School of Physics

Numerical and Analytical Approaches to Modelling 2D Flocking Phenomena.

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Abstract

In the first section of this thesis, the motion of self-propelled particles (known as boids) in a 2D system with open boundaries is considered using a Lagrangian Individual-Based model. In fact, two different variations of this model are developed, one with a cohesion potential based on the soft core Morse potential and the other based on the hard core Lennard-Jones potential, both well understood in the fields of atomic and molecular physics respectively. The results obtained from these two different variations are then compared with one another, as well as with earlier work in the field, in order to determine the effectiveness and applicability of hard-core and soft-core cohesion potentials, the differences in flocking behaviour they produce, and context in which each one is applicable to real flocking systems.

Some of the flocking phases and shapes obtained from these two different models are then compared to a number of specific flocking situations observed in the real world. It is shown that a flocking model with a soft-core cohesion potential is particularly good at modelling the cluster type flocks most commonly seen in bird and fish schools, whilst a hard-core cohesion potential has a tendency to produce a distinctive wavefront type flock which has been well documented in the context of large herds of mammals, particularly wildebeest. It is also found that stable vortex states, observed in systems of bacteria, are only seen with a soft-core cohesive potential.

In the second section of this thesis, a novel approach is taken to model a flocking as a gas. An equation of state is derived analytically for a flocking system in 2D using the virial expansion. The relationships obtained from this equation of state are compared to
the results of a simple numerical simulation in order to establish the accuracy of this new approach to modelling flocking systems.

Finally, this new statistical mechanical approach to deriving a flocking model is applied to the Vicsek model, the most well understood flocking model derived from a physics perspective. It is found that the analytical relationships between a number of key variables of the gas system such as pressure, temperature, interaction length, entropy and heat capacity derived from the virial equation of state bear a close comparison to those same variables derived numerically from the standard Vicsek model, thus demonstrating the efficacy and veracity of this new approach to modelling flocking phenomena.
DECLARATION

This is to certify that:

(i) the thesis comprises only my original work towards the MPhil except where indicated in the Statement of Contributions,

(ii) due acknowledgment has been made in the text to all other material used,

(iii) the thesis is less than 50,000 words in length, exclusive of table, maps, bibliographies, appendices and footnotes.

Jason Adam Smith
This thesis topic and its theory, as presented in Chapters 2, 3 and 4 were formulated and developed in collaboration with my supervisor, Andy Martin. I have been primarily responsible for the code and numerical work presented in Chapter 2 as well as the analytical calculations undertaken in Chapters 3 and 4. The ideas and interpretation of the results were developed with input and guidance from my supervisor Andy Martin. Resources obtained from other publications and authors have been cited in the text where appropriate.
During the course of this project, the following article has been published, which is based on the work presented in Chapter 2 of this thesis. It is listed here for reference.

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Flocking is happening all around us, each and every day of our lives. One has only to look to the sky on a clear day to see groups of birds wheeling in unison, seemingly of a single mind, flying as if belonging to a single body, united in action and in purpose. Many of us have been diving, and swam amongst the shoals of fish which behave almost as a single entity, their movements occurring in a strange, synchronous harmony. We have experienced the throngs of people leaving a football stadium on a Saturday evening or the jostling motion as our fellow humans thronging to catch the peak hour train. In fact, we are the product of flocking processes ourselves, millions upon millions of cells, each interacting through the most basic of stimuli, creating the thinking, seeing, feeling person who is sitting here reading this today. Flocking is universal, a ubiquitous part of the world we live in.

There are many different types of flocking behavior, occurring on many different scales from the human world, to the animal world, to the cellular world. It is my personal hope that one day, we can unify all of these flocking behaviours into a single small set of core principles, a grand theory of flocking. But for now, each of these is tackled using slightly different (but often similar) approaches. The focus of this work is primarily on flocking as it occurs in the animal world, for example in flocks of birds [1, 2, 3, 4], schools of fish [5, 6, 7], swarms of locust [8, 9] and herds of wildebeest [10, 11, 12].
In physics, a flock is defined as the coherent motion of a group of self-propelled particles arising from a simple set of interactions between the constituents of that group. The field of flocking research emerged out of computer graphics, where animators were attempting to create realistic looking biological systems for film and cinema purposes. C. Reynolds [13] was the first researcher to codify a set of key principles for writing an effective flocking algorithm for computer graphics in 1987. For some time flocking research existed primarily in the realm of computer animation and biology and it was not until Tamás Vicsek first introduced the concept of flocking to the physics community in 1995 [14], through the consideration of a simple agent-based model, that the field became an intensive area of study for physicists, paving the way for a new branch of interdisciplinary research into the physical mechanisms which result in the emergence of flocking. [1, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28].

All flocking models created thus far fall roughly into one of two broad categories [29]. The first category of models are known as Individual-Based Models, or IBMs. In an IBM each member of a flock is represented as an individual particle (known as a boid). The boids interact with one another via forces which are constructed to mimic the rules that it is believed are responsible for flocking behaviour. Equations of motion can then be written for each individual particle, and the simulation propagated forward through time. The second broad category are continuum models, of which hydrodynamical models are the primary example. In these models a flock is described as a fluid moving through space, and can be modelled through the use of hydrodynamic equations similar to the Navier-Stokes equations for a classical fluid. In a continuum model, the behaviour of each fluid particle is not tracked, but rather it is the bulk behaviour of the flock as a whole which is modelled, the equations effectively averaging over the behaviour of all the constituent members. This means that rather than modelling the position and velocity of each individual in the flock over time, the bulk behaviour of the flock itself is described and modelled.

Typically, IBMs are more amenable to numerical calculation and hydrodynamical models more open to analytical investigation, although this is not always the case. Another type
of flocking model which falls under the umbrella of continuum models is the modelling of a flock as a classical gas using a statistical approach. This avenue of research has not received a significant amount attention to date [30], but could potentially bring new insights into the field. It is this novel approach that is taken in Chapters 3 and 4 of this thesis.

1.1 Early History of Flocking

In order to understand the current state of flocking research, it is essential to take a brief tour through the history of the field. This begins by following the path of IBM development from its beginnings in computer animation in the late 80’s through the present day, and then following up by tracing the history of hydrodynamical models. Finally, it will be seen how these two approaches have influenced the research being developed here, and how the IBM model developed in Chapter 2 builds upon the past work of others in the field, and how the classical gas model of flocking presented in Chapters 3 and 4 was developed as a novel mathematical way of looking at this complex biological behaviour, much in the same way as the hydrodynamical approach was developed over a decade ago.

The field of flocking first emerged as a scientific study in the late 1980’s as a result of work by computer graphics experts who wanted to create realistic looking examples of coherent motion, such as schools of fish and flocks of birds, for computer applications and movie animation. They found that if each boid moved separately, or if the groupings had a single leader, the behaviour of the flock did not adequately resemble that which was observed in nature. The flocks they were trying to create did not look realistic. A major breakthrough to this problem came when Craig Reynolds published ”Flocks, Herds, and Schools: A Distributed Behavioral Model” in 1987 [13]. In this work, Reynolds suggested that rather than using a ‘follow the leader’ type principle, or having the individual boids behaving independently of one another, the boids should simply try to match the behaviour of the boids around them, their neighbours. Reynolds suggested that three simple rules could be used to produce realistic looking flocking behaviour in a computer graphics context.
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These rules were:

(1) Separation: Boids steer to avoid colliding or crowding other members of the flock.
(2) Alignment: Boids steer toward the average heading of nearby members of the flock.
(3) Cohesion: Boids steer towards some preferred average position between other members of the flock.

Encapsulated in these simple rules are the fundamentals of flocking behaviour, and these rules are still used today as the basis for simulating realistic coherent biological motion for computer animation and movie production. In fact, the 1992 movie, 'Batman Returns' [31] used a modified version of Reynolds algorithm in order to create simulated bat swarms and penguin flocks whilst the movie 'The Lion King' included aspects on Reynolds model in the simulation of wildebeest herds.

In 1992 a new mathematical model was introduced by the theoretical biologists Huth and Wissel in order to describe the movement of fish in schools [5]. The specific interactions associated with this model are shown and described in Fig. 1.1. At the time, this paper was mostly of interest to biologists, but it would come to form the basis of many later physics models of flocking, and become one of the most widely cited papers in the flocking literature [1, 22]. The model used was an effort to simulate the behaviour of fish schools in a realistic fashion and was based on 5 basic assumptions [5]:

(1) The motion of a fish is only influenced by the position and orientation of its nearest neighbours.
(2) The new velocity and the turning angle of each fish is calculated by probability distributions (taking into account random influences).
(3) The movement of each model fish is based upon the same behaviour model (there is no leader).
(4) The motion of the model fish group is not affected by external influences (no destination).
(5) The models should be as simple as possible. Only simple models promote a comprehension of the results.

Figure 1.1: Basic behaviour regions of the Huth and Wissel flocking model. For $r < r_1$ the black fish repels nearby neighbours. For $r_1 < r < r_2$ nearby fish have a tendency to align with the black fish (represented in the centre of the figure) but tend to remain at approximately the same separation. For $r_2 < r < r_3$ nearby fish are attracted to the black fish. For $r > r_3$ there is no interaction between the black fish and its neighbours. Finally in the region $\omega$ behind the black fish, the behaviour of neighbours does not effect the black fish, as it cannot see them. [Figure reproduced from [5]]

Most notable amongst these, (and the reason why this biological model has become important to physicists) is perhaps assumption (5). Many earlier biological models were simply too complex to be derived analytically, or even semi-analytically, rendering them difficult for physicists to analyze quantitatively, and the results could only be interpreted
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qualitatively. However, the model presented by Huth and Wissel was simple enough that variants of it could later be used by physicists to investigate complex and realistic flocking behaviour, whilst keeping the model simple enough so that quantitative results can still be obtained for many flocking characteristics. In fact, Huth and Wissel’s model forms the basis of a particularly important physics model published by Y. Tu in 2000 [22], which we will return to later.

1.2 Individual-Based Models of Flocking

For some time, the study of flocking remained the realm of biology, numerical simulation and computer animation. That is, until Tamas Vicsek and a team from Budapest noted the similarities between self-propelled biological systems and condensed matter systems, in particular, ferromagnetic systems. Vicsek believed that analogies could be drawn between the way flocking systems and ferromagnetic systems work and his 1995 paper ”Novel Type of Phase-Transition in a System of Self-Driven Particles” [14] set out to demonstrate how simple flocking behaviour could be simulated using a very simple physical model based roughly on the model of a ferromagnetic system. The use of such a simple model to create a self-propelled biological system opened the door for complex biological systems to be investigated and analysed with more mathematical rigor than was previously possible, and for physical properties such as temperature, density, entropy and other thermodynamic variables to be applied in the context of flocking to enable a deeper physical description of their behaviour.

It is worth going into some depth about the details of Vicsek’s model and some of the more interesting results obtained from it. The Vicsek model of flocking is very straightforward mathematically, and it remains the gold-standard in flocking, being the most well understood, most investigated and most cited example in the field. It is, in effect, the measuring stick against which all models are compared against in terms of simplicity and tractability. An important thing to point out though is that while the Vicsek model is
extremely tractable due to its simplicity and similarities to known physical problems, it is not a terribly realistic simulation of flocking behaviour in nature. The power of the Vicsek model lies in the fact that it provides a very accessible model, both numerically and analytically, for investigating systems of self-propelled biological particles, and although the behaviours produced by the model are not entirely indicative of real-world flocking behaviour, they serve as important demonstrations of many of the key characteristics which are observed in real flocks. The Vicsek model also serves as a strong basis on which other more complex models which more accurately replicate actual flocking behaviours observed in nature can be based.

What Vicsek showed in the original simulations was the emergence of ordered states from a disordered initial condition. Starting with a 2D box with periodic boundary conditions, particles were distributed at random positions $r_i$ with a constant speed $|\mathbf{v}_i|$ in some direction $\theta_i$. At each time step, the new position and direction were given by:

$$\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i \Delta t, \quad (1.1)$$
$$\theta_i(t + \Delta t) = \langle \theta_i(t) \rangle_r + \Delta \theta. \quad (1.2)$$

where $\langle \theta_i(t) \rangle_r$ defines the average angle of all the boids within a distance $r$ of boid $i$, $\Delta \theta$ is a random value defining noise in the boid following angle, $t$ is the time and $\Delta t$ is the time increment.

Using this simple model, Vicsek and others discovered that a group of self-propelled particles displayed many of the same characteristics as a ferromagnetic system [14]. At high values of stochastic noise, $\Delta \theta$, the motion of the particles (known in flocking research as boids) was essentially random (completely disordered), analogous to a high temperature ferromagnetic system. As stochastic noise is reduced past a critical value, a phase transition occurs, whereby the direction of the boids suddenly becomes correlated (directionally ordered), and their direction of motion aligns. The 4 key phases observed in Vicsek’s model are shown in Fig. 1.2. This simple observation gave birth to the field of flocking
as a physics discipline. Since this time physicists have gained a deeper understanding of the analogies and relationships between physical condensed matter systems, and biological self-propelled systems.

Figure 1.2: 4 different behaviours observed in the original Vicsek model. (a) At high noise and low density the boids movement is uncorrelated. (b) At low density and noise, boids tend to form small clumps of correlated behaviour. (c) At higher density and noise values, the boids tend to move randomly but with some small correlations. (d) At high density but low noise, there are correlations between boids on all length scales. [Figure reproduced from [14]]

Over the following years, the Vicsek model has been the subject of a great deal of analysis over the nature and type of phase transitions that occur within the system. In particular, there has been significant differences of opinion as to whether the phase transition that
occurs when the direction of the birds becomes correlated is of first order [28, 32] or second order [14, 27, 33, 34]. This has been the subject of sometimes fierce debate over the years following the publication of Vicseks flocking model [35]. Vicsek’s model has also been expanded to include motion in both one dimension [18] and three dimensions [19], instead of the original two [14], aswell as the presence of an interbody cohesive force [36].

In 2000 a new model was introduced to the physics community in a paper by Y.Tu [22]. This model was derived from an earlier Individual-Based Model (IBM) model used by the biologists Huth and Wissel [5], discussed in Section 1.1. This model included pairwise interactions on top of the alignment interactions present in Vicsek’s model in order to encapsulate more possible variations of flocking behaviour.

In Tu’s model, the boids are initially placed at random, within a box of some fixed size. Thereafter, the net force on boid $i$ is calculated at each new time step and is given by:

$$
\mathbf{F}_i = \sum_j (a f_a(r_{ij})\hat{\mathbf{v}}_j + b f_b(r_{ij})\hat{\mathbf{r}}_{ij}) + \eta_i,
$$

where $a$ and $b$ are adjustable parameters governing the strength of the alignment force and the cohesion force respectively, and the above equation represents a generalized approach to deriving a flocking force where both these components are present, $\hat{\mathbf{v}}_j$ is boid velocity and $\hat{\mathbf{r}}_{ij}$ is a unit vector along the line of interaction between boids $i$ and $j$. $\eta_i$ represents the random stochastic noise, and is a force vector of some magnitude in a random direction. This may best be demonstrated graphically, with Fig 1.3 providing an example of one such possible force.

As noted above, the model itself consists of two forces, a cohesion force ($f_b(r_{ij})$) between the individual boids, and an alignment force ($f_a(r_{ij})$) which affects the boids directional alignment with regard to one another. The cohesion force includes a hard core repulsion at small separations (zone 1 in Fig. 1.4), to prevent collisions, a region where the force on the boid decreases linearly with distance (zone 2 in Fig. 1.4), a preferred region of
Figure 1.3: An example of a flocking potential of the form specified by Y. Tu in [22]. Zone 1 consists of a hard core repulsion, zone 2 is primarily alignment with some weak attraction, zone 3 is strong attraction and zone 4 has no interaction. [Figure reproduced from [22]]
separation (zone 3 in Fig. 1.4) and at long distances, no interaction (zone 4 in Fig. 1.4). In addition to this cohesion force, is the alignment force required for all flocking systems, which attempts to take into account the boids propensity to travel in the same direction as their nearby neighbours. This force is a tophat operating over zone 2, but falling to zero in all other regions [22].

