MASTERS DISSERTATION

Mathematical analysis of graphene grid structures with defects

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Declaration

I declare that this dissertation is my own, unaided work. It is being submitted for the Degree of Master of Science at the University of the Witwatersrand, Johannesburg. It has not been submitted before for any degree or examination at any other University.

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Date and time: 10/29/2022 at 9:56 a.m.

Abstract

In this dissertation, we explore the work by M. Archibald, S. Currie and M. Nowaczyk in their paper "Finding the hole in a wall." In this paper, the authors solve the inverse problem of locating the position of a single vacancy break using lengths of closed paths on an infinite hexagonal grid structure. In order to do this they transform the infinite hexagonal grid structure that models graphene into a brick wall structure. When a single vacancy break occurs, polygons of odd length are introduced into the grid structure. First, we explore lemmas that state which polygon the closed paths of shortest odd length circumnavigate. We then use these to provide a rigorous proof of the two main theorems in "Finding the hole in a wall". These depend on the region that the path originates from in the brick walls and tell us what the path is congruent to modulo 4. Finally, we study the algorithm for determining the exact position of the defect, and sometimes, provide alternative formulae for locating the defect. When this is the case, we show the formulas are equivalent to those in their work. Also provided are potential future studies in this area.

Acknowledgements

This work has been an interesting journey for me. This being a relatively fresh approach to studying graphene grid structures, I had little literature to go on. The support from my supervisors compensated for this challenge and I would like to extend my appreciation to them. I received a lot of support from my family and colleagues, which I am truly grateful for.

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Chapter 1

Some Background Information on Graphene

1.1 Introduction

This chapter introduces us to graphene as a hexagonal two-dimensional arrangement of carbon atoms. We explore what graphene is, its properties, defects that occur in graphene and how to locate them. We briefly discuss research on graphene from physics and mathematics disciplines.

1.2 What is Graphene?

Graphene is a two-dimensional arrangement of carbon atoms that closely resembles a honeycomb in structure [14]. Graphene is so special that a Nobel prize in physics was awarded to British scientists Andre Geim and Konstantin Novoselov for its discovery. Graphene's excellent electrical conductivity, heat conductivity, tensile strength and impermeability are some properties that make it one of the most important materials today [7, 10, 11]. These key attributes are all credited to the structural perfection of the hexagonal lattice of graphene [11]. Its possession of a wide range of outstanding properties makes it ideal for the development of electronics, membranes, biomedical technologies, sensors, transistors, energy harvesting and storage devices and composites and coatings [5, 10, 11, 17].

However useful it may be, growth and processing of graphene is rarely perfect and will often result in structural defects forming [14, 17]. Graphene can be represented by a hexagonal grid where the vertices are carbon atoms and the edges are chemical bonds. Figure 1.1 below is a representation of defect free graphene [2].

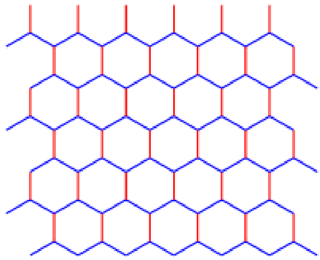

Figure 1.1: Graphene's honeycomb structure without defects.

1.3 Defects in the structure of Graphene

There are several types of defects that can occur in the structure of graphene. Some well-known defects include the Stone-Wales defect (SW), single vacancy (SV) and double vacancy (DV) defects.

1. A single vacancy defect is formed when a single lattice atom is missing. It is given geometrically by a pentagon below a nonagon [2, 11], see Figure 1.2 [2].

2. There is more than one type of double vacancy defect. Double vacancies are formed either by the joining or merging of two single vacancy defects or by removing two neighboring atoms. There are no dangling bonds present in a fully formed double vacancy defect. Instead, two pentagons and one octagon appear in place of the four hexagons in pristine graphene [14, 17], see Figure 1.3 (left) [2]. There is another route in which a graphene lattice structure can have two absent carbon atoms. Namely, by rotating one of the octagon bonds in the DV defect shown in Figure 1.3 (left), the double vacancy defect changes to a setup with three heptagons and three pentagons. This new arrangement of carbon atoms in the lattice takes less energy to form (one electron volt less) than the initially discussed double vacancy defect. There is yet another type of double vacancy defect that can be formed from this last configuration. In particular, a reconstruction involving the rotation of an additional bond will result in a configuration with four heptagons, four pentagons and one hexagon (see Figure 1.4 (right)). The last two double vacancy defects, have been observed experimentally [4].

3. The Stone-Wales break is formed by rotating one of the carbon bonds by 90 degrees. It is represented by two pentagons and two heptagons [14], see Figure

1.3 (right) [2].

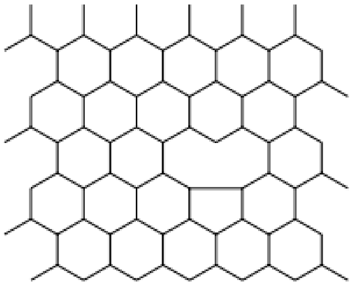

Figure 1.2: Graphene grid with a single vacancy defect.

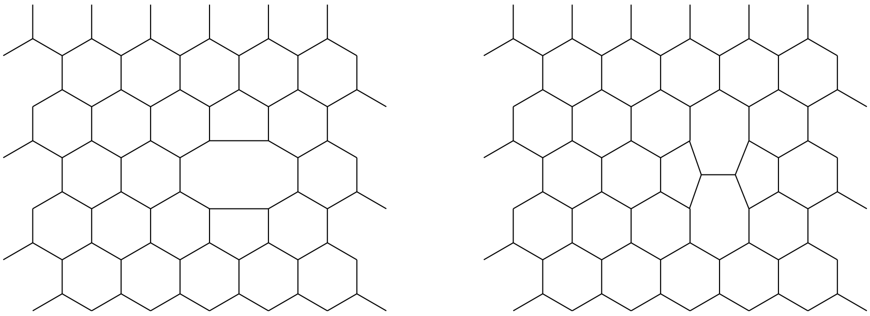

Figure 1.3: Hexagonal grid with a DV defect (left) and an SW defect (right).

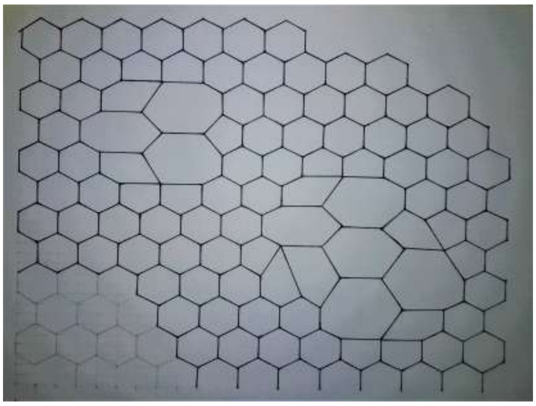

Figure 1.4: Graphene with other types of DV defects.

The length of the edges (chemical bonds)in Figures 1.2, 1.3 and 1.4 is not consistent with the actual lengths of bonds in defective graphene. For a more realistic picture of these defects, please see [4].

The defects introduced during growth and processing of graphene can affect some of its properties. The Young's modulus measures the elasticity of a material and is defined as the ratio of stress to strain [12]. In [11], the effect of the single vacancy, double vacancy and Stone-Wales defects on the elasticity of graphene are studied through the use of molecular dynamic simulations. It is evident from the simulations that the presence of these defects decreases the elasticity of graphene sheets. More precisely, an increase in the degree of the defects results in a decrease in the Young's Modulus of graphene. Here the defect degree of vacancies is defined as the numerical density of atoms removed from the pristine graphene sheet. In summary, the single vacancy, double vacancy and Stone-Wales defects all result in an inverse relationship between the Young's modulus of graphene sheets and the defect degree. The Young's modulus of a sheet of graphene with single vacancy defects decreases at a rate of approximately 0.0273 with respect to the defect degree. The Young's modulus of a sheet of graphene with double vacancy defects decreases at a rate of approximately 0.0253 with respect to the defect degree. Finally, the Young's modulus of a sheet of graphene with Stone-Wales defects decreases at a rate of approximately 0.0221 with respect to the defect degree [11].

The quality of graphene available today varies. Defective graphene can negatively affect development and performance of graphene-based devices [14, 17]. However, some studies have shown that imperfections in graphene's structure can be useful. For example, nanoengineering graphene-based devices for dedicated functions necessitates the introduction of structural defects that allow us to achieve the desired functionality, just like in conventional semiconductors [4]. This has caused many scientists from different fields, to take an interest in various studies involving defective graphene. These include studies in graphene production, effects of defects on graphene, locating defects etc [2, 4, 5, 7].

Studies in physics and chemistry have revealed that defects will affect the overall strength, conductivity (thermal and electrical) and even the lifespan of the graphene [11, 14]. For this reason it is useful to be able to locate the defects in graphene when they occur. This has led to the use of mathematical analysis in finding defects in graphene.

1.3.1 Locating Defects in Graphene

The best configuration for the study of defects in planar graphene would be the observation of crystalline foils with a thickness of about a single carbon atom, studied using a microscope with a single-atom resolution and the ability to record defect-formation and dynamics as they occur [15].

Transmission electron microscopy (TEM) is used in the imaging of nanoparticles at a scale close to a single atom. Factors like the type of image (bright and dark field) and magnification method affect the resolution of the measurement, the number of particles in each image, the contrast between particles and the background for images taken using TEM [18]. The authors of [15] state that, even though it may seem that TEMs are best suited for the study of defects in planar graphene, this is not the case. A low voltage is important for the stability of the membranes and traditional electron transmission microscopes lack the resolution required at these low operating voltages (80 kV). They go on to present results obtained using a microscope designed with the ability to resolve every carbon atom in the graphene lattice. The aberration-corrected, monochromated TEAM 0.5 TEM confirmed and imaged defects like the Stone-Wales in real-time. The scanning electron transmission microscope (STM) is another type of electronic microscope that is considered useful in the study of planar graphene [4].

1.3.2 Graphene in Mathematics and Physics

Ideally, it would be very convenient if we could locate a defect in a piece of graphene without having to examine the entire grid. Since the graphene grid structure is atomic, a natural question to ask would certainly be: "How can you locate what you can not see?". A viable idea would be to use a different sense (i.e. other than sight) to map out what the structure of the grid would look like. This would be the equivalent of a bat using echolocation to accurately locate its prey. In fact, this idea is reminiscent of the question "Can one hear the shape of a drum" asked in [8]. Even though the answer to this question was a definite no, it inspired mathematicians to investigate inverse spectral problems on quantum graphs [9, 13].

In [9], Gutkin and Smilansky answer the question: "Can one hear the shape of a graph?". They demonstrate that the spectrum of the Schrödinger operator defined on a metric graph (finite) decides uniquely what the connectivity matrix and the bond lengths should be. The results hold as long as the lengths are non-commensurate, and the connectivity is simple (no parallel bonds between vertices and no loops connecting a vertex to itself). Put more simply, yes, one can hear the shape of a graph. Using mathematical analysis it is possible to locate a defect in a piece of graphene without having to examine the entire grid.

A quantum graph is a linear network of vertices/nodes connected by edges. The edges have a finite length and a differential equation is imposed on each edge. In particular, the Laplace operator together with natural/Kirchhoff and matching conditions at the vertices is studied in [1]. The trace formula provides a relation between the spectrum of an operator and the periodic orbits on a quantum graph. In [1], additional information provided by the trace formula such as data about the transition and reflection coefficients is made use of.

Let G be a connected graph with V vertices v_i and E edges e_j, where $l(e_j)$ is the length of edge e_j and d_i is the degree of the vertex v_i. The degree of a vertex is the number of edges entering or exiting it. We define the following:

- A set P containing all periodic orbits (closed path lengths p) in G;
- $l(p)$ is the geometric length of the periodic orbit p;
- The total length of G given by $\mathcal{L} = l(e_1) + l(e_2) + \cdots + l(e_V)$;
- prim(p), the primitive periodic orbit of p (the shortest orbit such that p is a repetition of prim(p));
- k_j^2 the spectrum of the Laplace operator on L on G with natural/Kirchhoff boundary conditions;
- $\delta(k)$ is the Dirac delta function;
- $\mathcal{A}_p$ consists of the product of all entries in the matrix

$$S(v_i) = \sigma_{ij}^m = \begin{pmatrix} \frac{2-d_i}{d_i} & \frac{2}{d_i} & \cdots & \frac{2}{d_i} \\ \frac{2}{d_i} & \frac{2-d_i}{d_i} & \cdots & \frac{2}{d_i} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{2}{d_i} & \frac{2}{d_i} & \cdots & \frac{2-d_i}{d_i} \end{pmatrix}$$

along the periodic orbit p and $l(prim(p))$. More precisely,

$$\mathcal{A}_p = \left(\prod_{\sigma_{ij}^m \in \mathcal{B}} \sigma_{ij}^m \right) l(prim(p).$$

$\mathcal{B}$ is the set containing all entries of the matrix $S(v_i)$.

The trace formula is given by:

$$
\begin{aligned}
u(k) &\equiv \delta(k) + \sum_{j=1}^{\infty}[\delta(k-k_j) + \delta(k+k_j)] \\
&= -(V - E + 1)\delta(k) + \frac{\mathcal{L}}{\pi} + \frac{1}{2\pi}\sum_{p\in P}\mathcal{A}_p\left(e^{ikl(p)} + e^{-ikl(p)}\right).
\end{aligned}
$$

In [1], the authors study a finite rectangular grid. If a break was to occur on this rectangular grid, it would cause changes in the finite periodic orbits on this grid. By computing the extent to which the sum of the amplitude numbers over all periodic orbits changes in the event of a break for a fixed length, not only is it possible to pinpoint the location, one can also determine the type of defect by simply observing the unique sum of amplitude numbers (see [1]). This approach did, however, prove to become more tedious as grids became larger and hence motivated the authors of [1] to seek a different technique to use.

In mathematics and physics, an inverse problem computes from a set of observations/effects the factors that caused them. In [2] Archibald, Currie and Nowaczyk, give an approach to the problem of identifying the location of a single vacancy break in a hexagonal grid. They solve the inverse problem of identifying the position of a single vacancy break from the lengths of the closed paths. Here, the effect of the break is a variation in the parity of the length of closed paths on the underlying graph. By observing this variation in the length of closed paths, the authors calculate the exact location of the break.

