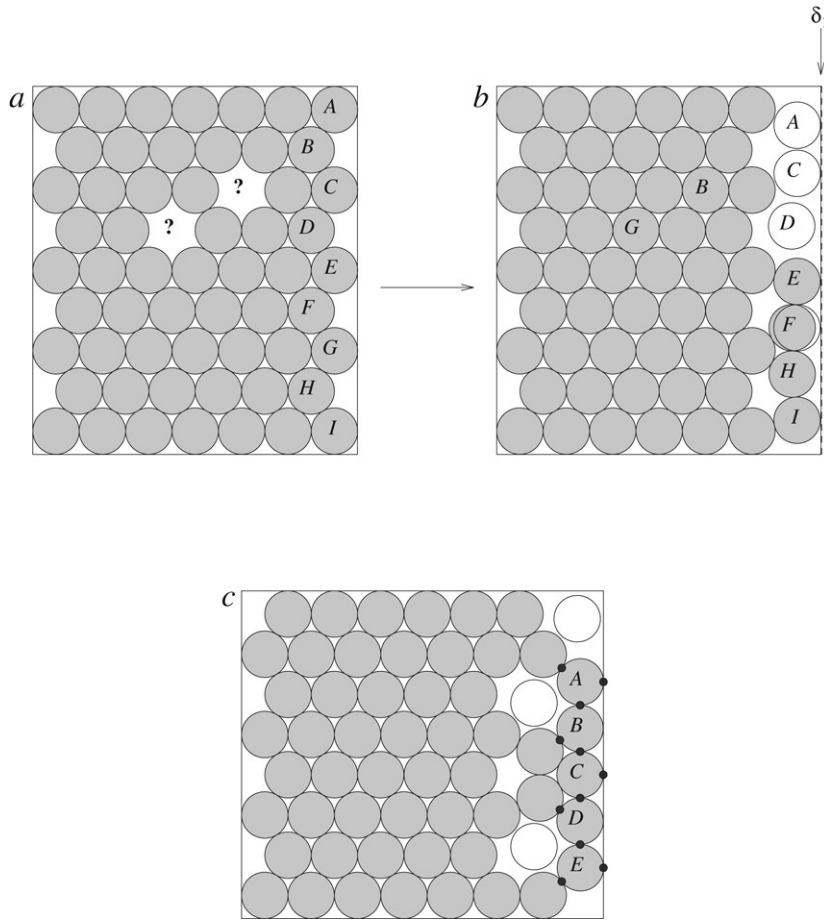
Fig. 4.5. Packings of 57 equal circles in rectangles: (*a*) with the smallest perimeter of the enclosing rectangle among the set R_{57}, (*b*) δ_2-improved packing *a*, (*c*) with the smallest perimeter of the enclosing rectangle we could find. Alternative position of circle *F* is shown in packing *b*. The black dots indicate bonds of the labeled circles in the packing *c*.

1 to 13 in Fig. 4.2*b* are assigned to the circles that occupy the positions in that figure which are similar to the corresponding circles 1 to 13 in Fig. 4.1*b*. The similarity, however, is not perfect. For example, the bond between circle 9 and the bottom boundary in Fig. 4.2*b* does not find its counterpart in Fig. 4.1*b*.

The remaining skipped entries in Table 3.1 are $n = 31$, 43, and 57. For these three values of n, unlike $n = 13$ or 21, the best in R_n packings all have holes, as seen in Fig. 4.3*a*, Fig. 4.4*a*, and Fig. 4.5*a*, and hence avail themselves for δ-improvements.

The improved packings labeled *b* in these three figures have perimeters, respectively

$P/r = 12(2 + \sqrt{3}) - 2\delta_3 = 44.74590240843\ldots$ for 31 circles,

$P/r = 14(2 + \sqrt{3}) - 2\delta_3 = 52.21000402357\ldots$ for 43 circles,

$P/r = 16(2 + \sqrt{3}) - 2\delta_2 = 59.59825161939\ldots$ for 57 circles.

Those improved perimeters still exceed the perimeters of the corresponding best packings found, which happen to be irregular, namely

for 31 circles $P^{\mathrm{opt}}/r = 44.7095500424198\ldots$ is smaller than P/r by at least 0.035,

for 43 circles $P^{\mathrm{opt}}/r = 51.99029827020367\ldots$ is smaller than P/r by at least 0.2,

for 57 circles $P^{\mathrm{opt}}/r = 59.4543998853414\ldots$ is smaller than P/r by at least 0.14.