The flocking behaviours emerging from this model consisted of 5 different phases occupying some region of parameter space in the $a - b$ plane. The phase diagram of these phases is shown in Fig. 1.4. At very small values of $b$, the tendency is for the boids not to cluster, and instead to travel independently, essentially at random, resulting in what resembles a gaseous state in condensed matter physics. This region is represented by the black bars at the bottom of Fig. 1.4. At small values of $a$ and $b$, a stationary liquid is observed, where boids move with respect to one another, but the centre of mass velocity of the flock as a whole is zero. At small values of $a$, but large values of $b$, the flock transitions to a moving liquid, where the flock as a whole moves ($v_{CoM} \neq 0$) as well as individuals moving with respect to other members of the flock. For large values of both $a$ and $b$, a moving solid is observed, $v_{CoM} \neq 0$ but where the boids do not move position relative to other boids in the flock. Finally, for large $a$ and small $b$, a stationary solid is observed where $v_{CoM} = 0$ and there is no motion of the boids relative to other members of the flock. This finding was particularly important because liquid/solid/gas phases are the most common phases in condensed matter physics. Additionally, previous research had concentrated almost exclusively on variations of the moving liquid phase, and this paper demonstrated that manipulation of the strength of a flocks alignment and cohesion can generate flocks with a wide range of different phases, and thus has the potential to explain much more diverse natural behaviours.

In 2005 the most complete review of the field to-date was completed in a paper by Toner, Tu and Ramaswamy [29], three researchers who have been heavily involved in the field since its early days. The paper features in depth analysis of both the most successful IBMs and fluid mechanical models to date, as well as some of the limitations of the work.
Figure 1.4: Phase diagram for the Y.Tu model in $a - b$ space. For high $a$, low $b$ flocks resemble a moving fluid, for high $a$, high $b$ they resemble a moving solid. For low $a$, high $b$ flocks resemble a stationary solid and for low $a$, low $b$ flocks resemble a stationary fluid. [Figure reproduced from [22]]
undertaken so far, and future directions for research in the field. Of particular note, the field has been lacking models with open boundary conditions. Most of the more successful models up until 2005 were simulated within reflecting or periodic boundary conditions [14, 19, 22, 36, 37]. However, this is not how flocking occurs in the real world. In the real world, flocks exist, form and move in free space, in the absence of fixed boundaries [2, 3].

This was considered one of the major limitations of the field at the time, and a barrier to having achieved flocking models which match up with reality [29]. Another limitation identified in the review, was the current dearth of experimental measurements. Although a small number of experimental papers, focused mainly on the movement of Dictyostelium (a soil living amoeba) [38] and Daphnia [39] along with several other bacteria types [40, 41, 42] had been conducted, there were few measurements of macroscopic flocking, and even though their were measurements of microscopic flocking, they were relatively few in number. Finally, deeper analysis of spontaneous vortex states was also suggested, although these had been touched on in a number of earlier papers [15, 17, 40, 43, 44], they had yet to be studied in depth, and since a number of bacterium have been observed to form spontaneous vortices these states were considered very amenable to experimental comparison [40, 42, 43].

Beginning in late 2006, several research groups (including our own) [45] have begun modelling flocking systems in free space [46, 45, 47, 48, 49], one of the important characteristics lacking in earlier flocking models. Additionally, a number of these have focused specifically on analysing the formation of spontaneous vortices, the stability of those vortices and the range of different behaviours exhibited by them. One particular set of papers by D’Orsogna et al [46, 47] used a cohesion force based on the Morse potential in free space in order to analyse the structure and stability of rotating flocking systems. Of particular note, it was found that double mill vortical structures (vortices that include boids rotating both clockwise and counter-clockwise) were only observed for soft-core cohesion potentials, and could not be replicated using a hard-core cohesion potential. Furthermore, it was found that these systems tend to be very fragile and hence more susceptible to breakdown than ordinary flocking systems. The model produced a number of different
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examples of correlated rotational motion including the rings shown in Fig. 1.5(c), the
vortices shown in Fig. 1.5(b) and mini-flocks circling a fixed centre of mass which are seen
in Fig. 1.5(a). This was considered particularly important as there are some well known
testcases of ring and vortex formations in microbiology which allow for the predictions of
this model to be accurately assessed in a laboratory setting. This model also formed the
basis for some of our own work in chapter 2.

In 2007 as part of efforts to remedy the lack of experimental data in the field, the
STARFLAG project was founded, with the significant backing of the European Union
through EC FP6 on scientific research. Centered in Rome, the project brought together
flocking experts from a number of institutions in Europe, with the aim of improving col-
aboration between academics specialising in flocking research and also to begin the first
computer aided experimental measurements of bird flocks [2, 3]. Rome was chosen as the
headquarters of the project partly because the city is famous for its spectacular starling
flocks [2, 3]. Headed by Andrea Cavagna the team at the INFM-CNR sought to track
the positions of flocking starlings above Rome in 3D using cameras erected on buildings
around the city. With the aid of computer simulation programs, the motion of individual
birds is recorded and can be compared with various models in the field to determine their
validity, accuracy and applicability to flocking birds. An example of this can be seen in
Fig. 1.6. Although less than 3 years old, a number of important papers have come about
through this collaboration, and the experimental work done has been invaluable for fur-
thering the field beyond its primarily theoretical roots [50, 51, 52, 53].

In 2008 the field expanded further, with a series of papers by S.-H. Lee focused on the ef-
fects of introducing a predator into a flocking simulation [54, 55]. Essentially, the predator
is represented by a simple short range repulsive potential and repels nearby prey boids,
which quite naturally, want to avoid getting close to the predator. In these papers, Lee
investigated how having a predator in close proximity to a flock, affects its formation,
structure and subsequent movement. He was also able to investigate how different angles
of attack effect predation success, opening the door for experiments to observe whether
predators in nature tend to attack from these optimized angles, and how it impacts their
Figure 1.5: Chaotic flock geometry in D’Orsogna model. (a) Rotating clumps observed at $l_r = 0.5, C_r = 0.6$, where $l_r$ is a measure of the width of the repulsive potential and $C_r$ is a measure of the strength of the repulsive potential. (b) When $l_r$ is increased, the clumps begin to coalesce forming a clumpy ring structure. (c) If $C_r$ is decreased from (a) but $l_r$ remains the same, a smooth ring structure is formed. (d) Ring radius as a function of $N$ (number of boids in system). [Figure reproduced from [46]].
1.2. INDIVIDUAL-BASED MODELS OF FLOCKING

Figure 1.6: A typical flock reconstructed in 3D by STARFLAG. (a)(b) Two images of the same flock taken simultaneous by 2 different cameras 25m apart. These two images allow for a 3D reconstruction of the flock to be created such that the position of each boid in the flock can be located in 3-dimensional space. (c)-(f) give computational reconstructions of how the flock would appear from 4 different angles. [Figure reproduced from [2, 3]].
hunting success in reality. Two examples of different predator attack angles are shown in Fig. 1.7, each resulting in quite different reactionary behaviours from the prey flock. A key point however, is that this model took the field beyond looking at single species interactions, into looking at cross-species interactions, possibly opening a new avenue for modelling the behaviour of simple ecosystems in the context of flocking.

A further outgrowth of predator-prey flocking models has been the recent interest within flocking research in investigating the flow of information through a flock. If each individual in a flock is influenced by their neighbours, and if one (or several) members of the flock are the first to observe a looming predator and react, how rapidly does that information wave expand to encompass the whole flock. This sort of model can be used to investigate whether the speed of the information flow through a flock depends on the number of boids which initially observe the stimuli (the predator), how many flock members are required to observe the stimuli in order to set off a stampede and how flock density and composition

Figure 1.7: S. H. Lee’s paper demonstrates how the response of a prey flock to the presence of a predator is critically dependent on the predator's angle of attack. The left panel shows an attack from $\theta < \theta_c$ which causes the flock to split undergoing a phase transition into an uncorrelated state. The panel on the right shows an attack from $\theta > \theta_c$ where the approaching predator induces a transition in the flock to a fully correlated state. [Figure reproduced from [54]].
effect the speed of the information wave travelling through the flock.

In 2008 an important paper by Sumpter, Couzin et al. [56] was published, investigating the flow of information through a 2D flocking system induced by the presence of a nearby predator. In it, the relationship between the flow of information through a flock, and the transition from disordered to order state was demonstrated, showing an important link between the two. Infact, it was demonstrated that information transfer is maximised at the point where a leaderless self-propelled particle model transitions from disorder to order. Fig. 1.8, taken from [56] shows the propagation of this information wave through a fish school at different time steps. This fascinating link should prove to be an important area of upcoming flocking research and in future and may help to answer very fundamental questions about flocking, such as giving quantitative answers for optimum flock sizes, compositions and densities in the presence of different predator and environment types. These results could then be compared experimentally to real flocks to see if these same values are observed in nature, where evolution should have shaped flocks toward their optimal effectiveness.

Another interesting problem in flocking physics is whether or not their are any energy benefits to birds flying in a flock as opposed to flying in open space. In general, it is quite difficult to analyse the energy of a flocking system, because in many cases the simple models used in physics are not energy conservative [20, 29]. Unlike a model of an ordinary fluid or gas, where the internal energy of the particles remains constant and thus the kinetic energy and potential energy of the system must also remain constant, for a flock, the internal energy of the boids is constantly being converted into kinetic energy via metabolic processes. The exact nature of these metabolic processes are far too complex to be encapsulated in a simple physics model, and hence they are often neglected completely. Since the motion of the boids is dependent upon the energy provided by their metabolic processes, and that energy pool is usually undefined or infinite for simple flocking models in physics, the models of flocking motion are themselves are not energy conservative.
Figure 1.8: Information propagation through a school of fish. (a) Motion of fish is initially uncorrelated (b) Information about the stimulus passes the fish on the right of the school, causing there motion to correlate (c) As information wave passes through the school, the fish school undergoes a phase transition from disordered to ordered motion. (d) Once the information wave has passed through the entire school, the motion of the fish has become completely correlated. [Figure reproduced from [56]].
1.3. HYDRODYNAMICAL MODELS OF FLOCKING

There has however been some research undertaken into the possible energy incentives or disincentives associated with being in a flock as opposed to travelling alone [4, 57]. It has indeed been shown that the classical 'V' shaped flock seen in some ducks and geese is associated with aerodynamic energy benefits [4], which could explain why this particular flock formation is chosen by these long range migratory birds. However, in general, only a few species of birds display this characteristic pattern, and typically they are larger species where the aerodynamic benefits are more pronounced. In fact for more typical cluster flocks, as seen in pigeons for instance, it was shown by Usherwood et. al. in Nature [57] that there is actually an energy disincentive to flying in a flock [57]. That is, the constituent boids in one of these flocking formations actually consume significantly more energy by being a member of a cluster flock than they would flying alone. This of course means that other incentives must override the energy cost, such as increased safety from predation. To date however, these metabolic considerations have not been included in more conventional physics flocking models.

The late 2000’s has also seen further interest in flocking algorithms from military sources and military contractors, interested in applying flocking algorithms to robotics. Using swarms of robots with 'dispersed intelligence' has become a popular area of research particularly in military fields for purposes such as bomb disarmament, inspecting building interiors to identify possible combatants and general reconnaissance [58, 59, 60, 61]. The general purpose of many of these projects is similar however, with a long term aim to reducing the need to risk human soldiers for these purposes and to instead use the more dispensable AI technology being developed.

1.3 Hydrodynamical Models of Flocking

As discussed previously, the other main branch of flocking research involves the use of fluid mechanical models, usually used in analysing fluid flows to model the bulk properties of a flock. This branch of research began with a paper by Toner and Tu in 1998 entitled...
'Flocks, herds, and schools: A quantitative theory of flocking' [20]. In it, they presented
an alternative approach to flocking research, in contrast with previous work which had
concentrated exclusively on IBMs. Instead, the flocks were analysed as classical fluid flows.
Toner and Tu produced the first continuum model of flocking, and demonstrated that for
d = 2 dimensions, flocks exhibit a true long-range broken symmetry state. That is, long
range order which occurs spontaneously through short range interactions.

The continuum model derived by Toner and Tu has many similarities to the Navier-Stokes
equations of fluid dynamics. The model was designed to simulate the behaviour of any
large flock of particles $N$, which obeys certain symmetry conditions. Thus, it should be
capable of describing realistic flocking situations, provided that the flocks are large enough
such that they can be considered as a continuum. The two symmetries required are that
the flock be translationally and rotationally invariant. What this means is that moving
the flock to a different position in space has no effect on the physics of the flock (space
is homogenous). Additionally there is no preferred direction of travel for the flock, one
direction is equivalent to another, and any direction chosen by the flock will be a result of
random symmetry breaking and not be chosen a priori.

There are also a number of important differences in Toner and Tu’s model compared to
a classical hydrodynamic model such as the Navier-Stokes equations. Firstly, energy and
momentum are not conserved [20]. This is because the internal workings of the boids are
not included in the model. Since energy is always being converted from the internal work-
ings of the boids (ie. food digestion) into forward motion, and because we cannot know
how much internal energy each of the boids has, there is too much uncertainty to try and
introduce energy conservation into hydrodynamic equations. Additionally, the model does
not possess Galilean invariance. This can be explained due to the fact that all flocks move
through a restrictive medium, which puts them in a special Galilean reference frame. In
fact there is only one conservation law present in Toner and Tu’s hydrodynamical model of
flocks. We may call this ‘boid conservation’ as the number of boids cannot change. Boids
cannot be born or die, and the number of boids in the flock is invariant.
With the conservation laws now understood, the hydrodynamical variables are defined. These include the coarse-grained bird velocity field \( v(r, t) \) and the coarse-grained bird density \( \rho(r, t) \). \( v(r, t) \) is an average of individual bird velocities over a given volume, \( V \), centered on \( r \). It is important that this volume is large enough to contain enough boids to get a suitable average, but small enough so that the behaviour is still localized with respect to the size of the entire flock. \( \rho(r, t) \) is simply the number of particles in a coarse-grained volume divided by the volume. The precedent of the Navier-Stokes equation is taken, in that instead of trying to explicitly coarse-grain the microscopic dynamics of the system, the simplest continuum equation which is consistent with the symmetries and conservation laws is instead written, which allows for random processes and uncertainties to be buried in a few phenomenological parameters.

Thus, Toner and Tu derived the most general hydrodynamical equations of motion for flocking to be:

\[
\begin{align*}
\frac{\partial \vec{v}}{\partial t} &+ \lambda_1 (\vec{v} \cdot \vec{\nabla}) \vec{v} + \lambda_2 (\vec{\nabla} \cdot \vec{v}) \vec{v} + \lambda_3 \vec{\nabla} (|\vec{v}|^2) \\
&= \alpha \vec{v} - \beta |\vec{v}|^2 \vec{v} - \vec{\nabla} P + D_B \vec{\nabla} (\vec{\nabla} \cdot \vec{v}) \\
&+ D_T \vec{\nabla}^2 \vec{v} + D_2 (\vec{v} \cdot \vec{\nabla})^2 \vec{v} + \vec{f}
\end{align*}
\]

\[ P = P(\rho) = \sum_{n=1}^{\infty} \sigma_n (\rho - \rho_0)^n \]

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\vec{v} \rho) = 0
\]

where \( \beta, D_B, D_2, D_T \) are all positive, \( \alpha < 0 \) for the disordered state and \( \alpha > 0 \) for the ordered state. The \( \Lambda \) terms are analogous to the same \( \Lambda \) terms in the Navier-Stokes equations, except that due to absence of Galilean invariance, all 3 combinations of one spatial gradient and two velocities to be non-zero. The \( \vec{f} \) is a random driving force representing the noise. This is taken to be a white noise gaussian. \( P \) is simply the pressure, and the final equation represents the fact that birds cannot be born or die ‘on the wing’.
Figure 1.9: A typical hydrodynamic model of a flocking system from [20], with a direction of flow being from left to right. Note that due to coarse graining, fluid dynamical flocking systems are usually far bigger and involve far more particles than an equivalent IBM. However, this also means that information about finer properties is lost. [Figure reproduced from [20]].