1.4 Conclusion

Having explored graphene and some of its properties, we are now ready for much more detailed discussions on the dissertation subject. This chapter is a brief and informative discussion of graphene and its properties. The next chapters will focus on the single vacancy defect.

Chapter 2

Finding the hole in a wall

2.1 Introduction

It is not uncommon to transform a problem into a mathematical setting that is more useful to scientists. This is done in [2]. In this chapter, we will explore in great detail the discussions of [2]. In particular, detailed proofs of the two main theorems in [2] will be provided and discussed.

2.2 Building the brick wall

When a single vacancy break occurs in the hexagonal grid, a single carbon atom in the hexagonal lattice goes missing. This results in the lower two of the three bonds that are without a node (carbon atom) joining to form one bond. The third bond then leads to a node with only two incident edges forming. The dangling third bond is excluded in our diagrams as it does not play any role in the analysis. Because of this, a pentagon and nonagon are formed in the hexagonal grid (see Figure 1.2). Since each edge is given a length of one unit, any closed orbit encompassing either the pentagon or nonagon (but not both) will be of odd length. The existence of a single vacancy break in the grid therefore immediately implies there will exist a closed path of odd length. This is key to the analysis used in [2].

To make referencing within the hexagonal graphene grid easier, the authors convert it to a rectangular grid (resembling a brick wall) and place it in the usual two-dimensional Euclidean plane (see Figure 2.1).

The transformation makes it appear as if Figure 1.2 is compressed downwards by vertical forces until the non-vertical slanted lines of the hexagons become horizontal

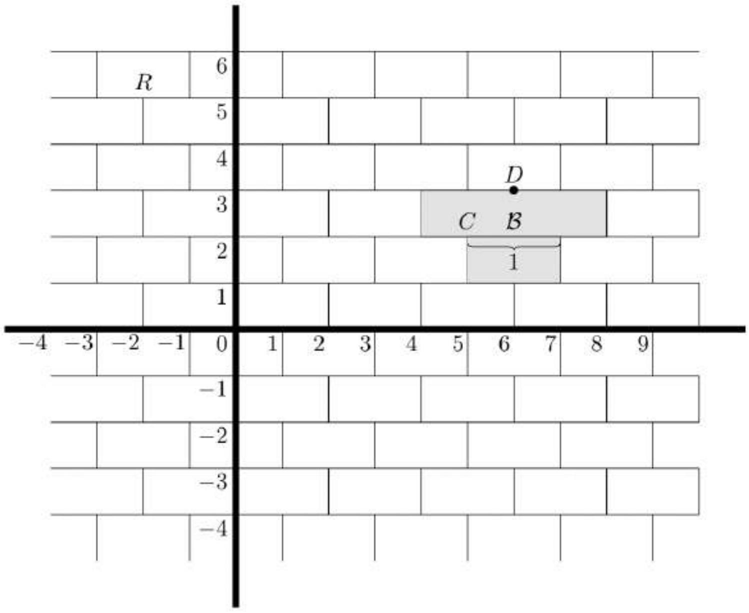

Figure 2.1: Transformed graphene grid.

and flat (looking more like brick wall). Vertical lines from the hexagonal grid on Figure 1.2 remain unchanged. The result is a brick wall on which it is possible to impose a coordinate system to simplify the task of locating where the defect occurs. To emphasize, the transformation is purely to allow us the ability to impose a coordinate system on the grid structure. In Figure 2.1, the nonagon and pentagon that are formed because of the removal of a carbon atom from the original perfect hexagonal graphene grid structure are shaded. $\mathcal{B}$ represents the position of the single vacancy break. And $D = (D_x, D_y)$ represents the carbon atom (node) directly above the break. Due to the third dangling bond (vertical line) on D not being joined to any carbon atom, the nonagon looks as if it joined two bricks on the wall to make one. Since two bonds joined to make a single bond, the length of the edge at the top of the pentagon is one unit. Now that we can reference where the break is located, we will make observations based on the length of closed paths circumnavigating either the nonagon or pentagon from different positions in the brick wall. For the reason given on the next page, the brick wall in Figure 2.1 is divided into regions $A = A_1 \cup A_2 \cup A_3$ (shaded brown) and $B = B_1 \cup B_2 \cup B_3$ (shaded green). See Figure 2.2.

Note that C labels the top left vertex of the pentagon in Figure 2.2, this vertex will be significant in the discussions of the next section. Now it is possible to discuss the main results in [2].

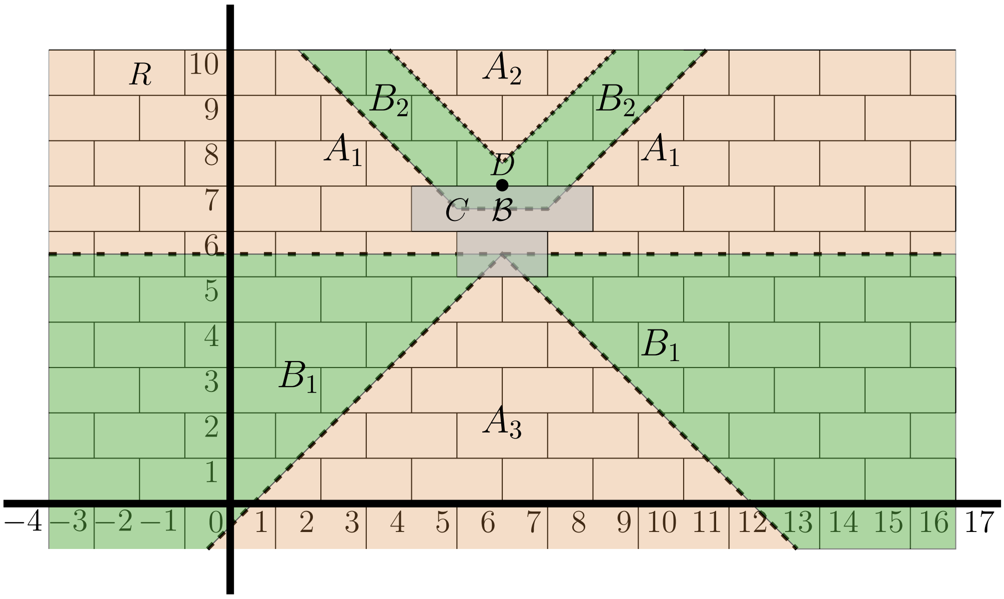

Figure 2.2: Transformed graphene grid.

We would like to make use of the shortest closed path of odd length from a chosen reference point R. In a two-dimensional plane, the shortest distance between two points is a straight line. Looking at the grid, we can not always move in a straight line towards the pentagon or nonagon. The next best thing is to, however, zig-zag around the grid in such a way that we approach the defect area in the straightest fashion.

We now provide some motivation/intuition as to how and why the regions in Figure 2.2 were chosen. Set S to be the length of a shortest path with odd length starting and ending at R (see Figure 2.2), where R is a chosen reference point of degree 3 (not directly above the break). All closed paths of odd length are either congruent to $1 \mod 4$ or congruent to $3 \mod 4$. This fact led to the partitioning of the grid into regions A_1, A_2, A_3, B_1 and B_2. That is, all closed paths of odd length obey one of the two congruence equations depending on which region (A or B) of the brick wall they originate from. The following results given in [2] show this relationship.

Theorem 1. *Let R be positioned at the top of a vertical line. Then:*

(a) R lies in Region A if and only if $S \equiv 1 \,(mod\, 4)$,
(b) R lies in Region B if and only if $S \equiv 3 \,(mod\, 4)$.

Theorem 2. *Let R be positioned at the bottom of a vertical line. Then:*

(a) R lies in Region A if and only if $S \equiv 3 \,(mod\, 4)$,

(b) R lies in Region B if and only if $S \equiv 1\,(mod\,4)$.

These two results are proved in the following section.

2.3 The Main Results

If S enclosed both the nonagon and pentagon, then the length of S would be even as $5+9$ (length of the nonagon plus pentagon) is even. The rest of the path encloses at least one hexagon (if the path covers more than one hexagon, then any edge that is repeated is subtracted twice) and will therefore be even in length, immediately contradicting that S is of odd length. Therefore, the path S will enclose either the nonagon or the pentagon, but not both. Degree in this context refers to the number of bonds (edges) incident from the carbon (node) atom.

The shortest closed path of odd length is not necessarily unique. For example, there could be one path of odd length going around the nonagon and another distinct path of odd length going around the pentagon. In fact, if S represents the length of a shortest odd path, then it is common for there to be other paths with the same length as S. One reason behind this is that because of the way the brick wall is structured, it is not always possible to go straight down or up. We will often have a choice to either go left or right before we can move up or down. This choice whether to go left or to go right results in many alternative paths possibly of the same length.

Definition 1. *Let P be a path on the grid. The horizontal length of the path P is defined to be the number of horizontal edges of length* 1 *that the path travels.*

Definition 2. *Let P be a path on the grid. The vertical length of the path P is defined to be the number of vertical edges of length* 1 *that the path travels.*

Definition 3. *Let P be a path on the grid. The length of the path P is defined to be the sum of the horizontal and vertical length of the path P.*

There is an interesting observation to make here. Even though the shortest closed path is not unique, the following claim holds for all these alternate paths that exist.

Proposition 1. *Let V_1 and V_2 be any two arbitrary vertices on the grid such that $V_1 \neq V_2$. If P is a shortest paths starting at V_1 and ending at V_2, then all alternative shortest paths starting at V_1 and ending at V_2 have the same vertical and horizontal length as P.*

Proof. Let P' denote an arbitrary alternative shortest path starting at V_1 and ending at V_2. Let λ_v denote the vertical length of $P^{'}$, λ_h denote the horizontal length of $P^{'}$ and $\lambda = \lambda_h + \lambda_v$ denote the length of $P^{'}$. From how the grid is structured, it is not always possible to go straight up or down. However, if the aim is to move downwards, the path will not go back up again because the vertical length of the path will become longer than necessary. A similar argument holds if the aim is to move up. Consequently, P and $P^{'}$ will have the same vertical length and since P and $P^{'}$ have the same length as well, then $\lambda_h = \lambda - \lambda_v$ will be same for both paths. As our choice of $P^{'}$ was arbitrary, then all other alternative shortest paths starting at V_1 and ending at V_2 have the same vertical and horizontal length as P.

□

This last proposition gives us assurance that, whenever we discuss multiple alternative shortest paths between two vertices, we will be certain that all such paths share the same vertical and horizontal length. This comes into play for the results that follow. It will later on in our discussion be important to know whether the shortest closed path of odd length circumnavigates the nonagon or pentagon. The following results form a criterion for the polygon that the shortest closed path of odd length circumnavigates, depending on the region in which R is placed.

Lemma 3. *Let $R = (R_x, R_y) \in A_1$ such that $R_y \geq D_y$ and P be a shortest closed path of odd length starting and ending at R. Then P could circumnavigate either the nonagon or the pentagon.*

Proof. Let $R = (R_x, R_y) \in A_1$ such that $R_y \geq D_y$ and P be a shortest closed path of odd length circumnavigating the nonagon. Now, if $\mathcal{B}$ (see Figure 2.2) is to the right of R the path P consists of the portion from R to the top left vertex of the nonagon, the portion around the nonagon and the portion from the top left vertex of the nonagon back to R. We can, however, take an alternative path after moving from R to the top left vertex of the nonagon. Instead, the path that goes down and across to the top left vertex of the pentagon around the pentagon and back to the top left vertex of the nonagon is also the same length as the path around the nonagon. If $\mathcal{B}$ is to the left of R a similar argument as to the one above holds. Thus P is not unique. P can circumnavigate either the nonagon or pentagon.

□

Lemma 4. *Let $R = (R_x, R_y) \in A_1$ such that $R_y < D_y$ and P be a shortest closed path of odd length starting and ending at R. Then P does not circumnavigate the nonagon and must go around the pentagon.*

Proof. Assume, on the contrary, that P circumnavigates the nonagon. If $R \in A_1$ such that $R_y < D_y$ then R has coordinates $(R_x, D_y - 1)$. As before, let C_n be the bottom right or bottom left vertex of the nonagon. More precisely C_n is the vertex closest to R. The path P has 3 components. Namely, the portion moving from R to C_n, the path around the 9 edges of the nonagon back to C_n and then the path from C_n back to R. λ_h is the horizontal length of the portion from R to C_n and λ_v is the vertical length of the portion from R to C_n (which in this case is 0) then the length of P is given by $2\lambda_h + 9$.

Define C_p to be the top left or top right vertex of the pentagon. Let $P^{'}$ be a shortest closed path of odd length starting and ending at R circumnavigating the pentagon. Just like P, the path $P^{'}$ has 3 components. Now since C_p is one unit away from C_n in this case the horizontal length for the path $P^{'}$ is given by $\lambda_h + 1$. The vertical length for the path P' is $\lambda_v = 0$ (there is never a need to make a vertical movement as the points lie on the same line). So the length of $P^{'}$ is

$$2(\lambda_h + 1) + 5 = 2\lambda_h + 7 < 2\lambda_h + 9$$

contradicting the claim that P is a shortest closed path of odd length starting and ending at R. Since our choice of R and P was arbitrary, P does not circumnavigate the nonagon and must go around the pentagon.