The patterns of the irregular packings *c* in Figs. 4.3–4.5 somewhat resemble each other, especially the packings of 43 and 57 circles. Moreover, the best found packing of 43 circles in Fig. 4.4*c* is an exact subset in the best found packing of 57 circles in Fig. 4.5*c*. In both packings, the dots attached to 5 circles labeled *A* to *E* indicate the bonds of these circles. Thus, for example, the circles *B* and *D* do contact the circle *C*, but do not contact the right side of the rectangle, where the gap is 0.00957…of the circle radius, too small to be discerned in the diagrams. Similarly, the circle *C* does contact the right side of the rectangle but does not contact either of the two unlabeled circles immediately at *C*'s left. Between the pairs that do not include at least one labeled circle the bonds exist in the obvious places, and they are not specifically indicated by dots in the figures. As before, it is possible to *prove* the existence of the irregular packings *c* in Figs. 4.3–4.5. This existence might be non-obvious, especially, for the latter two packings.

5. Double optimality and related properties

As mentioned in Introduction, minimizing the perimeter and minimizing the area of the rectangle lead to generally different optimal packings for the same number of circles n, if the rectangle aspect ratio is variable. Are there packings optimal under both criteria at the same time? Fig. 5.1 displays such conjectured double optimal packings that were obtained by comparing the list of smallest area packings reported in [4] with that of the smallest perimeter packings reported here. For a particular n and a particular optimality criterion, there may be several equivalent optimum packings. For example, two minimum-perimeter packings exist for $n = 11$ according to Table 3.1 and two minimum-area packings exist for $n = 15$ according to [4]. However, no more than one packing was found to be double optimal for any n.

Since we will show in Section 7 that for $n \to \infty$ the L/S ratio of the minimum-perimeter rectangles tends to 1, and it is conjectured in this case that the L/S ratio for the minimum-area rectangles tends to $2 + \sqrt{3}$ (see [4]), then, conjecturally, there may be only a finite number of double optimal packings. In fact, we believe Fig. 5.1 lists all double optimal packings. For larger n, best rectangular shapes found under the two optimality criteria become noticeably different from each other, e.g., see the best packings found under either criteria for $n = 200$ in Fig. 5.2.

Consider a configuration C^{opt} of n equal circles which supplies the global minimum perimeter for its enclosing rectangle and suppose the C^{opt} happens to be *not* the one that supplies the global minimum to the area of the enclosing rectangle. We believe, however, that the rectangle of this C^{opt} still holds a record of being a rectangle of the minimum area, albeit locally. Specifically, if we vary slightly the ratio L/S of the rectangle around its value given by C^{opt} and for each such L/S find the rectangle of the densest possible packing of n unit-radius circles (this rectangle possesses both the minimum perimeter and the minimum area for its value L/S), then the area of the rectangle for the configuration C^{opt} will turn out to be the minimum among the areas of all those varied rectangles. We also believe that the statement which is obtained from the statement above by the interchange of the minimum-perimeter criterion with the minimum-area criterion is also true. That is, a configuration that delivers the global minimum of the area of the enclosing rectangle also holds a record of supplying the minimum of its perimeter, though perhaps only locally. Can the two sets of configurations, those that deliver the local minima for the rectangle area and those that deliver the local minima for the rectangle perimeter, be the same sets?

We have tested the former statement (that the global minimum-perimeter optimality implies the local minimum-area optimality) numerically for some values of n. If this conjecture is true, then the minimum-perimeter packings for some values of n have to be of a higher density than the densest packings of n equal circles in a square. Cases $n = 13$ and $n = 21$