These equations of motion were analysed in the broken symmetry state where it was demonstrated that for all $d < 4$, all flocking systems exhibit this broken symmetry state, while for $d \geq 4$ this broken symmetry does not exist. Deeper analysis reveals that, hydrodynamically, in $d \geq 2$, transport of information through the flock occurs via fast convective transport whereas for $d \geq 5$ the information disperses through the flock by slow diffusion, that is, it can only be passed sequentially from member to member. Since reality is composed of just 3 (macroscopic) dimensions, this means that spontaneous symmetry breaking
1.4 Hard-Core and Soft-Core Flocking Potentials in Free Space

can occur in any environment on earth. Even more striking is that for $d = 2$ (a common
dimensionality for flocks moving on land such as herds and bacterium), scaling exponents
can be calculated exactly, meaning that flocking at $d = 2$ exhibits true long range order
in the broken symmetry state. A snapshot of a 2D implementation of this system which
has reached a statistical steady state is shown in Fig. 1.9.

Later papers, have applied this basic continuum model, sometimes with modifications to
a number of more specific cases of flocking behaviour. Kulinskii et al. [62] in 2005 found
exact solutions for rotating vortex states in the continuum model which can be related to
the behaviour of a number of microbiological organisms such as E.coli and Dictyostelium
while Topaz and Bertozzi in 2006 [63] used a Non-Local variation of the continuum model
to show that aggregations of self-propelled particles can occur in 1D as well as the standard
2D case which is typically investigated in these models.

Additionally a paper by Cucker and Smale in 2007 [64] found particular resonance with
the mathematics community as it provided a very rigorous analytical solution to the time
evolution of a simple Vicsek-like flock in both discrete and continuous time limits. Of
particular importance was the finding that for a flock where the scale over which the
alignment potential operates is defined by $\beta$, then for $\beta < \frac{1}{2}$ the velocity of the individual
boids will naturally converge, whereas for $\beta > \frac{1}{2}$ this convergence is only guaranteed under
specific initial conditions and will not otherwise occur [64].

1.4 Hard-Core and Soft-Core Flocking Potentials in Free Space

A number of key states have been observed and analysed in flocking research since the
original discovery by Vicsek et al [14] of correlated alignment states in self-propelled par-
ticles. They include moving and stationary fluids, moving and stationary solid states, and
single vs multiple flock states [8, 14, 20, 22, 24, 25, 37]. The phase transitions which have
Figure 1.10: Example of boundary conditions in a number of typical flocking models. Reflecting boundaries at the top/bottom and periodic boundaries at the left/right. However, in the real world, flocks exist in unbounded space, and are not restrained by these boundary conditions.

The model presented in Chapter 2 extends several key models which have been discussed previously, as well as tackling some of the shortcomings of previous models identified in Toner, Tu and Ramaswamy’s flocking review [29]. Firstly, the models presented in Chapter 2 are free space models. In the past, most flocking models have depended on periodic or reflecting boundary conditions in order to hold the flock together, as shown in Fig. 1.10. It was not until 2007 that the earliest physics free space models of flocking began to develop [46, 47, 48, 49]. As we know, real flocks exist in free space, they do not exist within artificial barriers. Whilst periodic boundary conditions simplify the modelling and analysis of flocks, and have proved extremely useful tools in analysing the bulk properties
of a flock, they cannot be used effectively for analysing edge effects or for looking at the merging and splitting of flocks in open space. Both of these behaviours are important properties of real flocks that require a free space model in order for us to effectively investigate them.

Secondly, there is no general procedure for developing a new flocking model. Many are pieced together in a rather ad-hoc fashion whilst others use a number of different approaches for deriving equations of motion. The closest thing to a 'General Equation of Flocking' that exists is the equation of Y. Tu which specifies the coupling of a simple position based potential with an alignment based potential that is also restricted in spatial extent to avoid non-local interactions [22]. Using this as a starting point a more formulaic general approach to developing flocking models will be presented, based on the Lagrange Equations of classical motion. It is intended that this formalisation can then be used in the development of future models, in order to introduce some clarity and rigour into the development of these flocking models.

Finally, many of the models developed hitherto have concentrated primarily on modelling one aspect of flocking behaviour, such as vortex formation [17, 38, 39, 40, 42, 43, 46] or the moving liquid state [1, 4, 5, 14, 13, 12, 50, 54, 65] but have not demonstrated the ability to model the full range of flocking behaviours observed in nature. The models presented in Chapter 2 aims to approach flocking phenomena in a more holistic fashion, demonstrating realistic modelling in a wide range of flocking regimes through the adjustment of just a small number of parameters. Through this approach, the universal nature of flocking behaviour is demonstrated, showing that although these behaviours can be split up and modelled separately, they all arise naturally from the same set of basic conditions, and are really all just different manifestations of the same basic underlying principles which make up flocking.

In addition to this, although there has been a wide variety of different models used, almost all of these fall into two categories, those based on hard-core cohesion potentials, and
those based on soft-core cohesion potentials. A hard-core potential is a potential which approaches infinity as the separation between boids approaches zero. This effectively means that collisions between boids are strictly forbidden. On the other hand, soft-core potentials approach some finite value as the separation of boids goes to zero. This means that although they must overcome some finite potential barrier, boids can occupy the same position in space time (they can collide). In strict terms, both of these approaches introduce some element of unrealistic behaviour. Boids in a flock can collide, so a hard core potential is not strictly accurate, but it is also apparent that boids that do collide are unlikely to continue as part of the flock (they would effectively die on the wing) which is not taken into account in these models. To date there has been no in-depth analysis of the qualitative or quantitative differences which occur due to the differing nature of these two different families of potentials. Using the two models introduced in Chapter 2 the comparison will be made between the effects a hard-core and soft-core potential have on the structural and dynamical characteristics of the flocks which develop due to the differing potentials.

The model introduced in Chapter 2 extends previous work done in Tu [22] in that it depends on combining a cohesion potential with an alignment potential. However, in this case, two different cohesion potentials are used, one representing a soft-core potential and the other representing a hard-core potential. As discussed earlier these are used to give contrasting results based on infinite versus finite repulsion at close proximities. One major improvement the cohesive potential has over that used by Tu is that our body potentials are continuous at all places except for the core, leaving them amenable to deeper mathematical analysis. Additionally, whilst the potential used by Tu is simply put together as the kind of potential that might fit with the flocking physics, the Morse and Lennard-Jones potential arise out of molecular and atomic physics and are well understood in those contexts already, as well as matching the types of physics required for a sensible flocking model.

As in all previous flocking models, an alignment force is also an important aspect of our
model. The alignment force represents the tendency of nearby boids to match the directional heading of their neighbours. In Tu’s model, this is represented as a force in the average direction of motion of the boids neighbours within some region represented by a top hat function in space as shown in Fig. 1.3. Likewise, in this model, the alignment force is in the average direction of the nearby neighbours, but instead of the strength of the force being mediated by a simple top hat function in space, a Gaussian is used instead. This represents the fact that nearer neighbours have more impact on the direction the boid chooses than those far away. As with all flocking models, boid following is not perfect, and there is a random stochastic force applied to each boid to take this into account.

The density dependent phase transition from a single correlated flock to multiple independent flocks will be examined in detail with the effects of initial density (note that since this is a free space model, only the starting region can be specified, as all subsequent motion is allowed to occur in open space) and noise on the form of this phase transition analysed in particular for both the hard-core and soft-core cases.

It is hoped that through the use of potentials which are already well understood in nature, as well as modelling the solution in free space, that deeper and more accurate insights can be gained into the behaviour exhibited by flocking systems than that provided by the rather ad-hoc approaches taken to date. By imposing as few ad-hoc limitations as possible, the most natural flocking behaviour arising from the equations of motion will be apparent, allowing for a better understanding of how hard and soft core potentials affect the evolution and behaviour of the flock and the role edge effects play in the structure of the flock.

1.5 Flocking and the Virial Expansion

In Chapters 3 and 4 a continuum model of flocking based on a virial equation of state is derived for two different variations of flocking behaviour. This is the first time that attempts have been made to model flocking using a gas-type equation of state, although
the idea that flocking may be seen as a gas was first introduced by Vicsek as early as 1995 [30] and again later by Parravano and Reyes in 2008 [66]. The virial expansion is a technique used in statistical mechanics to derive an equation of state for classical gas systems with interactions [67, 68, 69], and additionally to find the partition function. This enables the important thermodynamic properties of a gas, such as internal energy, specific heat and entropy to be evaluated [70].

Using the virial expansion, the equation of state derived for a gas system is of the form:

\[ P\beta = B_1\eta + B_2\eta^2 + \ldots + B_N\eta^N \]  \hspace{1cm} (1.7)

where \( B_1, B_2, B_N \) are the terms of the expansion up to order \( N \), where \( N \) is the order of the expansion, and the maximum \( N \) is the total number of particles in the system. Physically, each term in the expansion corresponds to an increase in the complexity of the interactions considered. For example, \( B_1 \) considers only single-body (self) interactions, \( B_2 \) considers 2-body interactions, \( B_3 \) 3-body interactions, and so on, up to \( B_N \). In practice the dominant gas behaviours are usually encapsulated in the early terms of the expansion, up to 2nd or 3rd order, with the higher order terms introducing ever smaller corrections.

In a typical gas, the only interaction between particles is some inter-molecular potential based on the relative separations of the constituent particles. This can take the form of a simple repulsive potential, or a more complicated potential such as a Morse or Lennard-Jones potential. One particularly well known form of the virial equation of state is the Van der Waals equation [71, 72], which adds a simple Sutherland-like potential contribution to the equation of state of an ideal gas by way of considering an additional term of the virial expansion for this interaction.

Describing flocking as a gas however, has some important differences to modelling a typical gas. In a flocking gas, not only are their interactions based on the relative positions
1.5. FLOCKING AND THE VIRIAL EXPANSION

of the particles, but also on the direction of motion of the particles. This is because the constituent particles of a flock (boids) have a preference to align their direction of motion with their nearest neighbours such that the flock while form a cohesive entity.

What this means is that the simple non-interacting momentum term that is used in the case of an ordinary gas will become a somewhat more complicated interacting term, in the case of a flocking gas. It is this additional consideration that makes a flocking gas unique to the types of ordinary gases that have been previously described using the virial expansion, and allows for the complexity of flocking behaviour to be modelled as a simple gas using the virial expansion.

In Chapter 3 this approach will be used to model a very simple form of flocking gas, with a repulsive interaction based on relative position and an alignment potential operating over all space which generates a lowest energy state when the direction of all boids are aligned. Using such a simple model means that the virial equation of state and partition function can be solved analytically to order $N$, and the results of interesting physical quantities such as pressure and specific heat can be compared to a corresponding computational model to investigate the accuracy of this approach.

In Chapter 4 the virial expansion is used to investigate possibly the most well understood flocking model in existence, the Vicsek model. The Vicsek model is both simple enough to be solved analytically using this method, but complicated enough to give deeper insight into more realistic flocking regimes than the toy model investigated in Chapter 3. The behaviour of the Virial-Vicsek equation of state is then compared to computational models of the same system to again analyse the veracity of this new approach to modelling flocking systems. The behaviour of the internal energy $U$, entropy $S$ and specific heat, $C_V$ with respect to the temperature $T$ is then plotted in order to examine whether this approach to modelling a Vicsek flock is correctly able to predict the phase transition between order and disorder in the Vicsek flock.
Much like when hydrodynamical models were first used to analyze flocking over a decade ago, it is hoped that this approach will open up new insights into flocking behaviour, and allow different types of information to be obtained when compared to current flocking models. In particular, it is hoped that by studying flocking models in this manner, the relationships between pressure, temperature, interaction strengths and noise can be better understood and that a new avenue will be opened up for calculating phase transitions in flocking systems through the analysis of thermodynamic quantities such as the specific heat capacity.

Finally, modelling flocking as a gas allows three important gas theories to be brought to bear on the problem, thermodynamics, kinetic theory and statistical mechanics. Importantly, thermodynamics is a continuum theory, while kinetic theory is a discrete theory. This means that it will now be possible to investigate the same problems from both a continuum and discrete point of view, much more simply compared to current flocking models where hydrodynamic and individual-based models are generally considered quite separately and different from one another. It is hoped that this method could bring these two disparate families of models closer together and allow for better cross-examination of the results obtained in the discrete and continuous limits.
1.5. FLOCKING AND THE VIRIAL EXPANSION
2.1 Introduction to Individual-Based Flocking

In this chapter, the development of two non-local flocking models based on the Morse and Lennard-Jones potentials is presented. Both of these models are derived with open boundaries in an attempt to model more realistic flocking behaviour than has typically been modelled in the past. Whilst some research into free space flocking has begun in recent years [46, 47, 48, 49], most flocking models continue to be based on periodic boundary conditions, which places restrictions upon their applicability to real world situations. Additionally, many of the newer models, in free space, focus on modelling bacterial systems, in particular, the simulation of vortex states which have been observed in a number of bacterial colonies, as mentioned in the previous chapter [38, 39, 42, 43, 46].

The model developed here is designed to be a simple, robust and independent of scale in order for it to be capable of accurately simulating a large number of biological systems, over a wide range of length scales, from bacterial colonies [38, 39, 41, 42] right up to ungulate herds [10, 12, 73]. Rather than attempting to model a specific instance of flocking behaviour very accurately, the models proposed will instead be aimed at exploring the generality of flocking behaviour, clearly showing how many of the characteristics of seem-
ingly quite different grouping behaviours, from the very small to the very large scale, can in fact be encapsulated through a single model with a small number of free parameters. Thus flocking can be seen as a universal behaviour with a unique set of characteristics which transcend any particular biological organism.

A Lagrangian approach is taken in order to derive the equations of motion [74], and the flock is then analysed as a non-local field, where each boid makes a contribution to the potential of the region. A comparison is made between the use of a cohesion potential characterised by the hard-core Lennard-Jones potential or the soft-core Morse potential to determine the similarities and differences observed when modelling flocking using these two potentials. The Lennard-Jones potential [75, 76, 77] and the Morse potential [78] provide suitable features for modelling flocking and are well understood in the context of atomic [79, 80] and molecular [81, 82] physics respectively.

Despite the importance of the Vicsek model to flocking research in physics, it does have a number of short-comings when used to model realistic flocking systems. Two key issues are the lack of short-range repulsion to prevent particle collision and the reliance on periodic boundary conditions to effectively force continued interaction over long time periods and prevent dispersion. This means that the full range of realistic flocking behavior is not observed using this model.

A number of different approaches have been attempted in order to overcome these short-comings. Often, the approach taken includes the ad-hoc introduction of some short range repulsion or alignment dependent equations of motion [15, 16, 18, 19, 23, 32, 28, 24, 36, 37, 83]. The approach taken here is similar, but instead follows in the footsteps of Huth and Wissel [5], Y. Tu [22] and others [46, 47, 54] by introducing a well understood potential, and then deriving the associated equations of motion. In this instance, two different non-local potentials are chosen, in order to contrast the behaviour of flocks based on hard-core and soft-core potentials. The two potentials which are used are the Lennard-Jones Potential (LJP) and the Morse Potential (MP). After a randomized initial placement these
systems evolve in free space, allowing a wider range of possible flocking phenomena to occur. This approach extends previous studies [5, 22, 46, 47], by consideration of open boundary conditions and direct comparison of the effects of hard (LJP) and soft (MP) core potentials on such parameters as flock density, cohesion and behaviour around the critical points.