□

Lemma 5. *Let $R = (R_x, R_y) \in A_3 \cup B_1$ and P be a shortest closed path of odd length starting and ending at R. Then P does not circumnavigate the nonagon and must go around the pentagon.*

Proof. Assume, on the contrary, that P circumnavigates the nonagon. Then we have two cases:

Case 1: If $R \in B_1$, let C_n be the top right or top left vertex of the pentagon. More precisely, C_n is the top left vertex of the pentagon if R is to the left of the break $\mathcal{B}$ and C_n is the top right vertex of the pentagon if R is to the right of the break $\mathcal{B}$. Observing the grid, it becomes apparent that the path P can be broken down into the portion moving from R to C_n, the path around the 8 edges of the nonagon to the bottom corner of the nonagon closest to C_n and then the path from bottom corner of the nonagon closest to C_n back to R. If λ_h is the horizontal length of the portion from R to C_n and λ_v is the vertical length of the portion from R to C_n then the length of P is given by $2\lambda_h + \lambda_v + (\lambda_v + 1) - 2 + 8 = 2(\lambda_h + \lambda_v) + 7$. We make slight adjustments to the horizontal length because we leave the nonagon at vertex one unit away from C_n. Define C_p as the bottom left or bottom right vertex of the pentagon. C_p is whichever vertex closer to R. Let $P^{'}$ be a shortest closed path of odd length starting and ending at R circumnavigating the pentagon. The path $P^{'}$ can be broken down into the portion moving from R to C_p, the path around the 5 edges of the pentagon to C_p and then the path from C_p back to R. Now, since C_p is one unit below C_n, in this case, the vertical length of the vertical portion from R to C_p for the path $P^{'}$ is given by $\lambda_v - 1$. The horizontal length of the horizontal portion from R to C_P for the path $P^{'}$ is not greater than λ_h. Therefore, the length of $P^{'}$ is at most

$$2\left[\lambda_h + (\lambda_v - 1)\right] + 5 = 2(\lambda_h + \lambda_v) + 3 < 2(\lambda_h + \lambda_v) + 7$$

contradicting the claim that P is a shortest closed path of odd length starting and ending at R. Since our choice of R and P was arbitrary, P does not circumnavigate the nonagon and must go around the pentagon.

Case 2: If $R \in A_3$, let C_n be the top left vertex or top right vertex of the pentagon. Again, λ_h is the horizontal length of the portion from R to C_n and λ_v is the vertical length of the portion from R to C_n. If R is directly below the break, then we can use either vertex. We can break the path P down into the portion moving from R to C_n, the path around the 9 edges of the nonagon back to C_n and then path from C_n to R. In this case, because the two vertices that combined at the bottom of the nonagon have a length of 1 unit we can not traverse exactly 7 units on the nonagon. The length of the path P is at least $2(\lambda_h + \lambda_v) + 9$.

Let C_p be the central vertex at the bottom edge of the pentagon. Let $P^{'}$ be a shortest closed path of odd length starting and ending at R circumnavigating the pentagon. The vertical length for the portion from R to C_p will be $\lambda_v - 1$ since C_p is again one unit below C_n. Since C_n is one unit away (horizontally) from C_p the horizontal length of the portion from R to C_p is at most $\lambda_h - 1$ making the length of $P^{'}$ at most equal to

$$2(\lambda_h - 1 + \lambda_v - 1) + 5 = 2(\lambda_h + \lambda_v) + 1 < 2(\lambda_h + \lambda_v) + 9$$

contradicting the hypothesis. By the above argument, if $R = (R_x, R_y) \in A_3 \cup B_1$ and P is a shortest closed path of odd length starting and ending at R, then P does not circumnavigate the nonagon and must circumnavigate the pentagon.

□

Lemma 6. *Let $R = (R_x, R_y) \in B_2 \cup A_2$ and P be a shortest closed path of odd length starting and ending at R. Then P does not circumnavigate the pentagon and must go around the nonagon.*

Proof. We use the same idea as in Lemma 5, consequently we will leave out some details that have already been included in previous lemmas from now on. Assume, on the contrary, that P circumnavigates the pentagon. If $R \in B_2$, let C_p be the top right or top left vertex of the pentagon. From observing the grid it becomes apparent that the path P can be divided into the portions moving from R to C_p, the path around the 5 edges of the pentagon back to C_p and then the path from C_p back to R. If λ_h is the horizontal length from R to C_p and λ_v is the vertical length from R to C_p then the length of P is given by $2(\lambda_h + \lambda_v) + 5$.

Define C_n to be one of the vertices adjacent to D on the nonagon. C_n is the vertex adjacent to D on the left if R is to the left of the break and C_n is the vertex adjacent to D on the right if R is to the right of the break. Let $P^{'}$ be a shortest closed path of odd length starting and ending at R circumnavigating the nonagon. The path $P^{'}$ contains 3 components, the portion moving from R to C_n, the path around the 9 edges of the nonagon to C_n and then path from C_n back to R. Now since C_p is one unit below C_n in this case, the vertical length for the portion from R to C_n is given by $\lambda_v - 1$. The horizontal length of the portion from R to C_n is at most $\lambda_h - 2$ (since you must either go right, down then left or left, down then right to get to C_p). So the length of $P^{'}$ is at most

$$2\left[(\lambda_v - 1) + (\lambda_h - 2)\right] + 9 = 2(\lambda_v + \lambda_h) + 3 < 2(\lambda_h + \lambda_v) + 5$$

contradicting the claim that P is a shortest closed path of odd length starting and ending at R circumnavigates the pentagon. Since our choice of R and P was arbitrary, P does not circumnavigate the pentagon and must go around the nonagon.

If $R \in A_2$, C_p is the top left vertex or top right vertex of the pentagon. Again, let λ_h be the horizontal length from R to C_p and λ_v be the vertical length from R to C_p. The length of the path P is $2(\lambda_h + \lambda_v) + 5$. Let C_n be one of the two vertices next to D. Define $C_n^{'} \neq C_n$ to be the second neighbouring vertex of D. Now you notice that the path taken from R to the nonagon and from the nonagon to R is different. This is because we never actually return to the point C_n before going back to R. However, the horizontal length does not change. The path P' can be broken down into the portion moving from R to C_n, the path around exactly 7 edges of the nonagon to C_n' and then the path from C_n' to R. The horizontal length for the portion from R to C_n is at most $\lambda_h - 2$ (since you must either go right, down then left or left, down then right to get to C_p) and the vertical length of the portion from R to C_n is $\lambda_v - 1$. The length of P' is at most equal to

$$2(\lambda_h - 2 + \lambda_v - 1) + 7 = 2(\lambda_h + \lambda_v) + 1 < 2(\lambda_h + \lambda_v) + 5$$

contradicting the hypothesis. By the above argument, if $R = (R_x, R_y) \in A_2 \cup B_2$ and P is a shortest closed path of odd length starting and ending at R. P does not circumnavigate the pentagon and must go around the nonagon.

□

To summarize Lemmas 3 to 6 we have the following:

Let R be a chosen reference point of degree 3 (not directly above the break i.e. $R \neq D$).

- If $R = (R_x, R_y) \in A_1$ such that $R_y \geq D_y$, then P can circumnavigate either the pentagon or nonagon.
- If $R = (R_x, R_y) \in A_1$ such that $R_y < D_y$ or $R = (R_x, R_y) \in A_3 \cup B_1$ then P does not circumnavigate the nonagon but goes around the pentagon.
- If $R = (R_x, R_y) \in B_2 \cup A_2$ then P does not circumnavigate the pentagon but goes around the nonagon.

The length of shortest path of odd length is unique as all these different shortest paths have the same odd length. However, the actual shortest closed path of odd length is not unique. The results of Lemmas 5 and 6 may make it seem that P is unique in those specific cases. However, as already mentioned earlier, P is almost never unique. For example, when $R = (R_x, R_y) \in A_3 \cup B_1$ we know P must go around the pentagon, but this doesn't mean P is unique. There might be multiple alternative paths that go around the pentagon, one going left where another might go right on its way to the pentagon.

Definition 4. *Let $A = (A_x, A_y)$ and $B = (B_x, B_y)$ be vertices on the grid. We define the vertical distance between A and B as $\mid A_y - B_y \mid$.*

Definition 5. *Let $A = (A_x, A_y)$ and $B = (B_x, B_y)$ be vertices on the grid. We define the horizontal distance between A and B as $|\, A_x - B_x \,|$.*

The theorems on the following pages are the main theorems discussed in [2].

2.3.1 R lies at the top end of a vertical line

Theorem 7. *Let R be positioned at the top of a vertical line. Then*

(a) R lies in Region A if and only if $S \equiv 1\,(mod\,4)$;

(b) R lies in Region B if and only if $S \equiv 3\,(mod\,4)$.

Proof. We verify the forward implication for (a) directly. Suppose $R = (R_x, R_y) \in A = A_1 \cup A_2 \cup A_3$. Then either $R \in A_1$ or $R \in A_2$ or $R \in A_3$. Each of these cases will be considered separately. We show that in any of the previously mentioned cases, $S \equiv 1 \mod 4$. Define P to be a shortest closed path of odd length, starting and ending at R.

Case 1: If $R = (R_x, R_y) \in A_1$. Let C be the top left or top right vertex of the pentagon. More precisely, C is the top left vertex if the reference point of choice R is to the left of the break and C is the top right vertex if the reference point R is to the right of $\mathcal{B}$. Recall that S is the length of the shortest closed path of odd length starting at R. We must know first the horizontal and vertical distance from R to C. The horizontal distance from R to C is given by the formula

$$\Delta x = \begin{cases} |\, R_x - (D_x - 1)\,|\,, & R_x \leq D_x \\ R_x - (D_x + 1)\,, & R_x > D_x. \end{cases} \tag{2.1}$$

We subtract 1 from the x-coordinate of D when the reference point is to the left of the break because in this case C is the top left vertex of the pentagon. Similarly, we add one to the x-coordinate of D when the reference point is to the right of the break because in this case C is the top right vertex of the pentagon. We define the vertical distance between R and C by

$$\Delta y = R_y - (D_y - 1) \tag{2.2}$$
$$= R_y - D_y + 1. \tag{2.3}$$

Similarly, we subtract 1 from the y-coordinate of D because in this case C is one unit below D in terms of vertical distance. We can split the path P into 3 components: the path from R to C represented by $\Delta x+\Delta y$; the path around the pentagon, which is five units in length and the path from C to R represented again by $\Delta x+\Delta y$. Therefore,

$$S \equiv 2(\Delta x+\Delta y)+5 \mod 4.$$

The path circumnavigating the nonagon could also be another shortest path but because of Lemma 3 it is sufficient to just consider only the path circumnavigating the pentagon because both paths are of the same length. It remains to show that

$$S \equiv 2(\Delta x+\Delta y)+5 \mod 4 \equiv 1 \mod 4.$$

We make the following observations;

- If D_x and R_x are both even, because of the structure (bricks are staggered) the grid forms, D_y and R_y are odd, thus Δx is odd (subtracting two even numbers and adding 1 gives an odd number) and Δy is odd (subtracting two odd numbers initially gives an even number, adding 1 then makes the final number odd).
- If D_x and R_x are both odd, then D_y and R_y are even and consequently Δx is odd and Δy is odd.
- If D_x is odd and R_x is even, then D_y is even and R_y is odd and consequently Δx is even and Δy is even.
- If D_x is even and R_x is odd, then D_y is odd and D_y is even and consequently Δx is even and Δy is even.

From here on, we will use a table like the one below in summarizing observations of this nature

D_x and R_x are even.	D_y and R_y are odd.	Δx and Δy are odd.
D_x and R_x are odd.	D_y and R_y are even.	Δx and Δy are odd.
D_x is odd and R_x is even.	D_y is even and R_y is odd.	Δx is even and Δy is even.
D_x is even and R_x is odd.	D_y is odd and R_y is even.	Δx is even and Δy is even.

Table 2.1: Theorem 7, $R \in A_1$.

In any of these 4 cases, $\Delta x + \Delta y$ is an even number.

Therefore

$$\begin{aligned} S &\equiv 2(\Delta x + \Delta y) + 5 \mod 4 \\ &\equiv 2(2k) + 5 \mod 4 \quad (k \text{ an integer since } \Delta x + \Delta y \text{ is even.}) \\ &\equiv 4k + 5 \mod 4 \\ &\equiv 0 + 5 \mod 4 \\ &\equiv 1 \mod 4. \end{aligned}$$

Case 2: If $R = (R_x, R_y) \in A_2$. Let C be one of the two vertices adjacent to D. Define $C' \neq C$ to be the second neighbouring vertex of D. Fix the vertex to the left of D as C and the vertex to the right of D to C'. Now you notice that the shortest closed path going around the nonagon does not use the same edges from R to the nonagon as it does from the nonagon back to R. This is the reason why it is necessary for us to have a separate formula calculating the distance back to the nonagon. The path P can be broken down into the portion moving from R to C, the path around exactly 7 edges of the nonagon to C' and then path from C' to R. In this situation, we will denote the horizontal distance between R and C by

$$\Delta x = \begin{cases} R_x - D_x + 1, & R_x > D_x \\ |\, R_x - D_x + 1 \,|, & R_x \leq D_x. \end{cases} \tag{2.4}$$

In a similar fashion, we will denote the horizontal distance between C' and R by

$$\Delta x' = \begin{cases} |\, R_x - D_x - 1 \,|, & R_x \leq D_x \\ R_x - D_x - 1, & R_x > D_x. \end{cases} \tag{2.5}$$

Since C is on the same level as D in this case we have that the vertical distance between R and C is

$$\Delta y = |\, R_y - D_y \,|. \tag{2.6}$$

Observe that even though Δx and $\Delta x^{'}$ always share the same parity they do not have the same congruence modulo 4. Since C and $C^{'}$ are two units apart on the grid

$$\Delta x = \begin{cases} \Delta x^{'} - 2, & R_x \leq D_x \\ \Delta x^{'} + 2, & R_x > D_x. \end{cases}$$

Therefore,

$$S \equiv \Delta x + \Delta x^{'} \pm 2 + 2\Delta y + 7 \mod 4. \tag{2.7}$$

Substituting Δx for $\Delta x^{'} \pm 2$ gives

$$S \equiv 2\left(\Delta x + \Delta y\right) + 7 \mod 4. \tag{2.8}$$

We make the following observations:

D_x and R_x are even.	D_y and R_y are odd.	Δx is odd and Δy is even.
D_x and R_x are odd.	D_y and R_y are even.	Δx is odd and Δy is even.
D_x is odd and R_x is even.	D_y is even and R_y is odd.	Δx is even and Δy is odd.
D_x is even and R_x is odd.	D_y is odd and R_y is even.	Δx is even and Δy is odd.

Table 2.2: Theorem 7, $R \in A_2$.