1 circle   2 circles   4 circles   6 circles

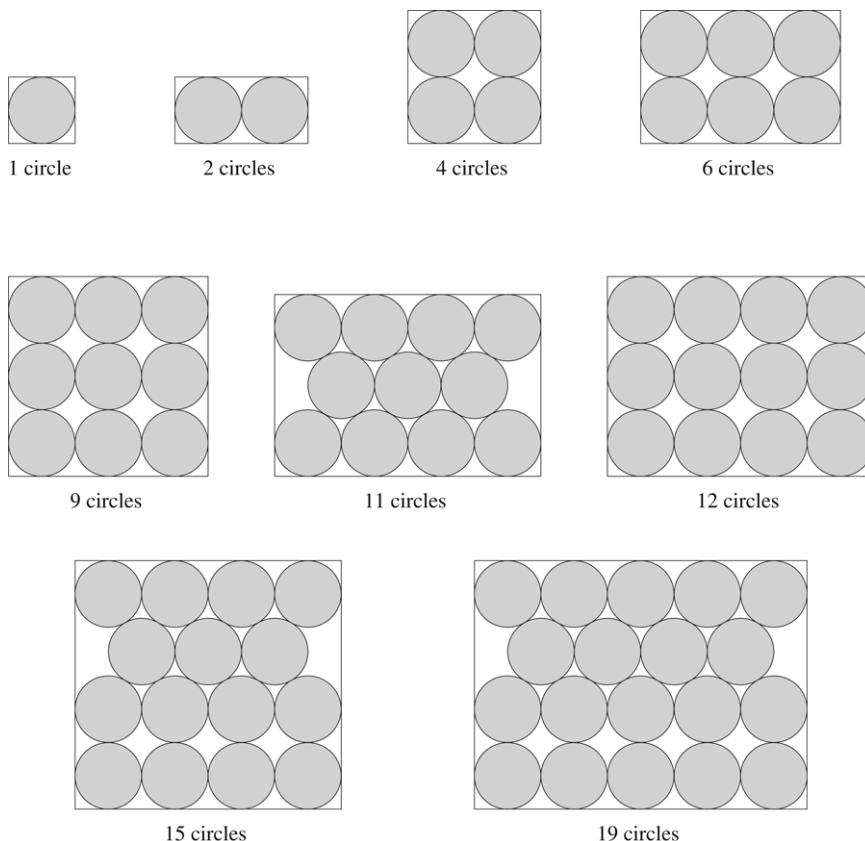9 circles   11 circles   12 circles

15 circles   19 circles

Fig. 5.1. The rectangle that encloses each of these packings has the smallest perimeter and the smallest area that we could find for their number of circles.
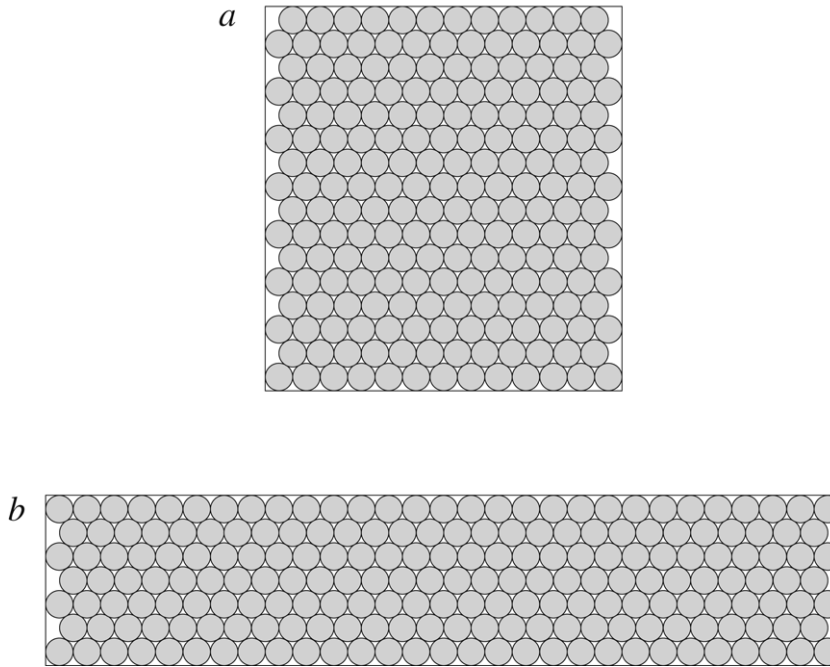
Fig. 5.2. The best packings found for $n = 200$ equal circles in rectangles of a variable shape: (a) under the criterion of the minimum perimeter, (b) under the criterion of the minimum area.

seem to be such occurrences. The configurations of 13 and 21 circles with the smallest found rectangular perimeter shown in Figs. 4.1 and 4.2b resemble the respective best found packings of 13 and 21 equal circles in a square, see for example, [3]. The only visible difference between the pairs for each n is in the positions of the bonds. The L/S ratios in either minimum-perimeter packing is very close to 1, so each respective densest packing in a square is a local neighbor of the corresponding minimum-perimeter packing. It can be verified that each of the two densest-in-a-square packings in [3] has a lower density than that of its minimum-perimeter counterpart reported here.