2.2 Formulation of a computational flocking model

As discussed briefly in Chapter 1, the model presented here is an extension of the Y. Tu model [22]. In that model a general form for the force between any 2 boids in a flock is given by:

\[ F_i = \sum_j (a f_a(r_{ij}) \hat{\mathbf{u}}_j + b f_b(r_{ij}) \hat{\mathbf{r}}_{ij}) + \eta_i, \]  

(2.1)

where \( a \) and \( b \) are adjustable parameters governing the strength of the alignment force and the cohesion force respectively, and the above equation represents a generalized approach to deriving a flocking force where both these components are present, \( \hat{\mathbf{u}}_j \) is boid velocity and \( \hat{\mathbf{r}}_{ij} \) is a unit vector along the line of interaction between boids \( i \) and \( j \).

Subsequently Y. Tu adopts two very simple functions for \( f_a \) and \( f_b \), with \( f_a \) consisting of 4 ‘zones’ of interaction separated by discontinuities and \( f_b \) as a simple top hat function in space with interaction only occurring in zone 2.

In the work presented here, we instead begin from a more fundamental basis, with a potential of the form:

\[ V_i(\hat{\mathbf{r}}, \hat{\mathbf{\theta}}) = \sum_{j \neq i} V_a(r_{ij}) \hat{\mathbf{r}}_{ij} + V_b(r_{ij}) \hat{\mathbf{\theta}}_j, \]  

(2.2)

where \( V_a \) is the function corresponding to the cohesion potential of the boids and \( V_b \) is the function corresponding to the alignment potential of the boids. \( \hat{\mathbf{r}}_{ij} \) is the unit vector pointing from boid \( i \) to boid \( j \) and \( \hat{\mathbf{\theta}}_j \) is a unit vector in the direction of motion of boid \( j \), in
an absolute coordinate system. Since we are considering two different cohesion potentials, one a hard-core (Lennard-Jones) and one a soft-core (Morse) potential, this can be further expressed as two equations:

\[ V_{M_i}^M(\hat{r}, \hat{\theta}) = \sum_{j \neq i} V_M(r_{ij}) \hat{r}_{ij} + V_A(r_{ij}) \hat{\theta}_{ij}, \]  
(2.3)

\[ V_{L_i}^{LJ}(\hat{r}, \hat{\theta}) = \sum_{j \neq i} V_{LJ}(r_{ij}) \hat{r}_{ij} + V_A(r_{ij}) \hat{\theta}_{ij}, \]  
(2.4)

where \( V_M \) is the Morse potential (MP), \( V_{LJ} \) is the Lennard Jones potential (LJP) and \( V_A \) is the alignment potential, described below.

Figure 2.1: Specification of parameters: a representation of two boids positioned at \( \mathbf{r}_i \) and \( \mathbf{r}_j \) with respective velocities \( \mathbf{v}_i \) and \( \mathbf{v}_j \) in directions \( \theta_i \) and \( \theta_j \), where \( r_{ij} = \mathbf{r}_i - \mathbf{r}_j \).

First, the interactions between two boids, \( i \) and \( j \) are considered, as shown in Fig. 2.1. \( r_{ij} \) is the distance separating any two boids while \( \mathbf{v}_i \) and \( \mathbf{v}_j \) are the velocities of boids \( i \) and \( j \), with their direction of motion being defined as \( \theta_i \) and \( \theta_j \), as measured from the horizontal.

To fully encompass the essential properties of flocking three key elements are required.
These can be encapsulated through the consideration of two boids separated by distance \( r_{ij} \). Boids have a tendency to avoid collisions thus a repulsive force is required for \( r_{ij} < r_{\text{min}} \). Boids have some preferred separation \( r_{ij} = r_{\text{min}} \), a balance between collision avoidance and predation risk. Boids cease to interact for large separations. Both the LJP and MP, satisfy the above criteria, as can be seen in Fig. 2.2(a). These potentials are qualitatively similar for \( r_{ij} > r_{\text{min}} \) but possess a significant quantitative difference for \( r_{ij} < r_{\text{min}} \). Specifically, as \( r_{ij} \to 0 \) the LJP has a hard-core with \( V \to \infty \) whereas the MP has a soft-core with the potential tending to a finite constant. This difference generates different bulk behaviour in the flock and also effects the behaviour of the flock around the critical points.

The LJP is given by:

\[
V_{\text{LJ}}(r_{ij}) = \sum_{j \neq i} \epsilon \left[ \left( \frac{r_{\text{min}}}{r_{ij}} \right)^{12} - 2 \left( \frac{r_{\text{min}}}{r_{ij}} \right)^{6} \right],
\]

where \( V_{i}^{\text{LJ}} \) is the potential between boid \( i \) and the rest of the flock, \( r_{ij} \) is the distance between boid \( i \) and boid \( j \) in the flock. \( r_{\text{min}} \) and \( \epsilon \) are constants associated with the strength and spatial extent of the potential.

The MP is specified as:

\[
V_{M}(r_{ij}) = \sum_{j \neq i} \epsilon \left[ 1 - \exp \left( -a(r_{ij} - r_{\text{min}}) \right) \right]^{2},
\]

where \( a \) is a constant defining the width of the potential well. In each case the depth of the potential is defined by \( \epsilon \) and the minimum potential between the two boids occurs at \( r_{\text{min}} \), which may be physically interpreted as the preferred distance between nearest neighbours in the flock. The functional form of the two cohesion potentials (\( V_{C} \), the LJP (red solid line) and MP (blue dashed line) are shown in Fig. 2.2(a) for the case of two interacting boids \( i \) and \( j \).
The final key element for flocking behaviour is alignment. For two boids \( i \) and \( j \) to be aligned, the relative angle between them must be \( \Delta \theta_{ij} = \theta_i - \theta_j \approx 0 \). This potential must be fairly localized since individual boids have a strong preference to align with nearest neighbours but no interaction with boids further away in the flock. This means that any boid will attempt to match the direction of motion of it’s nearest neighbours, but boids far away will have little to no effect on the direction of motion of the boid being considered.

In order to achieve this, a potential is introduced which includes both a separation and alignment dependence. The separation dependence is used to provide greater weighting toward boids which are close to one another and lesser weighting towards those which are further away. This ‘weighting’ is then multiplied by the alignment dependence which is simply the angular direction of the velocity vector of the interacting boid. Thus, what this potential means physically, is that the direction of boids close to boid \( i \) will have a large bearing on it’s direction of motion whilst boids further away will have less and less impact on the direction of motion of boid \( i \). This impact becomes vanishingly small as the separation \( r_{ij} \) between boids \( i \) and \( j \) becomes large. A representation of the spatial weighting of \( V_A \) is shown in Fig. 2.2(b).

A convenient representation of this behaviour as a potential can be found in the form of the error function, multiplied by the unit vector of the other particles \( j \) in the flock. This potential will be referred to as the ‘alignment potential’ of this model:

\[
V_A(r_{ij}) = \sum_{j \neq i} C \times \text{Erf} \left( \frac{r_{ij} - \alpha r_{\text{min}}}{\beta} \right),
\]

where \( C, \alpha \) and \( \beta \) are constants which determine the magnitude, position of the minima and the width of the potential respectively. In Fig. 2.2(b) the functional form the alignment potential in space is shown for two boids. This shows how the strength of the alignment force is weighted towards nearby boids and drops to zero for boids far way. \( \alpha \) and \( \beta \) from equation (2.7) are suitably chosen to be \( \alpha = 2 \) and \( \beta = 1 \) respectively as these values provide a maximum direction correlation at \( 2r_{\text{min}} \) ensuring that the interaction is
short range only.

\( V_i^{LJ}(r) \) and \( V_i^A(r) \) are added to obtain a potential of the form:

\[
V_i(r) = \sum_{j \neq i} \epsilon \left[ \left( \frac{r_{\min}}{r_{ij}} \right)^{12} - 2 \left( \frac{r_{\min}}{r_{ij}} \right)^{6} \right] \hat{r}_{ij} + C\beta \hat{\theta}_j \times \text{Erf} \left( \frac{\left( r_{ij} + \alpha r_{\min} \right)}{\beta} \right).
\] (2.8)

and likewise for \( V_i^M(r) \) and \( V_i^A(r) \):

\[
V_i(r) = \sum_{j \neq i} \epsilon \left[ 1 - \exp \left( -\alpha (r_{ij} - r_{\min}) \right) \right]^2 \hat{r}_{ij} + C\beta \hat{\theta}_j \times \text{Erf} \left( \frac{\left( r_{ij} + \alpha r_{\min} \right)}{\beta} \right).
\] (2.9)

The force on each boid is derived using a Lagrangian approach [74]:

\[
L = T - V,
\] (2.10)

where \( L \) is the Lagrangian of the system, \( T = \frac{1}{2}m \dot{x}^2 + \frac{1}{2}m \dot{y}^2 \) is the kinetic energy of the system, and \( V \) are the potentials described above. Using the generalized Euler-Lagrange equations in \( x \) and \( y \):

\[
\frac{d}{dt} \left( \frac{dL}{dx_i} \right) - \frac{dL}{dx_i} + \frac{dA_{x_i}}{dx_i} = 0,
\] (2.11)

\[
\frac{d}{dt} \left( \frac{dL}{dy_i} \right) - \frac{dL}{dy_i} + \frac{dA_{y_i}}{dy_i} = 0,
\] (2.12)
2.2. FORMULATION OF A COMPUTATIONAL FLOCKING MODEL

Figure 2.2: (a) The two cohesion potentials ($V_C$), namely, the Lennard-Jones (red line) and the Morse (blue line) Potentials. (b) The spatial extent of the alignment potential ($V_A$). This indicates the weighting ascribed to the direction $\theta_j$ of boid $j$ on boid $i$. Note that for small $r_{ij}$ the force is strongest, and drops to zero as $r_{ij}$ becomes large.
with $\Lambda_i = \frac{1}{2} \lambda x^2_i - \frac{1}{4} \omega x^4_i + \frac{1}{2} \lambda \dot{x}^2_i - \frac{1}{3} \omega \dot{x}^4_i$. $\Lambda_{x_i}$ and $\Lambda_{y_i}$ incorporate both a self damping and a self acceleration term, which effectively cause the flock to approach an average speed of $v = \sqrt{\frac{\lambda}{\omega}}$ [21, 47] whilst still allowing variation about this speed from individual boids within the flock.

Introducing damping in this way allows for a great deal of control over the flock's velocity, increasing the stability and cohesion of the flock. This is an important addition for flocks being modelled in free space, since the lack of a self-damping term can cause catastrophic buildup of kinetic energy within the model, which has been observed in previous attempts to model flocking in free space [45, 47].

From the Lagrange Equations, the equations of motion for the LJP are:

$$ F_i(r) = -\sum_{j \neq i} \frac{12\epsilon}{r_{\text{min}}} \left( \frac{r_{\text{min}}}{r_{ij}} \right)^{13/8} - \left( \frac{r_{\text{min}}}{r_{ij}} \right)^{7/8} \hat{r}_{ij} + A\hat{\theta}_j \exp \left( -\frac{(r_{ij} - \alpha r_{\text{min}})^2}{\beta^2} \right) \hat{r}_{ij} - (\lambda - \omega v^2) \dot{r}_i + \eta_i, \quad (2.13) $$

and likewise for the MP:

$$ F_i(r) = \sum_{j \neq i} 2\epsilon \left[ 1 - e^{-a(r_j - r_{\text{min}})} \right] e^{-a(r_j - r_{\text{min}})} \hat{r}_{ij} + A\hat{\theta}_j \exp \left( -\frac{(r_{ij} - \alpha r_{\text{min}})^2}{\beta^2} \right) - (\lambda - \omega v^2) \dot{r}_i + \eta_i. \quad (2.14) $$

Note that the new constant $A = \frac{4}{\beta \sqrt{\pi}}$ is defined for convenience and that $m = 1$ is set, giving all boids equal weighting. By setting $m = 1$ there is a loss of generality, since no individual boid can be set to have a greater weighting than any other (ruling out the modelling of behaviours where there is individual leadership). The term $\eta_i$ introduced here represents the stochastic noise which is a result of small errors in the boids’ ability to perfectly follow one another. $\dot{r}_i$ is the velocity of particle $i$ and variation of $\lambda$ and $\omega$ can
be used to adjust the average velocity of the flock. These equations now represent a set of equations of motion which can be used to model flocking in free-space on length scales defined in terms of $r_{\text{min}}$.

There are 4 important parameters which can be varied to simulate different flocking phases, $A$, $\epsilon$, $\eta$ and the initial density $\rho$. However, $\epsilon$ remains constant throughout these models and $A$ is only varied between 0 and a single finite number, in this case 1, which represents turning the alignment component of the potential on or off. This leaves $\eta$, the stochastic noise and $\rho$ the initial density, which are varied with respect to one another in order to examine the range of flocking behaviours observed within this parameter space.

In order to measure different states of the system and determine the locations of any phase transitions a set of 4 order parameters are defined, these being:

(i) the average separation, $\bar{x}$,
(ii) the fluctuation in the average separation, $\Delta \bar{x}$,
(iii) the average orientation of velocity, $\bar{\theta}$ and
(iv) the fluctuation in the average orientation of velocity, $\Delta \bar{\theta}$.

2.3 Computational Methodology

Initially, each boid is placed randomly within a box of side length $l$ at position $r_i$. Each boid starts with some randomized initial speed $v_i$ in some angular direction $\theta$, where $\theta$ is as defined in Fig. 2.1(a). The initial density is thus simply,

$$\rho = \frac{N}{l^2},$$

(2.15)

In the case of the LJP, an additional restriction that $r_{\text{init}} > r_{\text{min}}$ is imposed such that no boids start within the infinite repulsive region of the LJP. Earlier experimentation found
this restriction to be necessary since any boid beginning the simulation within the repulsive region of the Lennard-Jones potential will have extremely high kinetic energy with respect to the other boids [45]. This leads to flock breakdown and dispersion in almost all cases considered. Note that this is one of the major weaknesses in the LJ description of flocking presented here, and does result in a loss of generality when compared to the MP description. It is also a particularly significant modification since it is found that the future evolution of the flock is critically dependent on the initial flock density. Each simulation contains 200 boids and is performed over a total of 20000 time steps. At each time step, the new position of boid \( i \) is calculated using simple Newtonian kinematics. For each set of suitable parameters an ensemble of 100 runs was performed, and the average of each of the order parameters listed in the previous section are taken over the entire ensemble.

Key phases may then be defined in terms of the order parameters that are tracked during the simulation. The non-moving state is defined by \( \bar{v} \approx 0 \) while the correlated moving state is defined by \( |\bar{v}| \neq 0 \) provided \( \bar{x} \approx \text{constant} \) over time. To differentiate between liquid and solid, the fluctuation in the average velocity of the boids in the flock is analysed. If \( \Delta \bar{v} \approx 0 \) then the state is a solid and if \( \Delta |\bar{v}| > 0 \) then the state is a liquid.

Of particular interest in this case is the phase transition between a single correlated flock which occurs at high initial densities and multiple independent flocks, which occur at lower initial densities. This phase transition has not been explored in as much depth as the phase transition between stationary \( \bar{v} \approx 0 \) and moving \( \bar{v} \neq 0 \) flock which is typically the source of interest in these models.

The phase transition between a single correlated flock and multiple independent flocks is important to understanding how small flocks can merge to form larger flocks and how large flocks sometimes split to create multiple, largely independent smaller flocks. It also has important ramifications for understanding the more general processes that lead to flock formation in the first place and for understanding how flocks eventually dissolve.
The phase transition between the single and multi-flock states can be tracked using the order parameter $\Delta \bar{\theta}$. If the system contains a single correlated flock then $\Delta \bar{\theta} \approx 0$ and $\bar{x} \approx \text{constant}$ over time. As the flock passes through a transitionary phase where more than one distinct flock may exist, but the direction of motion is still correlated, $\Delta \bar{\theta} \approx 0$ as before, but $\Delta \bar{x}$ will begin to increase. Finally, as the transition occurs to multiple independent flocks it is expected that $\Delta \bar{\theta} \neq 0$ since the independent flocks will be travelling in random directions, uncorrelated with one another.