In any of these 4 cases, $(\Delta x + \Delta y)$ is an odd number.

$$\begin{aligned} S &\equiv 2\left(\Delta x + \Delta y\right) + 7 \mod 4 \\ &\equiv 2(2k+1) + 7 \mod 4 \quad (k \text{ an integer since } \Delta x + \Delta y \text{ is odd.}) \\ &\equiv 2 + 7 \mod 4 \quad (\text{note that all odd integers are congruent to 1 or 3} \mod 4.) \\ &\equiv 9 \mod 4 \\ &\equiv 1 \mod 4. \end{aligned}$$

Case 3: If $R = (R_x, R_y) \in A_3$. Let C be the bottom centre vertex of the pentagon. The path P here moves from R to C, around the pentagon back to C and then from C back to R. Here Δx, the horizontal distance between R and C is independent of where R lies and is given by the formula

$$\Delta x = |\, R_x - D_x \,| \,. \tag{2.9}$$

In addition, Δy is

$$\Delta y = |\, R_y - (D_y - 2) \,| \,. \tag{2.10}$$

Now,

$$S \equiv 2(\Delta x + \Delta y) + 5 \mod 4 \tag{2.11}$$

Once again, we must check the parity of Δx and Δy.

D_x is odd and R_x is even.	D_y is even and R_y is odd.	Δx and Δy are odd.
D_x and R_x are even.	D_y and R_y are odd.	Δx and Δy are even.
D_x and R_x are odd.	D_y and R_y are even.	Δx and Δy are even.
D_x is even and R_x is odd.	D_y is odd and R_y is even.	Δx and Δy are odd.

Table 2.3: Theorem 7, $R \in A_3$.

Again, in any of these 4 cases, $(\Delta x + \Delta y)$ is an even number. Therefore

$$\begin{aligned} S &\equiv 2(\Delta x + \Delta y) + 5 \mod 4 \\ &\equiv 2(2k) + 5 \mod 4 \quad (k \text{ an integer since } \Delta x + \Delta y \text{ is even.}) \\ &\equiv 4k + 5 \mod 4 \\ &\equiv 0 + 5 \mod 4 \\ &\equiv 1 \mod 4. \end{aligned}$$

Thus, if $R \in A$ then $S \equiv 1 \mod 4$. By the contrapositive argument, if $S \equiv 3 \mod 4$ then R lies in Region B. Thus proving the reverse implication of (b).

Similarly, we will now prove the forward implication for (b) and as a consequence obtain the reverse implication for (a), thereby completing the proof. Suppose that $R = (R_x, R_y) \in B = B_1 \cup B_2$. Then either $R \in B_1$ or $R \in B_2$. We have the following 2 cases

Case 1: If $R = (R_x, R_y) \in B_1$. Set C to be the bottom left or bottom right vertex of the pentagon. We want C to be the closest entrance point to the pentagon from R depending where in B_1 the point R is located. C is the bottom left vertex if the reference point of choice R is to the left of the break. C is the bottom right vertex if the reference point R is to the right of $\mathcal{B}$.

We must first know the horizontal and vertical distance from R to C. The horizontal distance from R to C is given by the formula

$$\Delta x = \begin{cases} |\, R_x - (D_x - 1)\,|, & R_x \leq D_x \\ R_x - (D_x + 1)\,, & R_x > D_x. \end{cases} \tag{2.12}$$

We subtract one from the x-coordinate of D when the reference point is to the left of the break because in this case C is the top left vertex of the pentagon. Similarly, we add one to the x-coordinate of D when the reference point is to the right of the break because in this case C is the bottom right vertex of the pentagon. We define the vertical distance between R and C by

$$\Delta y = |\, R_y - (D_y - 2)\,|\,. \tag{2.13}$$

We subtract two from the y-coordinate of D because in this case C is two units below D in terms of vertical distance. We can split the path P into 3 components: the path from R to C represented by $\Delta x + \Delta y$; the path around the pentagon, which is five units in length and the path from C to R represented again by $\Delta x + \Delta y$. Therefore,

$$S \equiv 2(\Delta x + \Delta y) + 5 \mod 4. \tag{2.14}$$

It remains to show that

$$S \equiv 2(\Delta x + \Delta y) + 5 \mod 4 \equiv 3 \mod 4. \tag{2.15}$$

We make the following observations:

D_x and R_x are even.	D_y and R_y are odd.	Δx is odd and Δy is even.
D_x and R_x are odd.	D_y and R_y are even.	Δx is odd and Δy is even.
D_x is odd and R_x is even.	D_y is even and R_y is odd.	Δx is even and Δy is odd.
D_x is even and R_x is odd.	D_y is odd and R_y is even.	Δx is even and Δy is odd.

Table 2.4: Theorem 7, $R \in B_1$.

In any case, $\Delta x + \Delta y$ is an odd number. Therefore

$$\begin{aligned} S &\equiv 2(\Delta x + \Delta y) + 5 \mod 4 \\ &\equiv 2(2k+1) + 5 \mod 4 \quad (k \text{ an integer since } \Delta x + \Delta y \text{ is odd.}) \\ &\equiv 4k + 7 \mod 4 \\ &\equiv 0 + 7 \mod 4 \\ &\equiv 3 \mod 4. \end{aligned}$$

Case 2: If $R = (R_x, R_y) \in B_2$. Set C to be one of the two vertices adjacent to D. C is the right-adjacent vertex if R is to right of the break. Similarly, C is the left adjacent vertex if R is to the left of the break. We can break the path P down into the portion moving from R to C, the path around the 9 edges of the nonagon back to C and then path from C to R. In this situation, the horizontal distance between R and C is

$$\Delta x = \begin{cases} R_x - D_x - 1, & R_x > D_x \\ |\, R_x - D_x + 1 \,|, & R_x \leq D_x. \end{cases} \tag{2.16}$$

The reasoning behind the formula above is the similar to the discussion in case 1. Since C is on the same level as D in this case we have that the vertical distance between R and C is

$$\Delta y = |\, R_y - D_y \,|\,. \tag{2.17}$$

We conclude that in this case

$$S = 2(\Delta x + \Delta y) + 9. \tag{2.18}$$

We make the following observations:

D_x and R_x are even.	D_y and R_y are odd.	Δx is odd and Δy is even.
D_x and R_x are odd.	D_y and R_y are even.	Δx is odd and Δy is even.
D_x is odd and R_x is even.	D_y is even and R_y is odd.	Δx is even and Δy is odd.
D_x is even and R_x is odd.	D_y is odd and R_y is even.	Δx is even and Δy is odd.

Table 2.5: Theorem 7, $R \in B_2$.

In any of these 4 cases, $(\Delta x + \Delta y)$ is an odd number. We then have that

$$\begin{aligned} S &\equiv 2(\Delta x + \Delta y) + 9 \mod 4 \\ &\equiv 2(2k+1) + 9 \mod 4 \quad (k \text{ an integer since } \Delta x + \Delta y \text{ is odd.}) \\ &\equiv 2 + 9 \mod 4 \quad (\text{note that all odd integers are congruent to 1 or 3} \mod 4.) \\ &\equiv 11 \mod 4 \\ &\equiv 3 \mod 4. \end{aligned}$$

Thus if $R \in B$ then $S \equiv 3 \mod 4$. By the contrapositive argument, if $S \equiv 1 \mod 4$ then R lies in Region A. And therefore, the reverse implication of (a) has been proved.

□

2.3.2 R lies at the bottom end of a vertical line

We now prove the analogous result for when the reference point is at the bottom of a vertical line, namely:

Theorem 8. *Let R be positioned at the bottom of a vertical line. Then*

(a) R lies in Region A if and only if $S \equiv 3\,(mod\,4)$.

(b) R lies in Region B if and only if $S \equiv 1\,(mod\,4)$.

Proof. The proof follows a similar technique to the proof of Theorem 7. We verify the forward implication directly and then use the contrapositive to show the backward implication. The only difference will be a change in the parity of Δy caused by the reference point R being at the bottom of a vertical line.

For part (a), let $R \in A$ and P be a shortest closed path of odd length, starting and ending at R. We need to consider 3 cases:

Case 1: If $R \in A_1$. Let C be the top left or top right vertex of the pentagon, depending on which side of the region A_1 the point R lies. The horizontal distance from R to C is given by

$$\Delta x = \begin{cases} \mid R_x - (D_x - 1) \mid, & R_x \leq D_x \\ R_x - (D_x + 1), & R_x > D_x. \end{cases} \tag{2.19}$$

The vertical distance from R to C will be given by

$$\Delta y = R_y - (D_y - 1). \tag{2.20}$$

The path P goes from R to C, around the pentagon and from C back to R. Therefore,

$$S \equiv 2(\Delta x + \Delta y) + 5 \mod 4$$

An analogous result to Lemma 3 justifies why we are at liberty to use only the pentagon in our analysis of this case. The staggering of the bricks on the wall means that R_x and R_y have the same parity whenever the reference point R is at the bottom of a vertical line. We will again observe the parity of Δx and Δy under this condition.

D_x and R_x are even.	D_y is odd and R_y is even.	Δx is odd and Δy is even.
D_x and R_x are odd.	D_y is even and R_y is odd.	Δx is odd and Δy is even.
D_x is odd and R_x is even.	D_y is even and R_y is even.	Δx is even and Δy is odd.
D_x is even and R_x is odd.	D_y is odd and R_y is odd.	Δx is even and Δy is odd.

Table 2.6: Theorem 8, $R \in A_1$.

In any case Δx and Δy have opposing parity and so $\Delta x + \Delta y$ is an odd number. Consequently,

$$\begin{aligned} S &\equiv 2(\Delta x + \Delta y) + 5 \mod 4 \\ &\equiv 2(2k+1) + 5 \mod 4 \quad (k \text{ an integer since } \Delta x + \Delta y \text{ is odd.}) \\ &\equiv 2 + 5 \mod 4 \quad (\text{note that all odd integers are congruent to 1 or 3} \mod 4.)) \\ &\equiv 7 \mod 4 \\ &\equiv 3 \mod 4. \end{aligned}$$

Case 2: If $R = (R_x, R_y) \in A_2$ then, as in Case 1 it is easy to see that Equations (2.4), (2.5), (2.6), (2.7) and (2.8) for Δx, $\Delta x'$, Δy and S respectively, from Theorem 7 (Case 2) hold. The only change occurs in the table as follows:

D_x and R_x are even.	D_y is odd and R_y is even.	Δx is odd and Δy is odd.
D_x and R_x are odd.	D_y is even and R_y is odd.	Δx is odd and Δy is odd.
D_x is odd and R_x is even.	D_y is even and R_y is even.	Δx is even and Δy is even.
D_x is even and R_x is odd.	D_y is odd and R_y is odd.	Δx is even and Δy is even.

Table 2.7: Theorem 8, $R \in A_2$.

In any of these 4 cases, Δx and Δy have matching parity. Therefore, $(\Delta x + \Delta y)$ is an even number. Now,

$$\begin{aligned} &\equiv 2\left(\Delta x + \Delta y\right) + 7 \mod 4 \\ &\equiv 2(2k) + 7 \mod 4 \quad (k \text{ an integer since } \Delta x + \Delta y \text{ is even.}) \\ &\equiv 0 + 7 \mod 4 \\ &\equiv 7 \mod 4 \\ &\equiv 3 \mod 4. \end{aligned}$$

Case 3: If $R = (R_x, R_y) \in A_3$, then Equations (2.9), (2.10) and (2.11) from Theorem 7 hold for Δx, Δy and S respectively. Once again, we must check the parity of Δx and Δy.

D_x is odd and R_x is even.	D_y is even and R_y is even.	Δx is odd and Δy is even.
D_x and R_x are even.	D_y is odd and R_y is even.	Δx is even and Δy is odd.
D_x and R_x are odd.	D_y is even and R_y is odd.	Δx is even and Δy is odd.
D_x is even and R_x is odd.	D_y is odd and R_y is odd.	Δx is odd and Δy is even.

Table 2.8: Theorem 8, $R \in A_3$.

Again, in any of these 4 cases, Δx and Δy have opposite parity. Therefore, $(\Delta x+\Delta y)$ is an odd number. Now,

$$\begin{aligned} S &\equiv 2(\Delta x + \Delta y) + 5 \mod 4 \\ &\equiv 2(2k+1) + 5 \mod 4 \quad (k \text{ an integer since } \Delta x + \Delta y \text{ is odd.}) \\ &\equiv 2 + 5 \mod 4 \quad (\text{note that all odd integers are congruent to 1 or 3} \mod 4.) \\ &\equiv 7 \mod 4 \\ &\equiv 3 \mod 4. \end{aligned}$$

Thus, if $R \in A$ then $S \equiv 3 \mod 4$. By the contrapositive argument, if $S \equiv 1 \mod 4$ then R lies in Region B. Thus proving the reverse implication (b).

We will now prove the forward implication of (b). Suppose that $R = (R_x, R_y) \in B = B_1 \cup B_2$. Then either $R \in B_1$ or $R \in B_2$. We have the following 2 cases.

Case 1: If $R = (R_x, R_y) \in B_1$, then Equations (2.12), (2.13) and (2.14) from Theorem 7 hold for Δx, Δy and S respectively. We make the following observations;

D_x and R_x are even.	D_y is odd and R_y is even.	Δx is odd and Δy is odd.
D_x and R_x are odd.	D_y is even and R_y is odd.	Δx is odd and Δy is odd.
D_x is odd and R_x is even.	D_y is even and R_y is even.	Δx is even and Δy is even.
D_x is even and R_x is odd.	D_y is odd and R_y is odd.	Δx is even and Δy is even.

Table 2.9: Theorem 8, $R \in B_1$.

Δx and Δy here have matching parity and so $\Delta x + \Delta y$ is an even number.

Therefore,

$$\begin{aligned}
S &\equiv 2(\Delta x + \Delta y) + 5 \mod 4 \\
&\equiv 2(2k) + 5 \mod 4 \quad (k \text{ an integer since } \Delta x + \Delta y \text{ is even.}) \\
&\equiv 4k + 5 \mod 4 \\
&\equiv 0 + 5 \mod 4 \\
&\equiv 1 \mod 4.
\end{aligned}$$

Case 2: If $R = (R_x, R_y) \in B_2$, then Equations (2.16), (2.17) and (2.18) from Theorem 7 hold for Δx, Δy and S respectively. We make the following observations;

D_x and R_x are even.	D_y is odd and R_y is even.	Δx is odd and Δy is odd.
D_x and R_x are odd.	D_y even and R_y is odd.	Δx is odd and Δy is odd.
D_x is odd and R_x is even.	D_y and R_y are even.	Δx is even and Δy is even.
D_x is even and R_x is odd.	D_y and R_y are odd.	Δx is even and Δy is even.

Table 2.10: Theorem 8, $R \in B_2$.