6. Minimum-perimeter packings for larger n

Because the results of the restricted search, available for all $n \leq 5000$, were supported by simulation only for all $n \leq 62$, our conjectures become more speculative for larger n.

For $n \leq 62$ the restricted search reliably predicts the best packings found by the simulation except those of the form

$$n = k(k + 1) + 1, \tag{10}$$

where $3 \leq k \leq 7$. All those predicted packings happen to be either regular or semi-regular. The optimal packings for the values of n of the form (10) appear to be exceptionally irregular. For which $n > 62$ are the best packings similarly irregular?

Our previous experience for packing equal circles in various shapes suggests that the numbers of circles which result in exceptionally "bad" or irregular optimal packings often follow immediately after the numbers which result in exceptionally "good" or regular optimal packings. For example, triangular numbers of circles $n = k(k + 1)/2$ arrange themselves optimally in regular triangular patterns inside equilateral triangles and in [2] we observed that the optimal arrangements of $n = k(k + 1)/2 + 1$ circles look irregular and disturbed.

The minimum-perimeter packings of $n = k(k + 1)$ equal circles inside rectangles with a variable aspect ratio, as conjectured by the restricted search for

$$4 \leq k \leq 33, \tag{11}$$

are regular hexagonal arrangements of $h = k + 1$ alternating rows with $w = k$ circles in each row. For $k > 33$ ($n > 1122$) this regular pattern with $w = k$, $h = k + 1$ does not serve as the optimum. The latter statement is proven at least for $n \leq 5000$. Thus we speculate that the 30 values of k in (11) also might correspond to the 30 cases of n as computed by formula (10) in each of which the minimum-perimeter packing of n circles in rectangles with variable aspect ratio is irregular.

The irregular minimum-perimeter packings, probably, also occur for some n which are *not* of the form (10). We believe $n = 66$ is the smallest such n. In fact, $n = 66$ is the smallest one with the properties: (A) it is not of the form (10) for any integer k, (B) the best in R_n packing, as delivered by the restricted search, has $h = 9$ alternating rows, $h_- = 4$ of which are one circle shorter, and $v = 2$ holes. The smallest n for which (B) holds is $n = 57$. The best in R_{57} packing is shown in Fig. 4.5a.

Table 6.1

Packings of n circles in rectangles of the smallest perimeter as found by the restricted search for several contiguous segments of n that were arbitrarily selected within the set $62 < n \leq 5000$

n	w	h	h_-	s	v	n	w	h	h_-	s	v	n	w	h	h_-	s	v
101	9	12	6	0	1	501	21	24	0	0	3	2001	44	46	23	0	0
102	9	12	6	0	0	502	21	24	0	0	2	2002	41	49	0	0	7
103	10	11	5	0	2	503	21	24	0	0	1	2003	41	49	0	0	6
104	10	11	5	0	1	504	21	24	0	0	0	2004	41	49	0	0	5
105	10	11	5	0	0	505	22	23	0	0	1	2005	41	49	0	0	4
106	10	9	4	2	0	506	22	23	0	0	0	2006	41	49	0	0	3
	11	9	4	1	0	*507	20	26	13	0	0	2007	41	49	0	0	2
107	9	12	0	0	1	508	21	25	12	0	5	2008	41	49	0	0	1
108	9	12	0	0	0	509	21	25	12	0	4	2009	41	49	0	0	0
109	10	11	0	0	1	510	21	25	12	0	3	2010	42	48	0	0	6
110	10	11	0	0	0	511	21	25	12	0	2	2011	42	48	0	0	5
...	..	..	.	.	.	...	..	..	.	.	.	...	..	..	..	..	..
251	14	18	0	0	1	1001	30	34	17	0	2	4991	64	78	0	0	1
252	14	18	0	0	0	1002	30	34	17	0	1	4992	64	78	0	0	0
253	15	17	0	0	2	1003	30	34	17	0	0	4993	68	74	37	0	2
254	15	17	0	0	1	1004	31	33	16	0	3	4994	68	74	37	0	1
255	15	17	0	0	0	1005	31	33	16	0	2	4995	68	74	37	0	0
256	16	16	0	0	0	1006	31	33	16	0	1	4996	65	77	0	0	9
257	14	19	9	0	0	1007	31	33	16	0	0	4997	65	77	0	0	8
258	15	18	9	0	3	1008	28	36	0	0	0	4998	65	77	0	0	7
259	15	18	9	0	2	1009	29	35	0	0	6	4999	65	77	0	0	6
260	15	18	9	0	1	1010	29	35	0	0	5	5000	65	77	0	0	5
...	..	..	..	..	..	...	..	..	..	..	..	...	..	..	..	..	..