### 2.4 Results and Discussion

The phase transition from disorder to order observed in Vicsek’s original model is observed in both the hard-core (LJP) and soft-core (MP) cases. Much like the Vicsek model, changes in initial density effect the size of the ordered clumps with high densities resulting in a single ordered flock whilst lower initial densities result in a number of independent but correlated flocks. More importantly, perhaps, is that all of the moving and stationary variants of the fluid and solid phases from Y. Tu’s model in both the multi-flock and single flock limits were successfully replicated using both soft-core (MP) and hard-core (LJP) potentials in free space by varying the noise amplitude, $\eta$, the initial density, $\rho$ for stationary flocks where alignment is switched off ($A = 0$) and moving flocks where it is switched on ($A = 1$).

This is an important result, since previous free space models have primarily concentrated on just the moving liquid phase as in Ref. [46] which examines vortex formation and stability of rotating flocks in free space. Here, it has been demonstrated that both hard-core and soft-core potentials generate all four of the key phases from Y. Tu in free space [22]. This shows that although the flocks formed by these two different types of potentials show some variation in structure and form it does not restrict the ability of either the hard or soft core potential to form flocks in any of any of these phases.
Importantly, it also shows that both models demonstrate similar qualitative behaviour, which is likely due to the fact that neither $\eta$ nor $A$ effect the LJ or Morse components of the potential, only the alignment component. Both the hard-core LJP and the soft-core MP produce the same types of phases, leading to a strong qualitative agreement between the two models. This indicates, from a qualitative point of view at least, that a kind of "model independence" exists for cohesive potential types which feature some short-length repulsion, a single minimum at $r_{\text{min}}$ and no long range interaction. Cohesive potentials of this form, coupled with an alignment potential should always display this same qualitative agreement.

The two models do however vary quantitatively in the results they produce. The selection of model (hard-core vs soft-core) effects the location and nature of the phase transitions and also the quantitative regions of $\rho$ vs $\eta$ phase space over which each model exhibits a given state.

Fig. 2.3 shows a sampling of some of the key phases that have been documented in flocking literature and which are observed in this model. Fig. 2.3(a) shows a single flock, Fig. 2.3(b) a phase consisting of multiple independent flocks in a low density regime, Fig. 2.3(c) a stationary lattice and Fig. 2.3(d) a stationary liquid exhibiting vortex like structures within the bulk. It is important to note that all these states were observed in free space, in the absence of any boundary conditions. Whilst the structures observed in Fig. 2.3(a) and Fig. 2.3(b) have been studied in previous models, few of these models have been examined in free space. Additionally, experimental observation and measurement is significantly lacking for structures like these [12, 73], which tend to form on macroscopic levels. The recent advent of the STARFLAG project means that experimental verification for some of these phases may soon be forthcoming, with a number of papers already published [2, 3, 50] outlining the experimental methods and data that will be collected. Despite this current lack of quantitative experimental data the state shown in Fig. 2.3(d) is in very good qualitative agreement, not just with several previous models looking at
2.4. RESULTS AND DISCUSSION

Figure 2.3: Examples of 4 different coherent states observed for the MP. (a) Single moving flock (b) Multiple Independent moving flocks (c) Stationary lattice-like flock (d) Stationary liquid flock (with vortex-like behaviour). The images are not in the same scale, so the bars on the left and bottom of each tile represent a length of $5r_{\text{min}}$ in each corresponding image.
Figure 2.4: Examples of breakdown modes in MP and LJP flocks. (a) Single moving flock governed by LJP (b) Single moving flock governed by MP (c) Fragmentation of LJP flock demonstrating characteristic ”tearing” (d) Fragmentation of MP flock demonstrating the characteristic ”train” behaviour. The bars on the left and bottom of each tile represent a length of $5r_{\text{min}}$ in each corresponding image.
2.4. RESULTS AND DISCUSSION

complex bacterial behaviour [38, 39, 40, 41, 43], but also with experimental measurements
made on E.coli [42].

Despite significant qualitative similarities in structure and behaviour between the two
models there are still some key differences between the flocks formed. Quantitative mea-
surements such as inter-boid distance, position and nature of the phase transitions and the
relative regions of phase space where these different phases are present are still dependent
on the finer structure of the different potentials and some variation between MP and LJP
cases. For instance, comparing Fig. 2.4(a) and Fig. 2.4(b) for the single flock state, the
MP forms a dense, regular teardrop shaped flock, whereas the LJP leads to a flock with
a dense frontal arc with a more dispersed region trailing. The positions and nature of
the phase transitions between the single flock and multi flock phases is model dependent.
Using the MP, the single-multi transition is far more abrupt, effectively occurring along
one plane in phase space. However in the case of the LJP, the single to multi flock tran-
sition occurs gradually, and there is not a sudden change between the single and multi
flock phases. Instead the flocks begin to disperse at some value of initial density $\rho$, but do
not become fully independent until a much higher $\rho$, with a transitional region existing in
between.

The form of the flock during transition is also substantially different. In the LJP, the
mode by which the single flock transitions into multiple flocks is quite different to that
which is observed in the MP case. The front of the flock begins to split as initial density
decreases, forming two separate "wavefronts" (the term which is adopted to describe this
mode hereafter). The evolution of this fragmentation with decreasing initial density is seen
clearly by comparing Fig. 2.4(a) to Fig. 2.4(c). In Fig. 2.4(a) there is a single, cohesive
front, whereas in Fig. 2.4(c) this single front has began to fragment into two or more
separate fronts. After splitting, each front then continues in a slightly different direction
to the other, and over long time scales, the single flocks resolves itself into two separate
flocks. As density decreases further, the two separate flocks become easier to define, until
at very low densities, a number of completely independent flocks can be observed.
This wavefront mode of flocking is observed in nature at the macroscopic level, with herds of wildebeest (and other ungulates) often forming distinct patterns qualitatively similar to those observed in the simulations presented here during their migratory marches. These wavefront flocks have been examined in some detail [10, 12, 73], but are primarily only understood qualitatively through qualitative observation, with few quantitative measurements of their characteristics having been made. Research has shown that there is a strong tendency for wildebeest herds to form these kind of long, spread out 'fronts' in order to make best use of foraging resources on a wide field or plain [11, 85, 86]. When combined with the natural tendency for flock members to follow one another, a breaking of the directional symmetry thus leads to the characteristic wavefront [10].

This characteristic shape is seen in Fig. 2.5(e), and the qualitative agreement with our model is seen by comparing this to Fig. 2.5(f). However, these models do not include the effects of resource gathering (feeding), yet the characteristic shape is still observed for moving phases with hard-core cohesive interactions. This indicates that instead of being purely a result of outside forces, the wavefront shape exhibited in moving ungulates could instead be caused by the interactions between the flock members themselves. Due to the slow speed of ungulates relative to one another, they are unlikely to undergo accidental collisions, and thus we believe their behaviour is more accurately described the hard-core potential we have used. Therefore, the question of whether the characteristic structure of ungulate herds is caused by interactions with the inhomogeneous resource pool, interactions with other flock members or some combination of the two, is a very pertinent one in the light of this combination of results.

For the MP, as density increases past the critical point, the flock splits into two or more independent flocks along the line of motion with the flocks travelling in the same direction. This characteristic splitting is clearly seen by comparing the regular teardrop shaped flock in Fig. 2.4(b) with the three separate flocks in Fig. 2.4(d) which occur at lower densities. The state observed in Fig. 2.4(d) is subsequently called the "train". As the density further
2.4. RESULTS AND DISCUSSION

Figure 2.5: (a) Simulated stationary fluid state, with flow lines observed. (b) Experimental image of E.coli bacterium exhibiting fluid-like behaviour. (c) Simulated single-flock MP state exhibiting distinctive teardrop structure. (d) A typical cluster bird flock (e) Simulated single-flock LJP state exhibiting distinctive wavefront structure. (f) Migrating wildebeest exhibiting typical wavefront structure. The images are not in the same scale, so the bars on the left and bottom of each tile represent a length of $5r_{\text{min}}$ in each corresponding image. [Images (b), (d) and (f) reproduced from [42], [84] and [10, 12, 73] respectively].
decreases, there is a breaking of the velocity directional symmetry, resulting in multiple independent flocks travelling in different directions. This holds true for all moving phases and noise regimes that were analysed in our simulations. Additionally, once the initial density is low enough for the directional symmetry to break, the independent flocks are free to move around and merge over time, with these mergers being observed in many of the simulations analysed in the low density regime.

The single-flock MP phase is of particular interest, as behaviour similar to this is exhibited in many biological flocks. In fact, spheroidal or amorphous flocks are amongst the most commonly encountered and include many types of bird flocks, fish schools and insect swarms. The qualitative similarities between the modelled single flock MP phase and an experimentally observed bird flock can be seen in Fig. 2.5(c)-2.5(d). However there is a significant lack of experimental data for flocking in 3D (fish and bird schools) and it is yet to be confirmed that similar cluster structures will form the 3D extension of the MP model used here.

It is also important to note the existence of vortex-like behaviour over a wide range of densities in our stationary state simulations $A = 0$ using the MP. This vortex behaviour warrants further analysis in the long-term due to its correspondence with observed behaviour in bacteria, in particular Dictyostelium [38], Daphnia [39] and E.Coli [42]. However, the vortex structures are quite sensitive to changes in noise and are only observed in the low noise regimes. In the medium and high noise cases, the vortex structure is broken down by random thermal motions. The fact that this state exists in our simulations at all is a good indication for the generality of the models presented here. Good qualitative agreement is found between the simulated case and experimental observations in E.Coli [42] in particular. This is shown in Fig. 2.5(a) and Fig. 2.5(b).

Fig. 2.6 and Fig. 2.7 show a set of phase diagrams for both the LJ and Morse based models with stochastic noise, $\eta$ plotted against $l = \frac{N}{\rho^{1/2}}$ in both cases for fixed values of $A = 1$ (moving states). Low noise corresponds to $\eta = 1$ for both models. In the MP case,
medium noise corresponds to $\eta = 20$ and high noise to $\eta = 40$ and in the LJP case medium noise corresponds to $\eta = 10$ and high noise to $\eta = 20$. This difference comes about due to the differing cohesive strengths of the two models.

As stochastic noise, $\eta$ increases, the liquid-like behaviour of the flock becomes dominant, and for small values of $\eta$ the solid-like behaviour is dominant. The formation of single flock or multi-flock states is highly dependent on the initial density $\rho$, even in the absence of boundary conditions. For high values of $\rho$ in the respective models, a single flock state will form, as $\rho$ is decreased, the flock transitions into an intermediate phase, and then at lower values of $\rho$, multiple independent flocks are observed. Fig. 2.6 and Fig. 2.7 show the results for the MP and LJP respectively in the moving regime ($A = 1$). In both cases, three distinct phases are observed as initial density decreases. In the MP, as $\rho$ decreases the flock splits along the line of motion, resulting in a phase transition between the single flock and train phases. Further decrease in $\rho$ eventually results in a further breaking of directional symmetry, whereby multiple independent flocks form each with random direction.

This is true in low [Fig. 2.6(a)], medium [Fig. 2.6(b)] and high [Fig. 2.6(c)] noise regimes, although the actual values of $\rho_{\text{crit}}$ vary slightly depending on the amount of stochastic noise in the system. Fig. 2.7 shows similar behaviour in the case of the LJP. In this case however the transitionary state is quite different. As shown in Fig. 2.5(d) as initial density decreases, the flock tears along the middle, resulting in splitting of the wavefront. As density decreases further these fragmented flocks cease to interact and the result in a multi-flock state with a number of independent flocks moving in free space, as for the MP case. Additionally, in the case of the LJP, the position of the phase transitions described above is more difficult to resolve than for the MP, resulting in larger regions of uncertainty and making the nature of the phase transition less clear. As for the LJP, the same general behaviour is observed in low [Fig. 2.7(a)], medium [Fig. 2.7(b)] and high [Fig. 2.7(c)] noise regimes, despite the actual values for $\rho_{\text{crit}}$ varying slightly. Thus, the positions of the phase transitions in the moving regime are not highly sensitive to noise, and in fact, variation of the stochastic noise seems to have only a small effect on the position of the
transitions in phase space.

![Figure 2.6: Phase Diagram for the MP in the moving regime ($A = 1$) plotted against $l = \frac{1}{\rho^{1/2}}$ for three different cases corresponding to, (a) low ($\eta = 1$), (b) medium ($\eta = 20$) and (c) high $\eta = 40$ values of stochastic noise. The dark bands represent regions of uncertainty.](image)

In the stationary regime where $A = 0$ the phase transitions are a somewhat simpler. In the MP case, two phases are observed with a phase transition between the single and multi-flock state. There is no intermediate phase between the single and multi-flock states, as we observed in the moving regime. At high densities a single flock is formed, and as the density is decreased, there is little change in this single flock state until the critical value is reached. There is some uncertainty as to the exact value at which the phase transition takes place, but Table 2.1 shows the approximate values of $l$ and $\rho$ where this takes place. At values lower than $\rho_{crit}$ two independent flocks are observed. Thereafter, further decreases in $\rho$ lead to an increase in the number of independent flocks present.

In this case it is important to note that position of the phase transition is more sensitive to stochastic noise than in the moving states, with a consistent increase in $\rho_{crit}$ which
2.4. RESULTS AND DISCUSSION

Figure 2.7: Phase Diagram for the LJP in the moving regime \((A = 1)\) plotted against \(l = \frac{1}{\rho^{1/2}}\) for three different cases corresponding to, (a) low \((\eta = 1)\), (b) medium \((\eta = 10)\) and (c) high \((\eta = 20)\) values of stochastic noise. The dark bands represent regions of uncertainty.

results in a transition between the single and multiple flock states as noise, \(\eta\) increases. For the case of the LJP, a decrease in density simply leads to an increasingly dispersed flock, but does not result in the formation of multiple independent flocks. It is not well understood why this should be the case, but it is believed that it is a consequence of the random placement algorithm used in these simulations in which boids are prevented from being placed too close together in the case of the LJP due to the infinite hard-core, since this has the effect of reducing the amount of initial inhomogeneities which subsequently form into the multiple independent flocks in the MP simulations.

<table>
<thead>
<tr>
<th>Noise((\eta))</th>
<th>Side Length((l_{crit}))</th>
<th>Density((\rho_{crit} \times 10^{-3}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20 - 22</td>
<td>2.5 - 2.1</td>
</tr>
<tr>
<td>20</td>
<td>18 - 20</td>
<td>3.1 - 2.5</td>
</tr>
<tr>
<td>40</td>
<td>16 - 18</td>
<td>3.9 - 3.1</td>
</tr>
</tbody>
</table>

Table 2.1: Phase Transition points in the stationary flock regime \((A = 0)\) for MP case at low, medium and high values of stochastic noise.
The behaviour of the two models near the phase boundary is significantly different in that the transition between single and multi flock phases as is described earlier. In the MP case the phase transition from single to multiple flocks is sudden. For some initial density \( \rho > \rho_c \) a single flock is formed, and form some value \( \rho < \rho_c \) multiple flocks are formed, there is only a very small transition region. In the case of the LJP however, this change is more gradual. With the primary flock losing slowly losing members and becoming increasingly fragmented as initial density decreases, until there are two clearly resolvable flocks. This is true in both the stationary and the moving regimes but is more significant in the stationary regime, since in the stationary regime the LJP does not undergo a transition into a true multi-flock state, but instead simply becomes more dispersed. Thus the MP will likely prove more useful in analysing critical phenomena close to the transition point than the LJP.