In any of these 4 cases, Δx and Δy have matching parity. $(\Delta x + \Delta y)$ is an even number. We then have that

$$\begin{aligned}
S &\equiv 2(\Delta x + \Delta y) + 9 \mod 4 \\
&\equiv 2(2k) + 9 \mod 4 \quad (k \text{ an integer since } \Delta x + \Delta y \text{ is odd.}) \\
&\equiv 0 + 9 \mod 4 \\
&\equiv 9 \mod 4 \\
&\equiv 1 \mod 4.
\end{aligned}$$

Thus if $R \in B$ then $S \equiv 1 \mod 4$. By the contrapositive argument, if $S \equiv 3 \mod 4$ then R lies in Region A. Thus proving the reverse implication of (a)

□

2.4 Conclusion

This chapter presents some of the work done in [2], with a significant amount of detail added to it. The introduction of six preliminary lemmas with proofs adds a great level of detail to the proof of major results in [2]. We provide a summary of the major findings at the end of some sections.

Chapter 3

The Algorithm

3.1 Introduction

In the previous chapter, we took a bottom-up approach. We first discussed smaller results and used those to build up to the bigger results (main theorems). In this section, we do the opposite. We will take a top-down approach, first looking at pseudo-code of the algorithm, then commenting on and justifying each step. In addition, examples of the algorithm being applied will be given.

3.2 Algorithm pseudo-code

3.2.1 R lies at the top of a vertical line

The following pseudo-code represents an algorithm that applies the previously discussed Theorems 7 and 8 to locate exactly where the hole (break) in our wall (grid) is. On the next page is the pseudo-code for this algorithm. The assumption is that all inputs given into the algorithm will be correct and obtained experimentally. The inputs are R_1 (a chosen reference point lying at the top of a vertical line), S_1 (the shortest path of odd length starting and ending at R_1) and S_2 (the shortest path of odd length starting and ending at R_2). The outputs of the algorithm are the co-ordinates of D, the node directly above the break $\mathcal{B}$.

Algorithm 1 Computes the co-ordinates of D

Input: R_1 (a chosen reference point lying above a vertical line), S_1 (the shortest path of odd length starting and ending at R_1), S_2 (the shortest path of odd length starting and ending at R_2)

Output: The co-ordinates of D (the node directly above the break) $\mathcal{B}$.

function CoordinatesOfD(R_1, S_1, S_2)
  $R_1 \leftarrow (0, 0)$
  $R_2 \leftarrow \left(\frac{S_1-1}{2}, 0\right)$ ▷ determine the regions of the reference points.
  if $S_1\%4 == 1$ **then**
    $R_1 \in A$
    if $S_2 == 2(S_1 - 1)$ **then**
      $R_2 \leftarrow \left(-\left(\frac{S_1-1}{2}\right), 0\right)$ ▷ Take in a new value for S_2
      if $S_2 == 7$ **then**
        $D \leftarrow \left(\frac{S_1-1}{2} - 1, 1\right)$
      else if $9 \leq S_2 \leq S_1$ **then**
        $D \leftarrow \left(R_{2x} - 2 - \left(\frac{S_2-9}{4}\right), -\left(\frac{S_2-9}{4}\right)\right)$
      end if
    else if $7 \leq S_2 \leq S_1$ **then**
      if $S_2 == 7$ **then**
        $D \leftarrow \left(\frac{S_1-1}{2} - 1, 1\right)$
      else if $9 \leq S_2 \leq S_1$ & $S_2\%4 == 1$ **then**
        $D \leftarrow \left(R_{2x} - 2 - \left(\frac{S_2-9}{4}\right), -\left(\frac{S_2-9}{4}\right)\right)$
      end if
    else if $S_1 < S_2 \leq 2(S_1 - 5)$ & $(S_2 - S_1)\%4 == 0$ & $S_1 \geq 13$ **then**
      $D \leftarrow \left(R_{2x} - 4 - \left(\frac{S_2-9}{4}\right), \left(\frac{5-S_1}{4}\right)\right)$
    else if $S_2\%4 == 3$ & $S_2 > S_1$ **then**
      $D \leftarrow \left(R_{2x} - 1 - \left(\frac{S_2-5}{2}\right) + \left(\frac{S_1-5}{4}\right), -\left(\frac{5-S_1}{4} + 2\right)\right)$
    end if
  else if $S_1\%4 == 3$ **then**
    if $S_2 == 2(S_1 - 1)$ **then**
      $R_2 \leftarrow \left(-\left(\frac{S_1-1}{2}\right), 0\right)$ ▷ Take in a new value for S_2
      if $5 \leq S_2 \leq S_1 - 2$ & $S_2\%4 == 1$ **then**
        $D \leftarrow \left(R_{2x} + 2 + \left(\frac{S_2-9}{4}\right), \left(\frac{S_2-9}{4} + 3\right)\right)$
      end if
    else if $5 \leq S_2 \leq S_1 - 2$ & $S_2\%4 == 1$ **then**
      $D \leftarrow \left(R_{2x} - 2 - \left(\frac{S_2-9}{4}\right), \left(\frac{S_2-9}{4} + 3\right)\right)$
    else if $S_1 < S_2 \leq 2S_1 - 3$ & $S_2\%4 == 3$ **then**
      $D \leftarrow \left(R_{2x} - 2 - \left(\frac{S_2-9}{2} + \left(\frac{S_1-7}{4}\right)\right), -\left(\frac{S_1-7}{4}\right)\right)$
    end if
  end if
  return D
end function

The pseudo-code alone is of course not a satisfactory guide to the logic behind finding the coordinates of D. As we study the formulae for computing the coordinates of the break, it will become clear that the form of the formulae provided in "Hole in a wall" are not cast in stone [2]. In fact, the geometric interpretation of the paths S_1 and S_2 determines the formula for locating the coordinates of D. However, even though formulae sometimes appear different, they must be equivalent since the location of the break is unique. We will show this equivalence by algebraic means. Firstly, we will elaborate on the Steps that must be followed in order to locate D.

1. Choose a reference point R_1 located at the top of a vertical line on the grid. Set $R_1 = (0, 0)$ so that we can have the entire grid on a co-ordinate plane with R_1 as the origin.

2. A value for the length of the shortest path of odd length starting and ending at R_1 can be obtained experimentally. Call the length of this path S_1. Recall that if $S_1 \equiv 1 \mod 4$ then R_1 lies in region A of our grid and if $S_1 \equiv 3 \mod 4$ then R_1 must lie in region B (see Theorem 7).

3. A second reference point R_2 is obtained by moving the detector $\frac{S_1-1}{2}$ to the right so that the coordinates of R_2 are given by $R_2 = \left(\frac{S_1-1}{2}, 0\right)$. Choosing R_2 this way ensures S_1 and S_2 have the same vertical length. We then use this to compute the horizontal length of S_2 which is used in finding the coordinates of D.

4. The value for S_2 (the length of the shortest closed path of odd length starting and ending at R_2 can again) be found experimentally. The results of Theorems 7 and 8 will then apply here again.

5. Now we provide some branching logic. If

$$S_2 = 2\left(\frac{S_1 - 1}{2} + \frac{S_1 - 5}{2}\right) = 2S_1 - 1$$

   then both R_1 and R_2 are in region A_1 or both are in region B_1 to right of the break. S_2 being much larger than S_1 implies we are moving much further away from the location of the break in choosing the second reference point. In this case, we must then repeat the last two Steps (Steps 3 and 4) but this time move the detector $\frac{S_1-1}{2}$ to the left of R_1 so that the coordinates of R_2 are given as $R_2 = \left(-\frac{S_1-1}{2}, 0\right)$.

6. If $R_1 \in A_1$ to the left of the break, then we will have that $R_2 = \left(\frac{S_1-1}{2}, 0\right)$. Recall that Δx is the change in horizontal length and Δy is the change in the

vertical length. Here the length of S_1 (as seen in the previous section) obeys the following congruence

$$S_1 \equiv 2(\Delta x + \Delta y) + 5 \mod 4.$$

In particular, if R_1 is located in region A_1 below D then $\Delta y = 0$ and R_1 has y-coordinates $D_y - 1$ (see Lemma 4 proof) and so

$$\begin{aligned} S_1 &\equiv 2(\Delta x + \Delta y) + 5 \mod 4 \\ &\equiv 2\Delta x + 5 \mod 4 \quad \text{since } (\Delta y = 0). \end{aligned}$$

Hence

$$\frac{S_1 - 1}{2} \equiv \Delta x + 2 \mod 4.$$

Note. By Theorem 7 since $R_1 \in A_1$ then $S_1 \equiv 1 \mod 4 \implies S_1 - 1 \equiv 0 \mod 4$. Therefore $\frac{S_1-1}{2}$ is divisible by 2.

So we can see that $\frac{S_1-1}{2}$ is congruent to the distance from R_1 to the top left corner of the pentagon plus 2 modulo 4. In this case R_2 is always given by $R_2 = (D_x + 2, D_y - 1)$ (one unit away from the pentagon's top right corner) and because of the location of R_2, the length of S_2 is equal to 7 . From the above argument we deduce that

$$D = \left(\frac{S_1 - 1}{2} - 1, 1\right) \quad \text{for } S_2 = 7. \tag{3.1}$$

Note that R_2 is one unit below D vertically and two units to the right of D horizontally. We subtract just 1 from $\frac{S_1-1}{2}$ because the distance from R_1 to the top left corner of the pentagon is one unit away from D horizontally.

If R_1 is located above or at the same level as D and still to the left of the break then as a consequence of Lemma 3 the path S_1 can circumnavigate either the nonagon or the pentagon. However both paths will be of the same length. Now R_1 will have y-coordinate $D_y + i$, for $i = 0, 1, 2, \ldots$. The vertical distance between R_1 and D is i. We will in this case then have that

$$\begin{aligned} S_1 &\equiv 2(\Delta x + \Delta y) + 5 \mod 4 \\ &\equiv 2(\Delta x + i) + 5 \mod 4 \quad \text{since } (\Delta y = i) \end{aligned}$$

and hence

$$\frac{S_1 - 1}{2} \equiv \Delta x + 2 + i \mod 4.$$

So $R_2 = \left(\frac{S_1-1}{2}, D_y + i\right)$ will be at the point $(D_x + 2 + i, D_y + i)$. Geometrically, R_2 is just below the border between B_2 and A_1. This line of reasoning then allows us to compute D as

$$D = \left(\frac{S_1 - 1}{2} - 2 - \frac{S_2 - 9}{4}, -\frac{S_2 - 9}{4}\right) \quad \text{for } S_2 = \{9, 13, 17, \ldots, S_1\}. \quad (3.2)$$

This last formula needs a bit more justification. Note that moving $\Delta x + 2$ Steps to the right horizontally from R_1 places us at the $x-$coordinate of the top left corner of the nonagon. Also, R_2 is i Steps away horizontally and i Steps away vertically from the top left corner of the nonagon. So by subtracting 9 from S_2 and dividing by 4 you get the vertical or horizontal distance between R_2 and the top left corner of the nonagon which we know is 2 units away horizontally from D. Therefore $\frac{S_2-9}{4} = i$.

7. If $R_1 \in A_1$ to right of the break then the conditions of Step 5 are satisfied. That is we now set

$$R_2 = \left(-\frac{S_1 - 1}{2}, 0\right)$$

and this change will be reflected in the formulae we gave in Step 6. The coordinates of D will become

$$D = \left(-\frac{S_1 - 1}{2} + 1, 1\right) \quad \text{for } S_2 = 7 \quad (3.3)$$

and

$$D = \left(-\frac{S_1 - 1}{2} + 2 + \frac{S_2 - 9}{4}, -\frac{S_2 - 9}{4}\right) \quad \text{for } S_2 = \{9, 13, 17, \ldots, S_1\}. \quad (3.4)$$

8. If R_1 is located in region A_2, then placing R_2 a distance of $\frac{S_1-1}{2}$ units to the right of R_1 places R_2 in region A_1 away from the diagonal boundary between B_2 and A_1. As a consequence of Theorems 7 we have that

$$S_1 \equiv 1 \mod 4 \quad \text{and} \quad S_2 \equiv 1 \mod 4$$

and so

$$\begin{aligned} S_2 - S_1 \equiv 0 \mod 4 &\implies S_2 - S_1 = 4k \quad \text{for some integer } k \\ &\implies S_2 = S_1 + 4k \\ &\implies S_2 \in \mathcal{A} := \{S_1 + 4k \, : \, k \geq 2\}. \end{aligned}$$

The restriction $k \geq 2$ is introduced because $k = \frac{S_2-S_1}{4}$ (the number of horizontal Steps between R_2 and the boundary) and R_2 being located in region A_1 away from the boundary between B_2 and A_1 implies that $\frac{S_2-S_1}{4} \geq 2$. Here, we will have that $R_2 = \left(\frac{S_1-1}{2}, 0\right)$ is in region A_1 at the top of a vertical line. The expression $\frac{S_2-9}{2}$ gives the length of the path from R_2 to the top right corner of the nonagon.

The path from R_2 to the top right corner of the nonagon has the same vertical length as the path from R_1 to one of the vertices adjacent to D on the nonagon. Therefore if we can compute the vertical length of the latter path then we would be able to calculate the horizontal length of the former path. In this case the computation of the vertical length of the path between R_1 and the nonagon using the same technique as in the previous cases is not possible because there are not as many vertical edges as there are horizontal edges. In this case we will have to subtract 5 from S_1 so that there are as many vertical edges as horizontal edges in the path from R_1 to the nonagon and this is not to suggest that the path S_1 circumnavigates the pentagon. We instead are just considering the length (vertical or horizontal) of the path from R_1 to the top (right or left) corner of the nonagon instead of the path from R_1 to the vertex (left or right) adjacent to D in order to solve the problem we have just described. The expression $\frac{S_1-5}{4}$ then gives vertical length of the path from R_1 to the nonagon. The coordinates of D can therefore be computed by the following formula.

$$D = \left(\frac{S_1 - 1}{2} - 2 - \left(\left(\frac{S_2 - 9}{2} \right) - \left(\frac{S_1 - 5}{4} \right) \right), - \left(\frac{S_1 - 5}{4} \right) \right). \quad (3.5)$$

This formula is different to the formula provided in [2] but the two formulae are however equivalent. It is in fact immediately clear that $-\left(\frac{S_1-5}{4}\right) = \frac{5-S_1}{4}$. We have as well that

$$\begin{aligned}
&\frac{S_1 - 1}{2} - 2 - \left(\left(\frac{S_2 - 9}{2} \right) - \left(\frac{S_1 - 5}{4} \right) \right) \\
&= \frac{S_1 - 1}{2} - 2 + \frac{S_1 + 13 - 2S_2}{4} \\
&= \frac{S_1 - 1}{2} - 1 + \frac{-2S_2 + S_1 + 13 - 4}{4} \\
&= \frac{S_1 - 1}{2} - 1 + \frac{-2S_2 + S_1 + 9}{4} \\
&= \frac{S_1 - 1}{2} - 1 + \frac{-S_2 + S_1 - S_2 + 9}{4} \\
&= \frac{S_1 - 1}{2} - 1 - \left(\left(\frac{S_2 - S_1}{4} \right) + \left(\frac{S_2 - 9}{4} \right) \right).
\end{aligned}$$

We have therefore demonstrated that these formulae are equivalent.