The packings shown are either regular (with $v = 0$) and then they all are believed to be globally optimal, with the exception of the case $n = 507$, or they are regular with holes (with $v > 0$) and then they can be δ-improved into semi-regular packings. The exceptional entry $n = 507 = 22 \times 23 + 1$ is marked with a star. The optimal packing for 507 circles might be of an unknown irregular pattern.

By attaching a column of 9 alternating circles at the left of Fig. 4.5a we obtain a diagram of the best in R_{66} packing. The best in R_{57} packing can be δ_2-improved as shown in Fig. 4.5b. The best in R_{66} packing can be δ_2-improved in the same way. In either one of these δ_2-improved packings all the circles can be "unjammed" so that there would be no contacts among them or with the boundary. Hence the perimeter of either one can be further reduced by subsequent "compaction" of the rectangle.

Our "compactor" simulation suggests that for $n = 57$ the irregular packing thus obtained does not overtake the conjectured optimum packing shown in Fig. 4.5c. However, we believe that its analogue for $n = 66$ might just be the optimum packing and it would be irregular. Approximately, each of the two "compacted" irregular packings might look similar to the packing in Fig. 4.5b. Unfortunately, obtaining their exact patterns, including the identification of the bonds, proved to be beyond our current computing capabilities. (The hardness of the computations might indicate existence of several local minima near the "unjammed" configurations.) Note that the pattern of the least perimeter packing for $n = 66$ would probably differ substantially from the patterns of the irregular least perimeter packings for $n = 13, 21, 31, 43$, and 57, those conjectured in Section 4.

The chance to encounter a non-regular n (which by definition has to correspond to either a semi-regular or irregular optimal packing) increases quickly with n. In Table 6.1 we list the packings found by the restricted search procedure for several segments of consecutive n. The segments are arbitrarily selected within the set $62 < n \leq 5000$. The structure of Table 6.1 is similar to that of Table 3.1, except that an additional column is provided for the number of holes v. The entries n with $v > 0$ are frequent in Table 6.1, unlike Table 3.1. Also, we choose to skip the δ column here. (Determining and presenting the higher-order δ_i would involve many details exceeding the reasonable limits for this paper.)

The discussion above suggests that, perhaps, some of the entries with multiple holes, $v > 1$, correspond to irregular packings, if their δ-improvements avail themselves to further improvements same as the packing in Fig. 4.5b.[2]

The larger values of n that would correspond to regular packings become rare. However, we do not believe regular n eventually disappear. In other words, we do not believe the largest such n exists. For the infinite sequence of values of n, all those of the form

$$n = \frac{1}{2}(a_k + 1)(b_k + 1), \quad k = 1, 2, \ldots \tag{12}$$

with

$$a_1 = 1, a_2 = 3, a_{k+2} = 4a_{k+1} - a_k, \quad b_1 = 1, b_2 = 5, b_{k+2} = 4b_{k+1} - b_k, \quad k = 1, 2, \ldots \tag{13}$$

---

[2] As reported in [4], for some $n \geq 393$ the configurations with the least area among the set R_n have multiple holes. In particular, the smallest n for which property (B) holds for the least rectangular area configuration among the set R_n is $n = 453$. The non-zero parameters of the configuration are $w = 51, h = 9, h_- = 4, v = 2$. The packing of 453 congruent circles which delivers the global minimum to the area of the enclosing rectangle is, probably, irregular.