2.5 Summary

It has been shown that both the Lennard-Jones and Morse potentials, when coupled with an alignment potential, are capable of simulating a wide range of flocking behaviour in free space, including those phases observed in Vicsek’s original flocking paper, that have previously only been studied with the aid of periodic boundary conditions. Additionally, it has been shown that while their are differences in the quantitative details, the bulk features of both the hard core LJP and the soft core MP are the qualitatively similar in most key regards. What this indicates is a kind of “model independence” meaning that all cohesive potentials which have the same key features of short-range repulsion, a preferred nearest-neighbour distance, and long range attraction that weakens with increasing inter-boid distance should yield qualitatively similar flocking systems.

However, significant quantitative differences appear upon deeper examination of the two potential types. The behaviour around the phase transitions differs in that the transition
between the single and multi-flocks states occurs discontinuously at some single value of density, $\rho$ whereas in the LJP, the breakdown of the single flock is gradual, taking place over a wide range of densities making it difficult to identify a single point where this phase transition occurs.

Additionally, the transition from single to multi-flock states happens in two stages. In the first stage, the flock is observed to split along the line of motion, with all flocks continuing to travel in the same direction. The second stage occurs as $\rho$ is further decreased, resulting in a breaking of directional symmetry, which leads to a number of independent flocks all travelling in effectively random directions. Once this state is reached, the individual flocks interact only minimally until they come into close proximity with one another. A number of behaviours can be observed when these independent flocks come into contact with one another including flock mergers, scattering of flocks off one another and flock collisions. All of these interactions have been observed in our model but have not yet fully investigated.

Finally, several vortex states were observed in the low noise regime of the stationary states for the MP. In the LJP these vortices were not observed, but instead solid lattice behaviour was observed in the corresponding regimes for this class of potential. The observation of these vortices is important since it is indicative of the ability of these models to effectively simulate bacterial behaviours which have already been observed in experimental situations and have been more extensively measured than most macroscopic examples of flocking.

Although a number of important observations have so far been made using these models, there is still much scope for future analysis of a number of flocking properties. The models presented have proven very effective in qualitatively simulating the behaviour of a wide range of different flocking behaviours over the entire spectrum of length scales, which was the original aim when they were developed.

The success of this model in simulating a wide range of flocking models will also prove
useful in the next chapter, where a novel analytic flocking model is derived based upon a classical gas equation of state. Some of the results of this new approach will then be compared to the results obtained from a numerical model similar to the one above (albeit significantly simpler) in order to check the accuracy of this new approach and to give a fuller picture of the entire flocking process. The derivations performed in Chapter 3 will also pave the way for using a classical gas model of flocking to investigate the Vicsek flocking model, and to demonstrate the efficacy and validity of using such an approach on an already widely understood model of flocking.
3.1 The Virial Expansion Introduced

To date, flocking has been primarily modelled using two different families of models, namely, individual based models (IBMs) and fluid dynamical models. In Individual-based models, each constituent member of the flock is modelled with its own distinct properties such as velocity, position, acceleration and so forth. The model we explored in Chapter 2 is a member of this family of models. IBMs tend to be more amenable to numerical simulation, but are often not analytically tractable, due to many-body considerations [4, 5, 13, 14, 15, 22, 23, 25, 32, 47, 54].

In order to explore flocking behaviour in a more analytically rigorous fashion the second family of models is typically used. Fluid dynamical models of flocking are based around the analogy between fluid flows and the behaviour of flocks through a medium, such as water or air [17, 20, 62, 64, 87]. In these models, the individual constituents of the flock are not represented, but rather the behaviour of the entire flock itself is described by a set of dynamical fluid flow equations. This is analogous to how fluid flow equations describe the motion of, for instance, the flow of water through a pipe, without describing the behaviour of each individual $H_2O$ molecule.
3.1. THE VIRIAL EXPANSION INTRODUCED

There is at least one additional model in statistical physics which is highly analogous to
the behaviour of flocks in free space, but which to date has not been extensively explored,
that being the behaviour of a simple gas modelled using statistical mechanics [30]. In
a simple gas, each particle in the gas interacts based on a separation dependent poten-
tial. Particles that get too close to one another are repelled and particles far from one
another do not interact. Additionally, each particle possesses kinetic energy based on its
momentum. Knowing the interaction potential, and the kinetic energy of the particles in
the system, a wide range of information about the system can be derived, including the
equation of state, the partition function, the internal energy, the specific heat and the
entropy.

One of the main strengths of modelling flocking using statistical mechanics is that it
makes the partition function immediately accessible. Once the partition function for a
given model is obtained, a number of parameters which have previously been difficult to
analyse are now more easily calculated, including the specific heat capacity, entropy and
the free and total energies of the system. There are a number of reasons these quantities
may prove interesting in the context of a flock. For instance, the specific heat would likely
give information about the location and nature of phase transitions, as it does for other gas
systems, whilst entropy would likely give information about the disorder and perhaps give
insight into the mechanisms of flocks breakdown and dissipation when disorder becomes
too high.

It is important to note that although the language of thermodynamics is being used here,
it may be that some thermodynamic quantities have a slightly different interpretation in
the context of a flocking gas. Temperature for example, as used throughout the follow-
ing calculations, does not refer to the ‘physical’ temperature in the same sense it would
for an ordinary gas. This is because temperature is really just a measure of energy in
a many body system. In an ordinary gas, the energy of the considered system is essen-
tially fixed but in a self-propelled gas, such as a flock, kinetic energy can be added or
subtracted from the system via changes in velocity (this energy is ultimately generated by
the internal metabolic processes of the flocking particle). Therefore it is not expected that
a flocking system will be energy conservative since the metabolic processes of the flock
members, which ultimately power their motion, are always neglected. Temperature will
still be closely related to the speed, stochastic noise and entropy of the flocking system,
but since the system being considered has some important physical differences to ordinary
gas systems, there may be some surprising consequences for the way these quantities are
related to one another.

One powerful technique for deriving an equation of state for a gas system is known as the
‘Virial Expansion’ (incidentally the word ‘virial’ is a Latin word related to ‘force’ denoting
that the terms of the expansion are calculated from the force of the interactions between
the particles of the system [88]). Typically, the virial equation of state is written in the
form:

\[ P\beta = B_1 n + B_2 n^2 + B_3 n^3 \ldots \ldots B_N n^N, \]  

where \( n = \frac{N}{V} \) (in 3 dimensions), \( B_1 = 1 \) trivially and \( B_2 \ldots B_N \) are known as the virial
coefficients and are temperature dependent terms derived from the virial expansion.

Physically, the virial coefficients correspond to the order of the interactions being con-
sidered in the model. For instance, \( B_1 \) considers only single body interactions (self-
interactions) whilst \( B_2 \) considers 2-body interactions, \( B_3 \) considers 3-body interactions
and so forth. In practice, \( B_1 \) is usually trivial to calculate, and \( B_2 \) is the most ‘important’
higher order term as it is the first term to consider genuine interactions between particles
in the gas system. \( B_3 \ldots B_N \) typically make increasing smaller corrections to the interacting
system as the number of particles, \( N \), increases.

The power of the virial expansion is that it can be used to model just about any classical
3.1. THE VIRIAL EXPANSION INTRODUCED

gas system, to as accurate an order as one likes. The more terms kept, the more accurate
and precise the result will be, the less terms kept, the easier it is to solve but the less
precise the result may be, particularly in certain limits [67, 68, 69, 70].

The weakness of the virial expansion is that as one increases the order of the expansion,
the complexity grows rapidly, making the expansion very difficult to work with in practice
if one desires a precision of 3rd order or higher. Additionally, due to the nature of the
mathematics, the physical significance of the results is not always immediately obvious and
some physical intuition is often required to obtain an accurate interpretation. In practice,
the virial expansion is usually only solved to 2nd or 3rd order, and only in rare situations
is it necessary to solve the expansion to higher orders.

In a somewhat convoluted fashion, the virial coefficients are dependent upon a series of
other terms, usually denoted as $b_1$...$b_N$. For instance, the first 3 virial coefficients are
equal to:

\begin{align*}
B_1 &= b_1, \\
B_2 &= -b_2, \\
B_3 &= -2b_3 + 4b_1^2
\end{align*}

Finally, $b_1$...$b_N$ are in turn dependent upon a set of terms called the configuration inte-
grals. It is these configuration integrals which form the core of the virial expansion. For
example, $b_2$, $b_2$, $b_3$ are related to the configuration integrals by:

\begin{align*}
b_1 &= 1, \\
b_2 &= \frac{1}{2V} (\Xi_2 - \Xi_1^2), \\
b_3 &= \frac{1}{6V} (\Xi_3 - 3\Xi_1\Xi_2 + 2\Xi_1^3)
\end{align*}
All the subsequent series terms used to find the equation of state ultimately depend on the configuration integrals $\Xi_1 \ldots \Xi_N$, as well as the partition function from which many of the useful thermodynamic quantities are derived. Thus it is the series $\Xi_1 \ldots \Xi_N$ which is where most of the mathematics for solving the virial expansion actually lies and it is these terms which will be the focus of most of the derivation. In general, the configuration integrals may be written as:

$$
\Xi_N = \int_0^V dx_1^3 dx_2^3 \ldots dx_N^3 \exp \left( -\beta H(x) \right),
$$

(3.8)

where $H(x)$ is the portion of the Hamiltonian including all the terms which involve inter-particle interactions.

Subsequently, this can be used to solve for the terms of the partition function, where:

$$
Z_N = \frac{1}{N!} \frac{1}{(2\pi \hbar)^2 N} \int d^3p_1 d^3p_2 \ldots d^3p_N \exp \left( -\frac{\beta p^2}{2m} \right) \Xi_N,
$$

(3.9)

and:

$$
Z = \sum_{N=0}^{N} \lambda^N Z_N,
$$

(3.10)

where $\lambda = e^{\mu \beta}$ is known as the fugacity, a function of the chemical potential $\mu$ which represents the amount by which the energy of the system would change if an additional particle is added.

It is important to note that the configuration integral depends only on the interacting portion of the Hamiltonian, meaning that for an ordinary gas, the entire integral over momentum can be neglected from $\Xi_N$ and solved explicitly for $Z_N$. This is because in an ordinary gas there are no intermolecular interactions that depend on relative momentum, only relative position. In general however, this need not be the case. For a flocking gas, momentum-based interactions (specifically those dependent on the direction of motion)
3.2. FLOCKING AND THE VIRIAL EXPANSION

form a key part of flocking behaviour. This is an important point which will be revisited later.

One example of a virial equation of state is the Van der Waals Equation [71, 72, 89]:

\[
(P + \frac{aN^2}{V^2})(V - Nb) = NkT. \tag{3.11}
\]

The Van der Waals equation is a refinement of the Ideal Gas Law which can be derived using the virial expansion to 2nd order for a Sutherland type potential. In this case, physical intuition leads to the understanding that the parameters \(a\) and \(b\) correspond to physical characteristics of the system with \(a\) being associated with the strength of the attractive intermolecular force and \(b\) being analogous to the volume occupied by the molecules themselves. Importantly, although the Van der Waals equation is based on a 2nd order virial expansion, it is a very robust and accurate equation, which is still oft used today in classical gases where quantum effects do not need to be taken into account.

3.2 Flocking and the Virial Expansion

What does all this have to do with Flocking though? Consider Fig. 3.1 which shows the interactions between particles in two different kinds of gas systems, one being a ordinary gas and the other what will be referred to as a flocking gas. In an ordinary gas system, the constituent particles interact with one another through potentials and hence forces which are dependent only on separation, not on the direction of motion of the particles. In a flocking gas, the particles (which are called boids in this context) not only interact based on their separation from one another, but also based on the alignment of their velocity vectors. This represents an entirely new degree of freedom which is related to the tendency for alignment found in flocking systems. Taking this alignment tendency into account produces a novel gas system which through the use of statistical mechanics techniques can be used uncover new information and make new predictions about the properties of
self-organised flocking systems.

There are two components of the configuration integral in this context, an integration over momentum, and an integration over space. Usually, the details of the integration over momentum can be considered outside the configuration integral, because particles in an ordinary gas don’t interact based on their momentum vectors. However, the virial expansion need not be considered this way, and it is entirely possible to analyse a system of particles which interact, not just based on separation, but also based on the direction of their velocity vectors. This is, in essence, the exact definition of a flock. A set of particles which interact based on their relative positions and on the alignment of their velocity vectors. The virial expansion can thus be used to derive an equation of state and the partition function for flocking behaviour, allowing a whole slew of new statistical mechanics tools to be bought to bear in analysing flocking systems.

As previously stated, virial equations of state are typically only solved to 2nd or 3rd order, but it is sometimes possible to write a geometric series to solve to N orders in principle, if not practice, for the simplest cases. In order to derive the system completely analytically, a very simple set of flocking potentials are chosen in this case. The aim here is not to derive a realistic flocking model, as the complexity of such a model may make it
3.2. FLOCKING AND THE VIRIAL EXPANSION

difficult to derive and interpret analytically. Instead a very simple case is examined to demonstrate that the virial expansion can, in principle, be used to derive equations of state and the associated quantities for flocking potentials. After the efficacy and robustness of this analytical approach is proven it is hoped that the technique can be used to analyse increasingly realistic flocking models in order to better understand this complex behaviour.

To start with, the flocking system being analysed here will be 2D rather than 3D, due to the relative complexity of modelling 3D systems compared to 2D systems, and the preponderance of previous flocking models in the literature being based on 2D systems. This means that what was the volume of the system, \( V \), in the general equations, will now be the area of the system, \( A \). Additionally, the form of some of the integrals and some other associated constants will change dimension due to this. Furthermore, the first step to actually finding the virial coefficients is to solve \( \Xi_N \), and from equation (3.8) it can be noted that in order to do so, the Hamiltonian of the gas system will be required. The Hamiltonian is the sum of the total energy of the system, including kinetic and potential components. However, the Hamiltonian which contributes to the configuration integral \( \Xi_N \), depends only on the interacting portion of the Hamiltonian, which means that the kinetic component is neglected from \( \Xi_N \) (although it will still appear in \( Z_N \)), yielding:

\[
H(x, \phi) = \sum_{i \neq j} V^C(r_i - r_j) + \sum_{i \neq j} V^A(\phi_i - \phi_j). 
\]  \hspace{1cm} (3.12)

A separation potential based on a simple Gaussian is considered along with an alignment potential of \( \sin^2 \) form, such that:
\[ V_{ij}^{(C)}(r) = B \exp(-\alpha^2 (r_i - r_j)^2), \]  
\[ V_{ij}^{(A)}(\phi) = C \sin^2 \left( \frac{\phi_i - \phi_j}{2} \right), \] 

where the constant \( B \) governs the strength of the Gaussian interaction and constant \( C \) governs the strength of the \( \sin^2 \) interaction.