9. If $R_1 \in A_3$, then $R_2 = \left(\frac{S_1-1}{2}, 0\right)$ and R_2 is at the top of a vertical in region B_1 to the right of the break. By Theorem 7(b) we know

$$\begin{aligned}
S_2 \equiv 3 \mod 4 &\implies S_2 - 5 \equiv 2 \mod 4 \\
&\implies S_2 - 5 = 4l + 2 \quad \text{for some } l \\
&\implies \frac{S_2 - 5}{2} \equiv 0 \mod 2.
\end{aligned}$$

So $\frac{S_2-5}{2}$ is an even number. The expression $\frac{S_2-5}{2}$ gives the number of edges (both vertical and horizontal) that S_2 passes through from R_2 to the bottom right corner of the pentagon. If we subtract from $\frac{S_2-5}{2}$ the quantity $\frac{S_1-5}{4}$ (which represents the vertical length of the portion of the path between R_1 and the bottom right corner of the pentagon), we will obtain the number of horizontal edges between the bottom right corner of the pentagon and R_2. This is justified because the vertical length of S_1 is equal to the vertical length of S_2. The coordinates of D can then be obtained as follows

$$D = \left(\frac{S_1 - 1}{2} - 1 - \left(\frac{S_2 - 5}{2} \right) + \left(\frac{S_1 - 5}{4} \right), \left(\frac{S_1 - 5}{4} \right) + 2 \right). \tag{3.6}$$

10. If $R_1 \in B_1$ to the left of the break, then the algorithm always places R_2 to be the first vertex to the right of the boundary between A_3 and B_1 at the bottom of a vertical line. The path S_2 goes around the pentagon (see Lemma 5) and crosses an equal number of horizontal and vertical edges whilst going to the bottom right corner of the pentagon. The number of horizontal edges between the pentagon and R_2 is $\frac{S_2-5}{4}$. The number of vertical edges therefore between the pentagon and R_2 is $\frac{S_2-5}{4}$. This formula follows a similar explanation to the one given in the last paragraph of Step 6. The coordinates of D are thus given by

$$D = \left(\frac{S_1 - 1}{2} - 1 - \left(\frac{S_2 - 5}{4} \right), \frac{S_2 - 5}{4} + 2 \right). \tag{3.7}$$

11. If $R_1 \in B_1$ to the right of the break, then we will proceed to Step 5 and set $R_2 = \left(-\frac{S_1-1}{2}, 0\right)$. It will be as if everything is as in the previous case only just reflected about the line $x = D_x$ on the y-axis. To elaborate, R_2 is the first vertex to the left of the boundary between A_3 and B_1 at the bottom of a vertical line. Justified by a similar rationale to Step 10, the coordinates of D are given by

$$D = \left(- \left(\frac{S_1 - 1}{2} \right) + 1 + \left(\frac{S_2 - 5}{4} \right), \frac{S_2 - 5}{4} + 2 \right). \tag{3.8}$$

12. If $R_1 \in B_2$ then R_2 is placed in region A_1 at the bottom of a vertical line. The quantity $\frac{S_2-9}{2}$ represents the length of the path from R_2 to the top right corner of the nonagon. The expression $\frac{S_1-7}{4}$ gives the vertical length of the paths S_1 and S_2. Therefore $2 + \left(\frac{S_2-9}{2}\right) - \left(\frac{S_1-7}{4}\right)$ gives the number of horizontal edges between R_2 and D. We can then obtain the coordinates of D as

$$D = \left(\frac{S_1 - 1}{2} - 2 - \left(\frac{S_2 - 9}{2} \right) + \left(\frac{S_1 - 7}{4} \right), - \left(\frac{S_1 - 7}{4} \right) \right). \tag{3.9}$$

Remark. The formulae given in Steps 10 and 11 are different to the formulae given in the paper "Hole in the wall". However, these formulae are equivalent. This last claim can be confirmed through a geometric justification. Lemma 5 states that S_2 circumnavigates the pentagon. This makes the formula $D =$

$\left(\frac{S_1-1}{2} - 2 - \left(\frac{S_2-9}{4}\right), \frac{S_2-9}{4} + 3\right)$ misleading. This is because one would expect that we are subtracting 9 because the path circumnavigates the nonagon when this is not the case. In this case subtracting 9 places us one unit to the right and one unit down from the pentagon's bottom right corner. In fact if you are 4 units away downwards from D the formula $D = \left(\frac{S_1-1}{2} - 3 - \left(\frac{S_2-13}{4}\right), \frac{S_2-13}{4} + 4\right)$ gives the coordinates of D.

Algebraically we observe that

$$\begin{aligned}\frac{S_1-1}{2} \mp 2 \mp \left(\frac{S_2-9}{4}\right) &= \frac{S_1-1}{2} \mp 2 \mp \left(\frac{S_2-5-4}{4}\right)\\ &= \frac{S_1-1}{2} \mp 2 \mp 1 \mp \left(\frac{S_2-5}{4}\right)\\ &= \frac{S_1-1}{2} \mp 1 \mp \left(\frac{S_2-5}{4}\right).\end{aligned}$$

Also,

$$\begin{aligned}\frac{S_2-9}{4} + 3 &= \frac{S_2-5-4}{4} + 3\\ &= \frac{S_2-5}{4} + 2\end{aligned}$$

and so we have confirmed algebraically that the formulae are equivalent.

3.2.2 R lies at the bottom of vertical line

We outline the key changes that occur when the reference point R_1 lies at the bottom of a vertical line. For a significant number of the cases, choosing R_1 to be at the bottom of a vertical line on the grid does not change the formulae for computing the coordinates of D. To keep this simple and interesting, we will draw up a table and, for all cases, check if the position of R_2 changes if R_1 is placed at the bottom of a vertical line. We will then explore in greater detail just a few of the cases.

1. Choose a reference point R_1 located at the bottom of a vertical line on the grid. Set $R_1 = (0, 0)$ so that we can have the entire grid on a co-ordinate plane with R_1 as the origin.

2. S_1, a value for the length of the shortest path of odd length starting and ending

at R_1 will be experimentally obtained. Recall that if $S_1 \equiv 3 \mod 4$ then R_1 lies in region A of our grid and if $S_1 \equiv 1 \mod 4$ then R_1 must lie in region B (see Theorem 8).

Steps 3 to 5 from Subsection 3.2.1 above still hold.

Step Number	**Position of R_1**	**Position of R_2**
6	$R_1 \in A_1$ (to the left of the break) at the bottom of a vertical line such that $D_y \leq R_y$.	$R_2 \in A_1$ (to the right of the break) at the top of a vertical line.
6	$R_1 \in A_1$ (to the left of the break) at the bottom of a vertical line such that $D_y > R_y$.	$R_2 \in A_1$ at the bottom of a vertical line. In particular, $S_2 = 7$ and R_2 is at the bottom right vertex of the nonagon.
7	$R_1 \in A_1$ (to the right of the break) at the bottom of a vertical line such that $D_y \leq R_y$.	$R_2 \in A_1$ (to the left of the break) at the top of a vertical line.
7	$R_1 \in A_1$ (to the right of the break) at the bottom of a vertical line such that $D_y > R_y$.	$R_2 \in A_1$ at the bottom of a vertical line. In particular, $S_2 = 7$ and R_2 is at the bottom left vertex of the nonagon.
8	$R_1 \in A_2$ at the bottom of a vertical line	$R_2 \in A_1$ at the top of a vertical line.
9	$R_1 \in A_3$ at the bottom of a vertical line.	$R_2 \in B_1$ at the top of a vertical line.
10	$R_1 \in B_1$ at the bottom of a vertical line to the left of the break.	$R_2 \in B_1$ at the bottom of a vertical line to the right of the break.
11	$R_1 \in B_1$ at the bottom of a vertical line to the right of the break.	$R_2 \in B_1$ at the bottom of a vertical line to the left of the break.
12	$R_1 \in B_2$ at the bottom of a vertical line.	$R_2 \in A_1$ at the bottom of vertical line.

Table 3.1: Algorithm, R_1 lies at the bottom of vertical line.

Below we explore cases in which the formula for computing the coordinates of D differs from that of an algorithm when the reference is at the top of a vertical line.

6. If $R_1 \in A_1$ to the left of the break, then Equations (3.1) and (3.2) hold.
7. If $R_1 \in A_1$ to right of the break then the conditions of Step 5 are satisfied. That is, we now set
$$R_2 = \left(-\frac{S_1 - 1}{2}, 0\right)$$
and this does not change the coordinates of D which are given by Equations (3.3) and (3.4).
8. If R_1 is located in region A_2, then placing R_2 a distance of $\frac{S_1-1}{2}$ units to the right of R_1 places R_2 in region A_1 away from the diagonal boundary between B_2 and A_1 at the top of a vertical line. Since $R_1 \in A$ at the bottom of a vertical line then Theorem 8 tells us that $S_1 \equiv 3 \mod 4$. Equation (3.5) does not apply in this case.

   The path from R_2 to the top right corner of the nonagon has the same vertical length as the path from R_1 to the vertices adjacent to D on the nonagon. We can use this to calculate the horizontal length of the former path as
$$\left(\frac{S_2 - 9}{2}\right) - \left(\frac{S_1 - 7}{4}\right).$$
   In this case the expression $\frac{S_2-7}{4}$ gives the vertical length of the path from R_1 to the vertex adjacent (right or left depending on R_1) to D. As a consequence of the above discussion, the coordinates of D are given by
$$D = \left(\frac{S_1 - 1}{2} - 2 - \left(\left(\frac{S_2 - 9}{2}\right) - \left(\frac{S_1 - 7}{4}\right)\right), -\left(\frac{S_1 - 7}{4}\right)\right).$$
9. If $R_1 \in A_3$, then $R_2 = \left(\frac{S_1-1}{2}, 0\right)$ and R_2 is at the top of a vertical in region B_1. By Theorem 8 we have $S_1 \equiv 3 \mod 4$. Hence Equation (3.6) does not hold in computing the coordinates of D.

   The path from R_1 to the bottom vertex of the pentagon does not have as many vertical edges as horizontal edges, yet we need that to be the case in order to calculate it's vertical length using the same strategy as before. To get around this problem, we will instead compute the vertical length as $\frac{S_1-3}{4}$, i.e. we will include the edges to the bottom left and right corners of the pentagon to ensure the number of horizontal edges is equal to the number of vertical edges. We can then calculate the horizontal length of the path from R_2 to the bottom right corner of the pentagon as $\left(\frac{S_2-5}{2}\right) + \left(\frac{S_1-3}{4}\right)$. Therefore, we can compute the coordinates of D as

$$D = \left(\frac{S_1-1}{2} - 2 - \left(\frac{S_2-5}{2}\right) + \left(\frac{S_1-3}{4}\right), \left(\frac{S_1-3}{4}\right) + 1\right).$$

10. If $R_1 \in B_1$ to the left of the break, then the algorithm always places R_2 at the first vertex to the right of the boundary between A_3 and B_1 at the bottom of a vertical line. The path S_2 goes around the pentagon (see Lemma 5) and crosses an equal number of horizontal and vertical edges whilst going to the bottom right corner of the pentagon. Therefore, the number of horizontal edges between the pentagon and R_2 is $\frac{S_2-5}{4}$. The number of vertical edges between the pentagon and R_2 is $\frac{S_2-5}{4}$. This formula follows a similar explanation to the one given on the last paragraph of Step 6 in Subsection 3.2.1. Therefore, the coordinates of D are given by Equation (3.7).

11. If $R_1 \in B_1$ to the right of the break, then Equation (3.8) stills holds in computing the coordinates of D.

12. If $R_1 \in B_2$ then, R_2 is placed in region A_1 at the bottom of a vertical line. The quantity $\frac{S_2-9}{2}$ represents the length of the path from R_2 to the top right corner of the nonagon. The expression $\frac{S_1-9}{4}$ gives the vertical length of the paths S_1 and S_2. Therefore, $2 + \left(\frac{S_2-9}{2}\right) - \left(\frac{S_1-9}{4}\right)$ gives the number of horizontal edges between R_2 and D. We can then obtain the coordinates of D as

$$D = \left(\frac{S_1-1}{2} - 2 - \left(\frac{S_2-9}{2}\right) + \left(\frac{S_1-9}{4}\right), -\left(\frac{S_1-9}{4}\right)\right).$$

3.3 Examples of reference point choices

Note that we are not aware beforehand of where the reference point R_1 lies. Rather, after obtaining experimentally a value for S_1 we employ Theorem 7 or Theorem 8 to then determine in which general region (A or B) R_1 lies. After using this information to produce a value for R_2 it then becomes possible to deduce a much more specific location for R_1 and R_2 i.e., to pinpoint in which specific A or B region they are. It must be pointed out that we choose apriori whether we place initially the detector (at the top or bottom of a vertical line) and then proceed to use Theorems 7 and 8 to deduce whether R_2 lies at the top or bottom of a vertical line. We now explore some examples of the algorithms being applied.

3.3.1 Example 1

In our first example the detector is randomly placed at the top of a vertical line on a piece of graphene with a SV defect. This is our reference point R_1, and we assign it coordinates $(0,0)$. The experimental value for S_1 obtained is 17. Since $17 \equiv 1 \mod 4$ then, by Theorem 7, R_1 is in region A. Now, R_2 has the coordinates $R_2 = \left(\frac{S_1-1}{2}, 0\right) = (8,0)$. A value for S_2 is determined experimentally. In this case, $S_2 = 25$. Having moved only an even number of steps from R_1 to R_2 we know that R_2 is at the top of a vertical line. $S_2 \equiv 1 \mod 4$ which implies R_2 is at the top of a vertical line in region A (by Theorem 7). Also S_2 is not equal to 7 (eliminating the special case in part 6 in the algorithm).