Table 6.2
Packings of n circles in a rectangle of the smallest found perimeter which are hybrid and/or exist in two differently shaped rectangles

n	w	h	h_	s	n	w	h	h_	s	n	w	h	h_	s
69	8	7	3	2	151	12	11	5	2	298	17	17	8	1
	9	7	3	1		13	11	5	1		18	17	8	0
78	9	7	3	2	176	13	13	6	1	316	18	17	8	1
86	9	9	4	1		14	13	6	0	371	19	19	9	1
	10	9	4	0	190	14	13	6	1		20	19	9	0
96	10	9	4	1	233	15	15	7	1	452	21	21	10	1
127	11	11	5	1		16	15	7	0		22	21	10	0
	12	11	5	0	249	16	15	7	1	541	23	23	11	1
139	12	11	5	1							24	23	11	0

All such cases $n > 62$ are listed in this table, except $n = 106$, which is listed in Table 6.1.

the minimum-perimeter packings are probably regular. The fractions a_k/b_k are (alternate) convergents to $1/\sqrt{3}$, and it has been conjectured by Nurmela et al. [8] that for these n, a "nearly" hexagonal packing of n circles in a square they describe is in fact optimal, that is, it has the largest possible density among those in a square. The beginning terms $n = 12, 120, 1512$ of sequence (12) are within the range $n \leq 5000$ for which we exercised the restricted search procedure. For these three n's the search delivers regular patterns as the minimum-perimeter packing in R_n: a 4×3 square-grid for $n = 12$, the hexagonal packing with $w = 10, h = 12$ for $n = 120$ and that with $w = 36, h = 42$ for $n = 1512$. Note that the latter two are the *exact* hexagonal packings and they have densities larger than that of the corresponding "nearly" hexagonal packings, those that are best in a square according to the conjecture in [8]. We believe the same relation between the best packings of n circles in a square and the minimum-perimeter packings of n circles in rectangles continues for all larger n of the form (12) and (13).

Increasing the value of n seems to diminish such phenomena as dimorphism and hybrid packings. Dimorphism of the optima is the existence of two different optimal rectangular shapes. The dimorphism occurs within the interval $1 \leq n \leq 62$ for $n = 11, 19, 28, 29, 40$ and 53, see Table 3.1. The hybrid packings, identifiable in the table by h and s being both positive, occur for $n = 11, 15, 19, 24, 28, 29, 34, 40, 47, 53$, and 61. Among the n's selected for Table 6.1, the two different optima exist only for $n = 106$. Both optima also happen to be hybrids and no other hybrid occurs in Table 6.1. The remaining cases of dimorphism and/or hybrid packings among $1 \leq n \leq 5000$ are all listed in Table 6.2. For either phenomenon, dimorphism or hybrid packings, the largest n for which the phenomenon still occurs appears to be $n = 541$. For comparison: both phenomena also occur for the criterion of the minimum area in [4], but both end much sooner, the largest n for which either phenomenon still occurs appears to be $n = 31$.

7. Optimal rectangles are asymptotically square

In this section we will show that as n goes to infinity, the ratio of L/S for the minimum perimeter rectangle in which n congruent circles can be packed tends to 1. This will follow from the following considerations. For a compact, convex subset X of the Euclidean plane, define the *packing number* $p(X)$ to be the cardinality of the largest possible set of points within X such that the distance between any two of the points is at least 1. Let $A(X)$ be the area and $P(X)$ be the perimeter of X. The following result of Oler (see [9,1]) bounds $p(X)$:

Theorem:

$$p(X) \leq \frac{2}{\sqrt{3}} A(X) + \frac{1}{2} P(X) + 1.$$

It is easy to prove the following lower bound on the packing number for a square $S(\alpha)$ of side α:

Fact:

$$p(S(\alpha)) \geq \frac{2}{\sqrt{3}} \alpha^2.$$

Suppose R is an optimal rectangle with side lengths $m + \epsilon$ and $m - \epsilon$. Thus, R has perimeter $4m$ and area $m^2 - \epsilon^2$. By the preceding upper bound on $p(R)$ we have

$$p(R) \leq \frac{2}{\sqrt{3}} (m^2 - \epsilon^2) + \frac{1}{2} (4m) + 1.$$

Since R is optimal, then we must have $p(R) \geq p(S(m))$. This implies that

$$\frac{2}{\sqrt{3}} (m^2 - \epsilon^2) + 2m + 1 \geq \frac{2}{\sqrt{3}} m^2.$$

From this it follows that

$$\epsilon \leq \left(\frac{\sqrt{3}}{2} (2m + 1) \right)^{1/2},$$

which is of a lower order than m, the order of the side lengths.

It is now straight-forward to convert this inequality to one for packing circles rather than points, and our claim is proved. As an example, if $m = 1000$ then $\epsilon < 41.623\ldots$, so that the ratio $L/S \leq 1.0869$.

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