The shape of these potentials is seen in Fig. 3.2. The repulsive potential \( V^{(C)}(r) \) decays rapidly to zero, such that only boids that pass close to one another will feel this repulsive potential. The alignment potential \( V^{(A)}(\phi) \) contains a minima at \( \phi_{ij} = 0 \), indicating a preference for alignment between boids. However, it should be immediately apparent that the alignment potential operates over all space. That is, boids will attempt alignment with every other boid in the flock regardless of the separation between them. This breaks one of the cardinal rules of modelling flocks, that is, that constituent members interact only with other members of the flock that are close to them. Strictly speaking then, this model allows for interaction that you wouldn’t expect to see in a real flock, however, this does not completely nullify the validity of this approach. Firstly, this particular model is still valid in situations that involve flocks with a small number of members, or inside very dense flocks where it would be expected that each individual boid is interacting with a large number of other boids. Finally, despite the limitations, the main purpose of this derivation is to show that in principle, flocking behaviour which involves both separation and alignment dependence, can produce meaningful results when solved using a virial expansion approach. The addition of coupling between separation and alignment dependence greatly increases the complexity of the problem, and considering how useful the results will remain without this, it is felt that such an approach would be inappropriate at this stage, but will be revisited later in Chapter 4.
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Figure 3.2: (a) The separation dependent potential $V^{(C)}_{ij}(r)$ with $B = 1$. (b) The alignment dependent potential $V^{(A)}_{ij}(\phi)$ with $C = 1$. Note that this potential allows alignment over the entire system, since there is no dependence on $r_{ij}$. 
3.3 Deriving a Flocking Equation of State

In ordinary gases, the momentum component can be explicitly excluded from the configuration integral since it is a non-interacting term, as previously discussed, in which case the form of $\Xi_N$ and $Z_N$ are given by equations (3.8) and (3.9). However, in the case of a flocking gas, the direction of the momentum vectors is now an interacting term, such that the momentum of each particle can no longer be considered in isolation from the other particles of the system. This means that although the magnitude of the momentum term still does not contribute to the configuration integral, the directional component does. So for a flocking gas, $\Xi_N$ and $Z_N$ may be written:

$$\Xi_N = \int_0^A d^2 x_1 d^2 x_2 \ldots d^2 x_N \int_{-\pi}^{\pi} d\phi_1 d\phi_2 \ldots d\phi_N \exp \left( -\beta H(x, \phi) \right),$$

$$Z_N = \frac{1}{N! \left( 2\pi \hbar \right)^2 N} \int_0^\infty \left| p \right| d\left| p \right|_1 d\left| p \right|_2 \ldots d\left| p \right|_N \left| p \right|_1 \left| p \right|_2 \ldots \left| p \right|_N \exp \left( -\frac{\beta \left| p \right|^2}{2m} \right) \Xi_N.$$

In order to find the equation of state for this flocking model, $\Xi_N$ must first be solved explicitly. Using $H(x, \phi)$ as defined in equation (3.12) then $\Xi_N$ becomes, after conversion to polar coordinates:

$$\Xi_N = \int_0^L dr_1 dr_2 \ldots dr_N \int_{-\pi}^{\pi} d\theta_1 d\theta_2 \ldots d\theta_N \int_{-\pi}^{\pi} d\phi_1 d\phi_2 \ldots d\phi_N r_1 r_2 \ldots r_N \times \exp \left( -\beta \left( \sum_{i<j} B e^{-\alpha^2(r_i-r_j)^2} + \sum_{i<j} C \sin^2 \left( \frac{\phi_i - \phi_j}{2} \right) \right) \right),$$

Note that $d\theta$ represents the trivial angular integral in position space, after converting to polar coordinates.

Although a Gaussian function gives an elegant representation for the separation dependent potential, solving the integral of the exponential of an exponential would prove very trou-
3.3. DERIVING A FLOCKING EQUATION OF STATE

blesome analytically. Instead the lower exponential can be expanded as a Taylor series, however this is also slightly problematic as it cannot be guaranteed that $\beta$ will be small. To get around this, a new parameter $\zeta$ may be introduced, with units of energy, such that $\beta\zeta < 1$. This allows for the lower exponential to be eliminated by performing a Taylor Expansion about $\beta\zeta$:

$$
\Xi_N = \int_0^L dr_1 dr_2 \ldots dr_N \int_{-\pi}^\pi d\theta_1 d\theta_2 \ldots d\theta_N \int_{-\pi}^\pi d\phi_1 d\phi_2 \ldots d\phi_N r_1 r_2 \ldots r_N \\
\times \left[ 1 - \beta\zeta \left( \sum_{i<j} b e^{-\alpha^2(r_i-r_j)^2} + c \sin^2 \left( \frac{\phi_i - \phi_j}{2} \right) \right) \right] \\
+ \frac{(\beta\zeta)^2}{2} \left( \sum_{i<j} b e^{-\alpha(r_i-r_j)^2} + c \sin^2 \left( \frac{\phi_i - \phi_j}{2} \right) \sum_{i<j} b e^{-\alpha(r_i-r_j)^2} + c \sin^2 \left( \frac{\phi_i - \phi_j}{2} \right) \right). 
$$

(3.18)

Note that $b = \frac{B}{\zeta}$ and $c = \frac{C}{\zeta}$ have been defined in order to preserve the dimensionality of the equation. Assuming $\beta\zeta \ll 1$, truncating the expansion to first order will give sufficient accuracy leaving a relatively simple integration:

$$
\Xi_N = \int_0^L dr_1 dr_2 \ldots dr_N \int_{-\pi}^\pi d\theta_1 d\theta_2 \ldots d\theta_N \int_{-\pi}^\pi d\phi_1 d\phi_2 \ldots d\phi_N r_1 r_2 \ldots r_N \\
\times \left( 1 - \beta\zeta \left( \sum_{i<j} b e^{-\alpha^2(r_i-r_j)^2} + c \sin^2 \left( \frac{\phi_i - \phi_j}{2} \right) \right) \right). 
$$

(3.19)

Now, given that each boid is indistinguishable from any other boid, that is, each boid has the same interaction form as any other, then in fact there exists $N^2$ couplings between the boids. However, since $r_{ij} = r_{ji}$ simply multiplying the integral by $N^2$ would result in a significant over count of the unique interactions. In fact, there exists only $\frac{N(N-1)}{2}$ unique interactions. However, since each interaction is, in principle, the same, the integral itself need only be solved once, then multiplied by $\frac{N(N-1)}{2}$. For simplicity, the integral solved will be labelled as boid 1 with boid 2:
\[ \Xi_N = (2\pi)^N \left( \left( \frac{L^2}{2} \right)^N - \left( \frac{L^2}{2} \right)^{N-2} \frac{N(N-1)}{2} \beta \zeta \right) \times \int_0^L dr_1 dr_2 r_1 r_2 \int_{-\pi}^\pi d\phi_1 d\phi_2 \left( be^{-\alpha^2(r_1-r_2)^2} + c \sin^2 \left( \frac{\phi_1 - \phi_2}{2} \right) \right). \tag{3.20} \]

The integrals may be separated to simplify the calculation, resulting in:

\[ \Xi_N = (A)^N - (A)^{N-2} \frac{N(N-1)}{2} \beta \zeta \times \left[ \int_0^L dr_1 dr_2 \int_{-\pi}^\pi d\phi_1 d\phi_2 r_1 r_2 e^{-\alpha^2(r_1-r_2)^2} + \int_0^L dr_1 dr_2 \int_{-\pi}^\pi d\phi_1 d\phi_2 r_1 r_2 c \sin^2 \left( \frac{\phi_1 - \phi_2}{2} \right) \right], \tag{3.21} \]

where \( A = \pi L^2 \) is the area of the entire system.

The \( \phi \) dependent function can then be integrated such that:

\[ \Xi_N = A - A^{N-2} \frac{N(N-1)}{2} \beta \zeta \times \left[ \frac{L^4 2\pi c}{4} + \int_0^L dr_1 dr_2 \int_{-\pi}^\pi d\phi_1 d\phi_2 \left( b r_1 r_2 e^{-\alpha^2(r_1-r_2)^2} \right) \right]. \tag{3.22} \]

However, the integral for relative separation requires a change of variables to a centre of mass coordinates system, with two new variables defined such that:

\[ r = \frac{r_1 + r_2}{2} \quad r_{12} = r_1 - r_2 \tag{3.23} \]
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After changing coordinate systems, the equation becomes:

\[
\Xi_N = A - A^{N-2} \frac{N(N-1)}{2} \beta \zeta \\
\times \left[ \frac{L^4}{4} \frac{2\pi c}{2} + \int_0^L \int_0^L drdr_{12} \left( 2\pi b \left( r^2 - \frac{1}{4} r_{12}^2 \right) e^{-\alpha^2 (r_1 - r_2)^2} \right) \right], \quad (3.24)
\]

which may again be split into 2 portions for ease of calculation:

\[
\Xi_N = A - A^{N-2} \frac{N(N-1)}{2} \beta \zeta \\
\times 2\pi \left[ \frac{L^4 c}{4} + \int_0^L \int_0^L drdr_{12} \left( r^2 e^{-\alpha^2 (r_1 - r_2)^2} \right) - \int_0^L \int_0^L drdr_{12} \left( \frac{1}{4} r_{12}^2 e^{-\alpha^2 (r_1 - r_2)^2} \right) \right], \quad (3.25)
\]

and finally solved to give a general expression for \( \Xi_N \):

\[
\Xi_N = A - A^{N-2} \frac{N(N-1)}{2} \beta \zeta \\
\times \left( \frac{2\pi c L^2}{4} - 2\pi b \left[ \frac{1}{3} \sqrt{\pi} L^3 \operatorname{Erf}(\alpha L) + \frac{L}{4} \left( \frac{e^{-\alpha^2 L^2}}{2\alpha^2} - \sqrt{\pi} \frac{\operatorname{Erf}(\alpha L)}{4\alpha^3} \right) \right] \right), \quad (3.26)
\]

where \( L \) is the radius of a circle of area, \( A \).

It should now be apparent that the constant \( \alpha \) has some length dependence. In fact having observed the form of the Gaussian potential earlier indicates that \( \alpha \) should be inversely dependent on length, since \( \alpha \) inversely governs the width of the Gaussian separation potential. In order to make the dimensionality of the equation of state more obvious, a new dimensionless constant \( a^2 = \alpha^2 L^2 \) is introduced such that:

\[
\Xi_N = A^N - A^{N-2} \frac{N(N-1)}{2} \pi^2 L^4 \beta \zeta \left( \frac{c}{4} - b \left[ \frac{1}{3} \sqrt{\pi} \frac{\operatorname{Erf}(\alpha a)}{2\alpha a} + \frac{1}{4} \left( \frac{e^{-a^2}}{2\alpha^2} - \sqrt{\pi} \frac{\operatorname{Erf}(\alpha a)}{4\alpha^3} \right) \right] \right). \quad (3.27)
\]
After a little consolidation, this results in a final value for $\Xi_N$ of:

$$\Xi_N = A^N - A^N \frac{N(N-1)}{2} \beta \zeta \left( \frac{c}{2} - b \left[ \frac{1}{3} \sqrt{\pi} \frac{\text{Erf}(a)}{a} + \frac{e^{-a^2}}{4a^2} - \frac{\text{Erf}(a)}{6a^3} \right] \right),$$

(3.28)

noting that $A = \pi L^2$ term has been absorbed into $A^N$.

From equations (3.2) - (3.7) $b_N$ and hence $B_N$ can then in principle be found, and a solution written for the virial equation of state to order $N$.

However, since the relationships leading from $\Xi_N$ to $b_N$ to $B_N$ are non-trivial, and there is no general form for converting $\Xi_N \to B_N$ it will not be attempted here in practice. Instead, for further analysis and comparison to numerical models, the virial expansion will be truncated to 2nd order in the solution of the equation of state and partition function.

For those interested in exploring the higher order perturbations of the virial expansion, $\Xi_N$ can be used and with increasing difficulty and computation, $B_N$ can be found to as many orders as desired. Much like the Van Der Waals Equation cited above, it is felt that a 2nd order expansion will be sufficiently accurate for the numerical models to be compared in this case, and that the corrections of terms 3rd order and above will decrease in magnitude as $N$ increases due to the increasing order of the density term $n$ as the order of the expansion increases.

Hence:

$$B_1 = 1$$

$$B_2 = A\beta \zeta \left( \frac{c}{2} - b \left[ \frac{\sqrt{\pi} \text{Erf}(a)}{3a} + \frac{e^{-a^2}}{4a^2} - \frac{\text{Erf}(a)}{8a^3} \right] \right),$$

(3.29)  

(3.30)
with the virial equation of state is given by:

\[
P_\beta = n + n^2 (A \beta \zeta) \left( \frac{c}{2} - b \left[ \frac{\sqrt{\pi}}{3} \text{Erf}(a) + \frac{e^{-a^2}}{4a^2} - \sqrt{\pi} \frac{\text{Erf}(a)}{8a^3} \right] \right) \tag{3.31}
\]

To tidy this up a little, a new variable \(f(a)\) will be defined:

\[
f(a) = \frac{\sqrt{\pi}}{3} \frac{\text{Erf}(a)}{a} + \frac{e^{-a^2}}{4a^2} - \sqrt{\pi} \frac{\text{Erf}(a)}{8a^3}, \tag{3.32}
\]

which simplifies the equation of state to:

\[
P_\beta = n + n^2 (A \beta \zeta) \left( \frac{c}{2} - bf(a) \right). \tag{3.33}
\]

For comparison to numerical simulations, this equation can be simplified still further. Firstly, it has been stipulated that \(\beta \zeta < 1\) as this is the range over which the first order Taylor series approximation of \(\exp(\beta \zeta x)\) is sufficiently accurate. However, the actual value of \(\beta \zeta\) is not fixed at this stage.

Hence, the value of \(\beta \zeta\) can be tuned such that \(A \beta \zeta = 1\), and since \(A\) can be changed arbitrarily in a computational simulation it can ensured that \(\beta \zeta << 1\). Additionally, since \(n\) is simply the number density of the simulation, which can also be tuned for any given simulation, hence:

\[
P_{\text{sim},\beta} = 1 + \left( \frac{c}{2} - bf(a) \right), \tag{3.34}
\]

where \(b = 1\) is set as the strength of the repulsive Gaussian potential.
Now by definition, the partition function to 2nd order is given by:

\[ Z = 1 + \lambda Z_1 + \lambda^2 Z_2, \]  

(3.35)

\[ Z_N \] can then be determined from equation (3.9) above.

This leads to a partition function to 2nd order of:

\[
Z = 1 + \lambda \left( \frac{1}{(2\pi \hbar)^2} \frac{2m}{\beta} A \right) \\
+ \lambda^2 \left( \frac{1}{(2\pi \hbar)^4} \frac{4m^2 A^2}{\beta^2} \left( 1 - \beta \zeta \left( \frac{c}{2} - f(a) \right) \right) \right),
\]

(3.36)

where \( f(a) \) is as defined in Equation (3.32).

Before progressing further, it is worth taking a moment to examine the physical significance of the interaction terms above, in particular, the strengths of the interactions \( a \), \( b \), and \( c \). As established earlier \( a \) is related to \( \alpha \) by \( a = \alpha L \) where \( L \) has dimensions of length and \( \alpha \) has dimensions of inverse length, making \( a \) dimensionless by definition. Both \( b \) and \( c \) come out of the expressions for the potential energy of the boids in the system as coefficients relating to the strength of the potential, specifically \( b = \frac{B}{\zeta} \) and \( c = \frac{C}{\zeta} \). Thus although both \( b \) and \( c \) are dimensionless, the magnitude of \( B \) and \( C \) define the strengths of the cohesion and alignment potential respectively. It is the magnitude of \( C \) which has units of energy, which governs the strength of the alignment potential, and this is particularly important when it comes to examining the difference between order and disorder in the system. To express it simply, when \( k_B T >> C \) one would expect to find the system in a disordered state, as the energy associated with thermal fluctuations, \( k_B T \) is far stronger than the magnitude of the potentials forcing the boids into correlated alignment. However when \( k_B T << C \) one would expect to find the system in an ordered phase, and somewhere in between, where \( k_B T \approx C \) will lie the transition between those 2 states.
3.4 **Comparison to Computational Flocking System**

Although this phase transition is not specifically dealt with for this model, it is instructive to understand how the choice of interactions strength for $B$ and especially $C$ will play a vital role in the location of any phase transitions in $k_BT$. Specifically, by choosing sensible values for strength of the alignment potential, the location of the phase transition can be contrived to lie at roughly some value of $k_BT = C$, thus making it far easier to search for and determine whether a transition is indeed occurring and the nature of that phase transition. This will prove a particularly important point in Chapter 4, where the phase transition in the Vicsek system is examined in detail.