Note that $S_2 \neq 2S_1 - 1$ since $2(17) - 1 = 33 \neq 25$, so R_1 and R_2 are not both in A_1 to the right of the break. Also, $S_2 > S_1$ so Steps 6 and 7 cannot be applied. Lastly, since R_1 and R_2 are both in region A we cannot use Step 9. Thus, we must have R_1 in A_2 and R_2 in A_1. Therefore, we use Step 8 of the algorithm and obtain D as follows:

$$
\begin{aligned}
D &= \left(\frac{S_1-1}{2} - 2 - \left(\left(\frac{S_2-9}{2}\right) - \left(\frac{S_1-5}{4}\right)\right), -\left(\frac{S_1-5}{4}\right)\right) \\
&= \left(8 - 2 - \left(\left(\frac{25-9}{2}\right) - \left(\frac{17-5}{4}\right)\right), -\left(\frac{17-5}{4}\right)\right) \\
&= (1, -3).
\end{aligned}
$$

See figure on the next page.

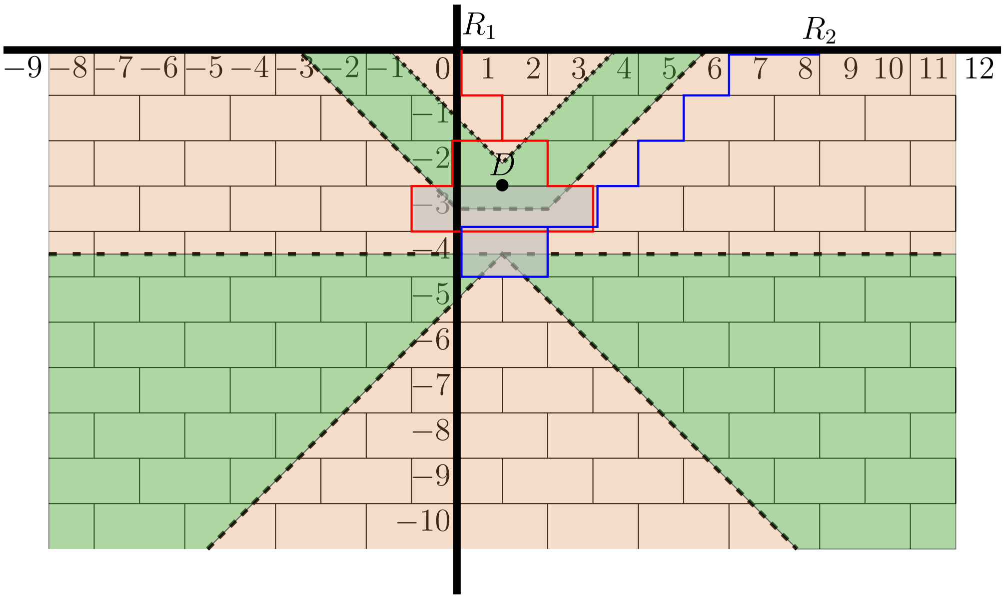

Figure 3.1: Example 1

3.3.2 Example 2

Place the detector at the top of a vertical line and call this point R_1. Set $R_1 = (0, 0)$. Obtain S_1 (the path in red) as $S_1 = 21$. Since $S_1 \equiv 1 \mod 4$ then R_1 lies in region A (by Theorem 7). Therefore

$$R_2 = \left(\frac{S_1 - 1}{2}, 0\right) = \left(\frac{21 - 1}{2}, 0\right) = (10, 0).$$

We obtain experimentally that $S_2 = 13$ and thus R_2 lies in region A at the top of a vertical line (since $S_2 \equiv 1 \mod 4$ plus we moved an even number of steps to the right from R_1 to R_2). Also S_2 is not equal to 7 (eliminating the special case in part 6 in the algorithm). Note that $S_2 \neq 2S_1 - 1$ since $2(21) - 1 = 41 \neq 13$, so R_1 and R_2 are not both in A_1 to the right of the break. Also, since R_1 and R_2 are both in an A region we cannot use Step 9. Now, $S_2 < S_1$, so Step 8 is not applicable. Therefore, by Step 6 we must have R_1 in A_1 to the left of the break and R_2 in A_1 to the right of the break. Using Step 6 of the algorithm, we obtain D as follows:

$$\begin{aligned} D &= \left(\frac{S_1 - 1}{2} - 2 - \left(\frac{S_2 - 9}{4}\right), -\frac{S_2 - 9}{4}\right) \\ &= \left(10 - 2 - \frac{13 - 9}{4}, -\frac{13 - 9}{4}\right) \\ &= (7, -1). \end{aligned}$$

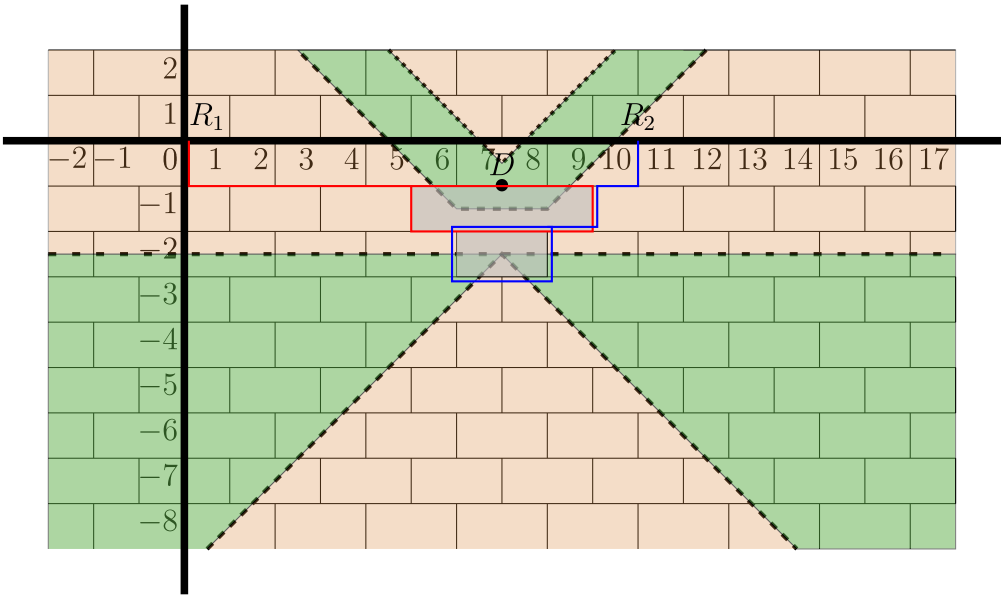

Figure 3.2: Example 2

3.3.3 Example 3

Set R_1 (chosen randomly at the top of a vertical line) to be $R_1 = (0, 0)$. The length of S_1 is obtained as 23. Now $23 \equiv 3 \mod 4$ and, as a consequence of Theorem 7, $R_1 \in B$. R_2 is obtained as

$$R_2 = \left(\frac{S_1 - 1}{2}, 0\right) = \left(\frac{23 - 1}{2}, 0\right) = (11, 0).$$

The value obtained for S_2 is $S_2 = 17$. We moved an odd number of steps to the right from R_1 to R_2, so R_2 will be at the bottom of a vertical line. $R_2 \in B$ since $17 \equiv 1 \mod 4$ (by Theorem 8). Now, $S_2 = 17 \neq 2S_1 - 1 = 45$ and so Step 5 of the algorithm is not invoked and R_1 and R_2 are not both in region B_1 to the right of the break. Therefore, Step 11 does not apply. Also, because both R_1 and R_2 are in region B then, Step 12 is not applicable. So, we use Step 10 to conclude that R_1 is in B_1 to the left of the break and R_2 is in B_1 to the right of the break. D is thus given as follows:

$$\begin{aligned} D &= \left(\frac{S_1 - 1}{2} - 1 - \left(\frac{S_2 - 5}{4}\right), \frac{S_2 - 5}{4} + 2\right) \\ &= \left(11 - 1 - \frac{17 - 5}{4}, \frac{17 - 5}{4} + 2\right) \\ &= (7, 5). \end{aligned}$$

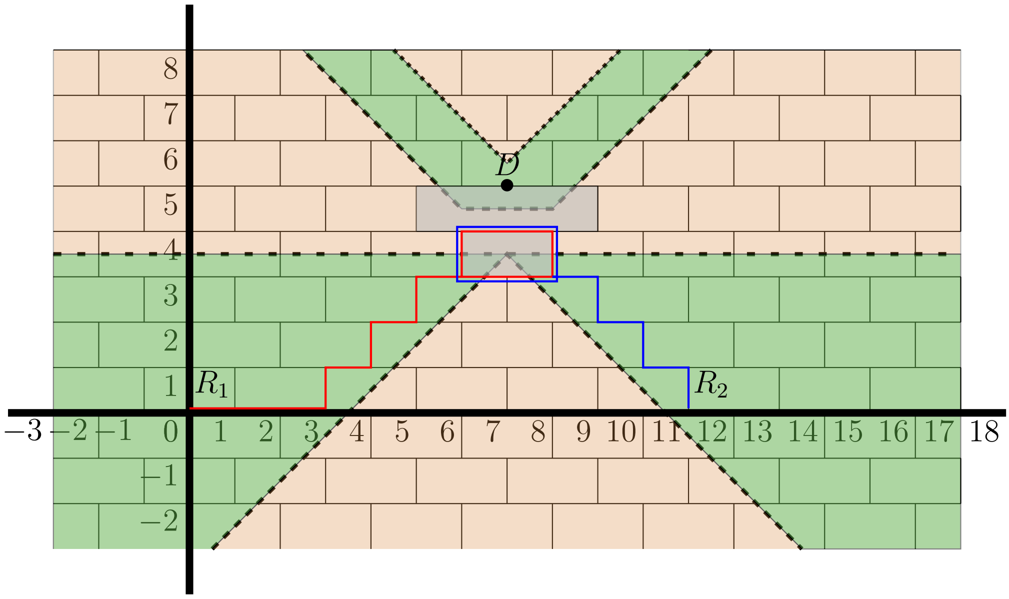

Figure 3.3: Example 3

3.3.4 Example 4

The next example is a mirror image of the previous. Let $R_1 := (0, 0)$ at the top of a vertical line. Experimentally we obtain $S_1 = 23$ and thus $R_1 \in B$ (Theorem 7). We set $R_2 = \left(\frac{S_1-1}{2}, 0\right) = \left(\frac{23-1}{2}, 0\right) = (11, 0)$. The value for S_2 is given to be 45. Therefore, $S_2 = 45 = 2S_1 - 1$ and hence Step 5 applies here. We must now set

$$R_2 = \left(-\frac{S_1 - 1}{2}, 0\right) = \left(-\frac{23 - 1}{2}, 0\right) = (-11, 0).$$

Thus, a new value for S_2 is obtained experimentally to be $S_2 = 17$ and so $R_2 \in A$ since $17 \equiv 1 \mod 4$ (by Theorem 8) as R_2 is at the bottom of a vertical line since we moved an odd number of steps. Note that, R_1 and R_2 were both in region B_1 to the right of the break before we changed the value of R_2 to $\left(-\frac{S_1-1}{2}, 0\right)$. Now, we have $R_1 \in B_1$ to the right of the break and $R_2 \in B_1$ to the left of the break. Therefore, Step 11 applies in this case. We can thus compute the coordinates of D as:

$$
\begin{aligned}
D &= \left(-\frac{S_1-1}{2}+1+\left(\frac{S_2-5}{4}\right), \frac{S_2-5}{4}+2\right) \\
&= \left(-11+1+\frac{17-5}{4}, \frac{17-5}{4}+2\right) \\
&= (-7,5).
\end{aligned}
$$

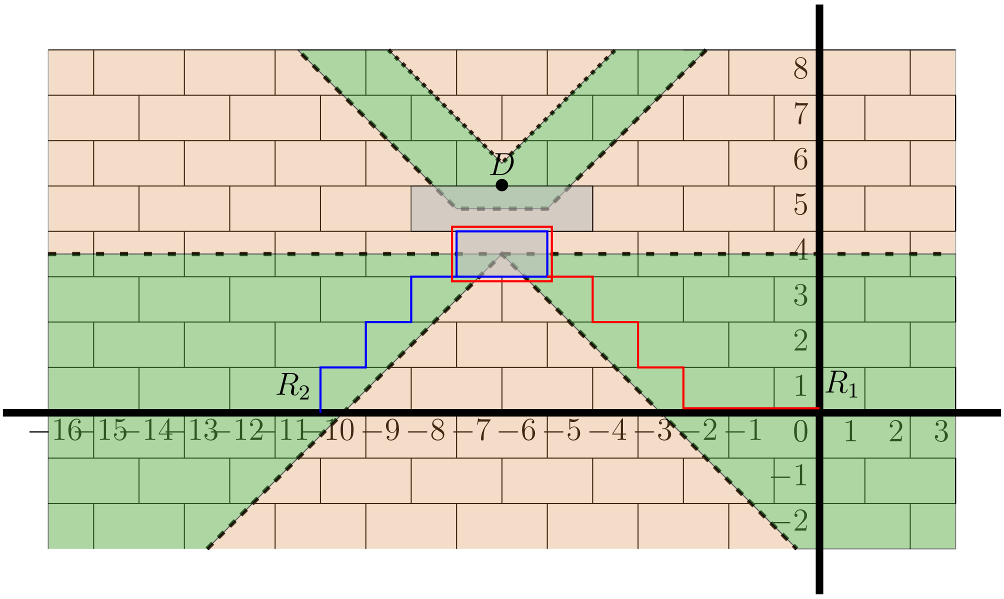

Figure 3.4: Example 4

3.3.5 Example 5

Set $R_1 = (0,0)$ to be at the top of a vertical line. The value obtained for S_1 is equal to $17 \equiv 1 \mod 4$ and hence R_1 is in the region A (Theorem 7). Now, $R_2 = \left(\frac{S_1-1}{2}, 0\right) = \left(\frac{17-1}{2}, 0\right) = (8,0)$. Here the value for S_2 is given to be $S_2 = 7$. Since $7 \equiv 3 \mod 4$ then R_2 lies in region A at the bottom of vertical line (Theorem 8 plus we moved an even number of steps to the right across from R_1 to R_2). The condition $S_2 = 2S_1 - 1$ is not satisfied. That is, R_1 and R_2 are not both in the region A_1 to the right of the break. Therefore, Steps 7 and 9 do not apply in this case. Also $S_2 < S_1$ so Step 8 cannot apply, and we must use Step 6. Also, since $S_2 = 7$ we use the special case of Step 6.

$$
\begin{aligned}
D &= \left(\frac{S_1 - 1}{2} - 1, 1\right) \\
&= \left(\frac{17 - 1}{2} - 1, 1\right) \\
&= (7, 1).
\end{aligned}
$$

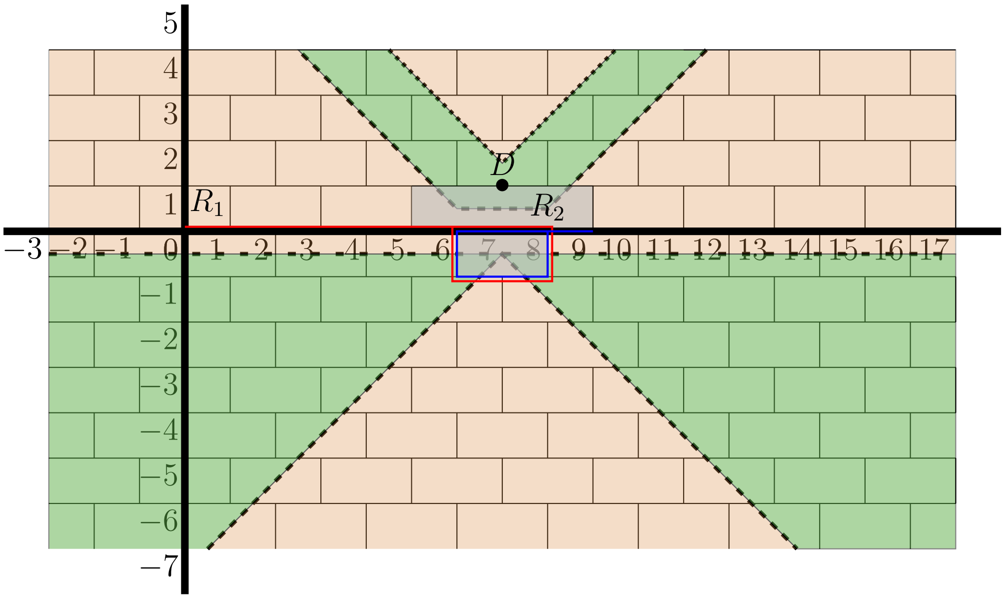

Figure 3.5: Example 5

3.3.6 Example 6

In this example, the detector is randomly placed at the bottom of a vertical line on a piece of graphene with a SV defect. This is our reference point R_1, and we assign it the coordinates $(0, 0)$. The value for S_1 is found to be $S_1 = 27$. Since $27 \equiv 3 \mod 4$, by Theorem 8, R_1 is in region A. Now, R_2 has the coordinates

$$
R_2 = \left(\frac{S_1 - 1}{2}, 0\right) = (13, 0).
$$

A value for S_2 is determined experimentally. In this case, $S_2 = 31$. Having moved only an odd number of steps from R_1 to R_2 we know that R_2 is at the top of a vertical line. Also, S_2 is not equal to 7 (eliminating the special case in part 6 in the algorithm). $S_2 \equiv 3 \mod 4$ which implies R_2 is at the top of a vertical line in region B (by Theorem 7). Thus, we must have R_1 in A_3 and R_2 in B_1 to the right of the break. Therefore, we use Step 9 of the algorithm and obtain D as follows:

$$D = \left(\frac{S_1 - 1}{2} - 2 - \left(\frac{S_2 - 5}{2} + \frac{S_1 - 3}{4}\right), \left(\frac{S_1 - 3}{4}\right) + 1\right)$$
$$= \left(13 - 2 - \left(\frac{31 - 5}{2} + \frac{27 - 3}{4}\right), \left(\frac{27 - 3}{4} + 1\right)\right)$$
$$= (4, 7).$$

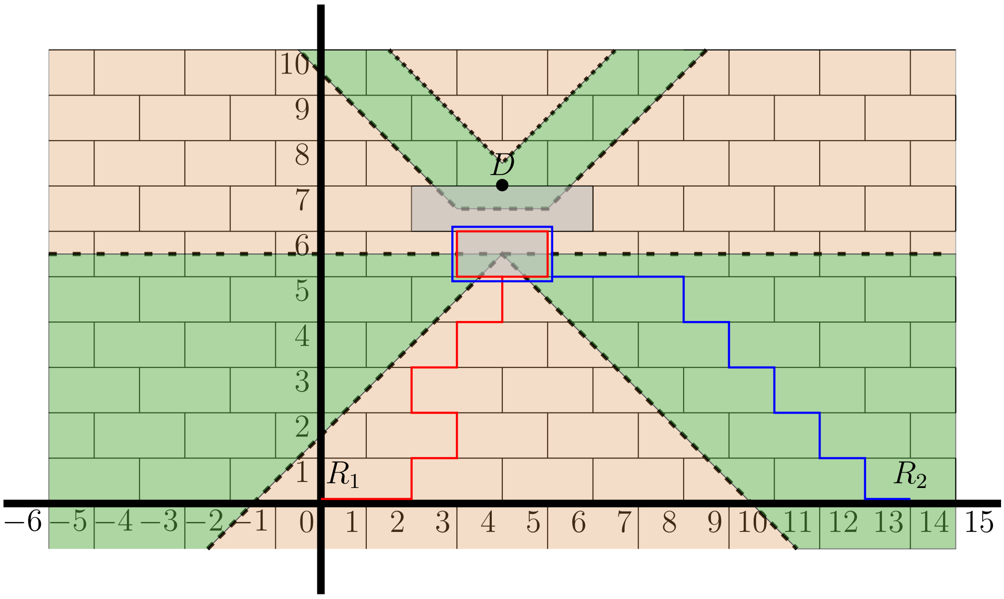

Figure 3.6: Example 6

3.3.7 Example 7

We set $R_1 = (0, 0)$ once again at the bottom of a vertical line. Our value obtained for S_1 is equal to 17. Therefore,

$$R_2 = \left(\frac{S_1 - 1}{2}, 0\right) = \left(\frac{17 - 1}{2}, 0\right) = (8, 0).$$

We moved an even number of steps across to the right between R_1 and R_2 so R_2 is at the bottom of a vertical line. Here $S_2 = 19$. Since $19 \equiv 1 \mod 4$ then R_2 lies in region A (Theorem 8).

Note that $S_1 \equiv 1 \mod 4$ and R_1 is in region B (Theorem 8). Consequently, we have moved from region B to region A and the only possibility for this to occur is when we move from B_2 to A_1 and hence Step 12 applies thus, by Step 12 we can compute the coordinates of D as

$$\begin{aligned} D &= \left(\frac{S_1 - 1}{2} - 2 - \left(\frac{S_2 - 9}{2}\right) + \left(\frac{S_1 - 9}{4}\right), -\left(\frac{S_1 - 9}{4}\right)\right) \\ &= \left(8 - 2 - \left(\left(\frac{19 - 9}{2}\right) + \left(\frac{17 - 9}{4}\right)\right), -\left(\frac{17 - 9}{4}\right)\right) \\ &= (3, -2). \end{aligned}$$

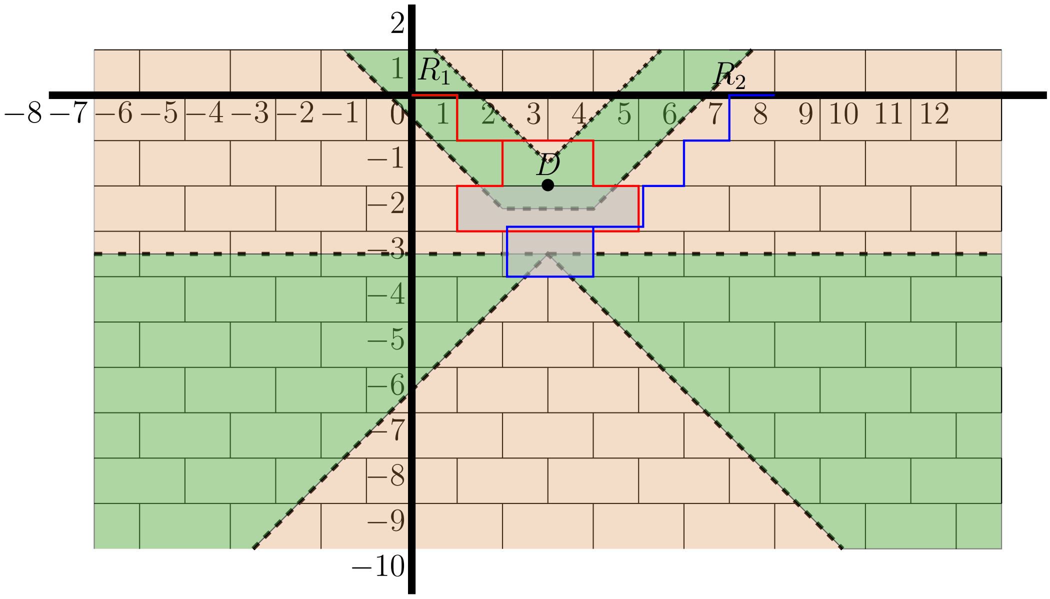

Figure 3.7: Example 7

3.4 Conclusion

This chapter presents an algorithm for locating single vacancy breaks with the detector placed at the top of a vertical line. We added detailed justifications on the steps of the algorithm and changes that would need to be made to the algorithm when the detector is placed at the bottom of the vertical line as an extension of the work done in [2]. We also provide a number of examples of the algorithm being applied.

Chapter 4

Further Explorations

4.1 Introduction

In this chapter we will reflect on the work done in this dissertation and discuss potential projects that could be covered in the future. This being a relatively new topic of study, there are still many avenues to pursue.

4.2 A reflection

A large portion of this dissertation's work was based on the paper "Finding the Hole in the Wall". We took a more detailed approach in that we first attempted to investigate how the location of the reference point R affected which polygons the path S circumnavigated. This was extremely beneficial because it made understanding the two main proofs in [2] a little bit easier. We were able to reach the following previously outlined conclusions through rigorous proof:

Let R be a chosen reference point of degree 3 (not directly above the break i.e. $R \neq D$).

- If $R = (R_x, R_y) \in A_1$ such that $R_y \geq D_y$, then P can circumnavigate either the pentagon or nonagon.
- If $R = (R_x, R_y) \in A_1$ such that $R_y < D_y$ or $R = (R_x, R_y) \in A_3 \cup B_1$ then P does not circumnavigate the nonagon but goes around the pentagon.
- If $R = (R_x, R_y) \in B_2 \cup A_2$ then P does not circumnavigate the pentagon but goes around the nonagon.

Consequently we were able to re-affirm Theorems 7 and 8 that were originally given in [2].

We then used these results to discuss an algorithm where the given inputs are R_1 (a chosen reference point lying at the top of a vertical line), S_1 (the shortest path of odd length starting and ending at R_1). From these inputs we then later obtain R_2 as $R_2 = \left(\frac{S_1-1}{2}, 0\right)$ and then S_2 (the shortest path of odd length starting and ending at R_2) experimentally. The output of the algorithm is the co-ordinates of D, the node directly above the break $\mathcal{B}$.

We occasionally derived formulae that looked different to the formulae in [2]. However, when this was the case, we went on to further show that these new formulae were in fact equivalent to the formulae in [2]. We also investigated what changes would occur if R_1 was placed at the bottom of the vertical line. In some cases, it did not matter whether the reference point was now at the bottom of a vertical line, as the results of the formulae for locating D remained unchanged. This was a rather interesting observation.

4.3 Potential future explorations

A possible alternative way of looking at these problems would be the following. If $V(P)$ is the set of vertices visited on a particular path P, and $E(G)$ is a set of edges on this path, then $G = (V(P), E(G))$ can be viewed as a graph. In addition, a path P_1 is the same length as another path P_2 if there is a bijection between $V(P_1)$ and $V(P_2)$. We can impose a metric $d(u, v)$ on the set V of all vertices on the grid. As such, we can study (V, d) as a metric space, where u and v are vertices on the grid. Here I believe that through the use of graph theory one can explore many results pertaining to the grid and use these facts to come up with a new perspective on the problem at hand and potentially extended results.

The authors of [2] have written other papers exploring other types of defects. In [3], the authors continue to use the brick wall model that they developed in [2] to locate the position of the Stone-Wales and double vacancy defects in a similar graphene nano-ribbon structure. They then proceed to use number theoretic arguments to define the regions where the reference points are located in order to obtain distinct numerical properties of the lengths of the shortest odd closed paths. Two algorithms that can pinpoint the location of either a Stone-Wales defect or the double vacancy defect using at most three reference points, are provided.

The case under discussion in this dissertation and subsequent papers on the subject is ideal. Where there is only one defect in the grid. We might have more than one flaw (vacancy) in the physical world. And, of course, that case would be more difficult to handle. The strategy here was divide and conquer. In many cases, dealing with simpler cases first allows us to use them as a building block for future solutions.

The potential areas of future investigation in this case are as follows:

- Expand the brick wall model to cases where multiple defects exist on the grid.
- Study of the hexagonal graphene grid using other mathematical models, such as graph theory.
- Study other types of defects that exist in graphene, like the authors have done in [3].
- Study and determine adaptations of the model to cases where graphene is not flat (3D graphene) [6].

Graphene may sometimes be subjected to stress, resulting in elongation or a potentially shortening of the C-C (bond between two carbon atoms) bonds [16]. In this case, we assume the edge length to still be similar enough for this model to work.

4.4 Conclusion

Graphene, in my opinion, is no longer receiving the same level of media attention that it did when it was first discovered. Because of its numerous potential applications, it is critical that research on it continue. I believe it is significant enough that we should continue to seek more information and a better understanding of the natural world, because even though failure is a possibility, success would have many exciting possibilities. As mathematicians, we can not stop making abstractions from what we see in nature.

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