### 3.4 Comparison to Computational Flocking System

In order to test the equation of state that has been derived, a simple computer simulation is created, similar to that used in Chapter 2, but with $V_C$ and $V_A$ altered to correspond to the potentials being used in this system, as in equations (3.13) and (3.14). Using this simulation, the average pressure, $P$ can be analysed for different alignment strengths $c$ and hence it can be determined whether the derived equation correctly predicts the right trending behaviour that is expected in complex flocking systems.

Each simulation was performed in a box with periodic boundary conditions. The system contains 100 particles in an square area of 100 arbitrary units, such that $n = \frac{N}{A} = 1$ and $\zeta\beta << 1$. Note that since the simulation is modelled in a square region, whereas the analytic calculations were performed in a circular region, there may be some slight discrepancies. However, by equalizing the overall area to 100 units, it is thought that these deviations will be fairly minimal and will not introduce large errors into the comparison. A diagrammatic comparison of the two regions can be seen in Fig. 3.3, where a circular area of 100 units corresponds to a circular region of radius $R = \sqrt{\frac{100}{\pi}} \approx 5.64$ and a square area of 100 units corresponds to a square region of width $W = 10$. 

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The initial particle positions are randomized such that any given particle has an equal probability of starting at any given position in the box. Additionally, the initial direction of motion is also randomized such that any particle has an equal chance of having an initial velocity in any given direction. Note however, that the magnitude of the velocity in this case is fixed.

The pressure in the computational model is measured using the typical kinetic theory methodology, however, since the system being considered is 2-dimensional there are some alterations to the standard result, since the quantity being measured is the force applied over 1D boundary of a 2D area, rather than a 2D boundary of a 3D volume. This means that there are some alterations to the standard kinetic theory definitions of pressure and temperature, since the standard results are derived in 3D.

Since the total force on the boundary of the 2D system is given by,

$$ F_{sim} = \frac{Nm\bar{v}_\perp^2}{L}, $$

(3.37)
3.4. COMPARISON TO COMPUTATIONAL FLOCKING SYSTEM

and the assumption of molecular chaos means that, \( \bar{v}_⊥^2 = \frac{v^2}{2} \) for a 2D system, yielding:

\[
F_{\text{sim}} = \frac{Nmv^2}{2W}, \tag{3.38}
\]

then the pressure on the boundary of the system is given by,

\[
P_{\text{sim}} = \frac{Nmv^2}{2A}, \tag{3.39}
\]

where \( N \) is the particle number, \( m \) is the particle mass, \( v \) the average particle speed and \( W \) is the box width, and \( A \) is the area of the system for equations (3.37)-(3.39).

Since the system is defined in arbitrary units, and each boid is indistinguishable, it is convenient to set \( m = 1 \) for ease of calculation. As in the Vicsek model [14] the speed of the particles is fixed, with a value of \( v = 1 \) for simplicity. Finally, the size of the system, is fixed, being a square of width \( W = 10 \), leaving:

\[
P_{\text{sim}} = \frac{N}{200}. \tag{3.40}
\]

In practice this means that the pressure is determined by counting the number of boids colliding with the periodic boundaries of the system, and dividing that quantity by 200.

Due to the crude nature of this approach to measuring pressure, there is expected to be a lot of noise on the small time scale in pressure, thus, the pressure is averaged over 1000 time steps and the simulation is run over 20000 time steps. Additionally, for every alignment strength \( c \) modelled, the pressure is averaged over an ensemble of 25 systems in order to reduce the impact of any behaviour that might be unique to any given initial conditions.

Three different alignment strengths were modelled with \( c = 1, 2, 5 \) and the results plotted on a pressure-time graph for each of these alignment strengths with \( \beta \) held constant. The strength of the Gaussian repulsion is also held constant at \( b = 1 \) whilst the constant \( a \)
is discussed below. The resultant graph, shown in Fig. 3.4, plots the numerical results obtained for \( c = 1, 2, 5 \) as solid lines. It is important to note that it is the long time scale behaviour which is important in this context. Any given system of this type with random initial conditions, will undergo a relaxation time as it settles into a steady state behaviour. It is the steady state behaviour that is calculated in the analytic work undertaken earlier and hence it is this state of the system which is used by way of comparison to the numerical model. It can be seen from Fig. 3.7 that for \( c = 1 \), \( P \) approaches a value where \( 1 < P < 1.5 \) in the long term and that for \( c = 2, 5 \) tend to \( P \approx 2 \) and \( P \approx 3.5 \) respectively.

![Figure 3.4: Comparison of predicted Pressure vs Time behaviour from virial equation of state (dashed lines) and observed Pressure vs Time from numerically simulated system (solid lines). Note that blue corresponds to alignment strength of \( c = 1 \), green to \( c = 2 \) and red to \( c = 5 \).](image)

The dotted lines represent the theoretically expected values for \( c = 1, 2, 5 \) of \( P = 1.5, 2, 3.5 \) respectively. However, it is not immediately obvious that this is the case from equation (3.34) since a couple of additional approximations are required. Firstly, the computational
3.4. COMPARISON TO COMPUTATIONAL FLOCKING SYSTEM

results are calculated for fixed $\beta$ such that $\beta = 1$.

In addition to this, the $f(a)$ term can also be simplified. As established earlier in this analysis, $a$ is a constant, which represents the width of the Gaussian potential. In a typical macroscopic system, the system is dominated by empty space. Much like a gas, the particles occupy only a small portion of the actual volume, and are separated by substantial amounts of empty space. So if the repulsive term $f(a)$ is taken to be representative of the boids in the system then $a$ inversely governs the size of the boids in the system. It is thus sensible to define large $a$ such that the width of the Gaussian is made very small. This rationalisation is borne out by considering that for $\alpha = 2$ (which is a corresponds to a sensible Gaussian interaction width) that $f(a) \rightarrow 0$, since $a = \alpha L = 20$. Fig. 3.5 shows the behaviour of the repulsive term $f(a) \rightarrow 0$ as $a$ increases.

![Figure 3.5](image.png)

Figure 3.5: The behaviour of the $f(a)$ term with respect to $a$. After an initial oscillation at low $a$, $f(a)$ rapidly approaches zero as $a$ increases. At realistic values of $a$, for instance, $\alpha = 2$ (corresponding to a significant repulsive interaction range of approximately 1 unit), $a = \alpha L = 20$ meaning that the size of $f(a)$ will be negligible in the equation of state.

Hence, assuming large $a > 2$ and keeping fixed $\beta$ as discussed previously, yields a very specific pressure vs alignment strength relationship.
\[ P_{\text{sim}} = 1 + \left( \frac{c}{2} \right). \]  

(3.41)

Meaning that pressure has a baseline of \( P = 1 \) for no alignment interaction, and increases in units of \( \frac{1}{2} \) for each subsequent unitary increase in \( c \). It turns out that this is exactly the behaviour observed in the computational model after the system has undergone an initial settling period. It is particularly evident in the cases of \( c = 2 \) and \( c = 5 \) where the correlation between analytically expected values and computationally observed values is very close in steady state timescales. Despite significant noise over time in the pressure measurements of all alignment strengths (which is to be expected given the method used to measure pressure), in all cases, and in particular for \( c = 2 \) and \( c = 5 \) the trending behaviour of pressure in the numerical simulation is very close to that predicted by the virial equation of state.

### 3.5 Discussion and Limitations

Despite the close agreement between the computational and analytic approaches, it can be also seen that the relationship is not completely precise. For \( c = 5 \) the long term trend for pressure in the numerical simulation lies almost exactly on the analytical line. However as \( c \) decreases, it can be noted that the numerical simulation starts to slightly diverge from the predicted behaviour given by the virial expansion and at \( c = 1 \) this is very obvious with the numerically modelled pressure being obviously less than that predicted by the virial equation of state.

It is believed that this could be due to the \( f(a) \) term which was neglected earlier from the equation of state earlier. When \( c \) is large, the alignment term, \( \frac{c}{2} \), is clearly dominant and \( f(a) \) can safely be neglected. However, it is suggested that for smaller alignment strengths, \( c \) the repulsive term could have more influence on the overall pressure, and that
is what could be resulting in slightly lower than expected pressures in the simulated cases. Modelling over a wider range of \( c \) values would be required to test this hypothesis.

Given the initial success of this simple virial expansion model to correctly predict some of the pertinent physical quantities associated with a system of particles with velocity alignment, it should now be considered time to move forward and look at a flocking system which is better understood and has a better connection to realistic flocking than this initial toy model.

Although this model has proved useful for the purposes of analytically solving for some important physical quantities and for demonstrating the analytical method for solving the virial expansion for a velocity aligned gas system, it has some substantial shortcomings and limitations as a serious flocking model. The biggest of these shortcomings is that the directional alignment operates over all space. This is akin to saying that a boid in a flock weights its directional behaviour against all other members of the flock directly, and equally. It is widely understood that this is not the case in real flocking behaviour.

In a real flock, any given boid gives substantially more weighting to his nearest neighbours whilst distant members of the flock only have a small direct influence on the alignment of the boid being considered. Any influence from distant members of the flock is generally passed through intermediary boids before it reaches a distant boid in the same flock [5, 10, 12, 14]. So, what does this mean for the robustness of the model presented here?

This means that there are quite a limited number of regimes where this model can be said to replicate realistic flocking behaviour. Primarily, this involves small regions within dense flocks where it would be expected that every boid in the given region would interact with every other boid in the given region. In the cases of macroscopic flocks, this would typically indicate a case with small \( N \), as most flocking interactions in macroscopic animals are believed to be governed by sight, and thus, there cannot be too many boids that sight lines within the region would be blocked. However, this model could prove useful for
modelling the interior of dense bacterium flocks, where the interactions generally occur via a different mechanism (usually chemical based) [90, 91, 92] and where the flocks tend to be denser conglomerations.

This new approach to modelling flocks using a virial equation of state will be continued in Chapter 4, where the virial equation of state will be derived for a Vicsek-like system, which is a far more robust, accurate and well understood model of flocking. Furthermore, this new technique will be used to derive a number of thermodynamic variables associated with this Vicsek-like system, including internal energy, entropy and specific heat. This will allow the phase transition from order - disorder in the Vicsek system to be examined in depth from a completely different approach than has been attempted previously.
A New Approach to the Vicsek Model

4.1 The Vicsek Model and the Virial Expansion

In the previous chapter, it was shown that the virial expansion could be used to create a simple gas model of flocking in order to obtain an equation of state and partition function for such a system, allowing for the investigation of some key physical properties of a flocking gas. However, a number of simplifying assumptions were made to this model, such as a long-range alignment interaction, and a very simple cohesion force in order to make it analytically tractable. Unfortunately, these assumptions, whilst useful in terms of allowing the problem to be solved analytically, mean that the resulting flocking model isn’t an especially realistic representation of real world flocking, and that its applicability is limited to a small number of regimes and flocking conditions.

Now that a virial treatment of flocking has been demonstrated to be consistent with numerical modelling, the next step is to derive a model which is capable of generating more interesting and rigorously defined flocking behaviour. Since the emergence of flocking research in the 90s, the Vicsek model [14] has remained the gold standard against which other flocking models are compared [18, 19, 22, 25, 27, 29, 33, 36, 49]. This model, whilst very simple, reproduces some of the more interesting collective behaviours present in real
4.1. THE VICSEK MODEL AND THE VIRIAL EXPANSION

world flocking systems [14, 18, 19, 36]. Additionally, it is by far the most recognised and well understood flocking model in physics literature, and for this reason, it would make an excellent cornerstone for comparison to any new approach to deriving flocking models, and in this case it happens to be particularly amenable to this treatment.

Once again, the virial expansion [67, 68, 69, 70] will be used to derive an equation of state, partition function and associated quantities of a flocking system, but this time, the potentials and Hamiltonian of the system will be based on the more robust Vicsek model [14]. Some of the key relationships and quantities derived using this semi-analytic approach will then be compared to the well understood computational characteristics of the Vicsek model in order to determine whether a gas model of flocking can be derived which encapsulates the important characteristics of the Vicsek individual-based model. This will help show that a gas based interpretation of flocking is a valid, useful and most importantly, accurate way of investigating flocking behaviour.

However, there are some trade-offs compared with the model discussed in Chapter 3. A small number of alterations will need to be made in order to make the problem tractable. Despite this, the gas model derived will still be primarily analytic, albeit to finite order in the virial expansion. Once an equation of state is obtained for the Vicsek model through this process, a number of physical quantities, can be calculated including, pressure, temperature and entropy.

In this case, deriving the virial expansion to N orders will not be attempted as it was in the previous chapter, and instead, the derivation will be limited to 2nd order, which considers 2-body interactions within the gas as well as the single body behaviour of the boids. It is at these low orders where the key interactions are expected to be most significant.

To start with, the Vicsek equations of motion are given by:
\[ r_i(t + \Delta t) = r_i(t) + v_i \Delta t, \]  
\[ \theta_i(t + \Delta t) = \langle \theta_j(t) \rangle_r + \Delta \theta. \]  

where \( \langle \theta_i(t) \rangle_r \) defines the average angle of all the boids within a distance \( r \) of boid \( i \) and \( \Delta \theta \) corresponds to a random number chosen from a uniform distribution between \(-\eta/2\) and \(\eta/2\).

Figure 4.1: A diagrammatic representation of the Vicsek model. The direction of boid \( i \) is determined by averaging the direction of motion of all boids within distance \( R \). Boid \( i \) does not interact at all with boids which are separated by more than distance \( R \).

This indicates that there is no cohesive inter-body potential of the kind typically found in ordinary gases. However, as opposed to the model examined in Chapter 3 there is
4.1. THE VICSEK MODEL AND THE VIRIAL EXPANSION

now a spatial dependence coupled with the alignment potential. In fact, the alignment potential is defined such that the direction of motion of boid \( i \) comes from averaging over the direction of all the boids within distance \( R \) of boid \( i \). Fig. 4.1 contains a diagram and description of the various components of the Vicsek model and how these interactions work based on the equations (4.1) and (4.2). However, the average of a directional heading is troublesome to express analytically as a potential, so instead the potential will be expressed as the sum of \( \sin^2 \left( \frac{\phi_{ij}}{2} \right) \) lying within region \( R \), which will give a similar (but not identical) result. This results in a set of potentials for a Vicsek-like system, with \( V^C_{ij}(r) \) denoting the cohesion potential and \( V^A_{ij}(r, \phi) \) denoting the alignment potential:

\[
V^C_{ij}(r) = 0 \quad (4.3)
\]

\[
V^A_{ij}(r, \phi) = \sum_{i < j} \zeta H(r_i - r_j) \sin^2 \left( \frac{\phi_i - \phi_j}{2} \right), \quad (4.4)
\]

where \( H(r_i - r_j) \) is a separation dependent Heaviside step function and:

\[
H(r_{ij}, \phi) = \sum_{i \neq j} V^C(r_i - r_j) + \sum_{i \neq j} V^A(r_i - r_j, \phi_i - \phi_j) \quad (4.5)
\]

The form of these potentials is shown graphically in Fig. 4.2.

A potential of the form in equation (4.4) should give results highly analogous to simply averaging over the directional heading of each boid, and although a \( \sin^2 \) form is an obvious choice, being naturally periodic, it is not the only functional form that generates similar behaviour. In fact there are a number of other potential types which follow a similar curve where a potential minima forms where \( \theta_i - \theta_j \approx 0 \) and where the potential energy rises rapidly away from this point, in order to encourage alignment. It may be insightful to examine a number of these different potentials in order to ascertain whether:

(1) Similar virial equation of state and partition function is observed for alignment poten-
Figure 4.2: (a) The interaction distance is represented by a simple Heaviside step function, at $r < R$, the step function has a value of 1, representing the fact that interaction occurs. At $r < R$ the value of the step function drops to zero, since no interaction occurs. (b) Instead of taking the average heading of all boids within distance $R$, this interaction is approximated as a potential between each boid of $\sin^2$ form, with an energy minima at $\phi_{ij} = 0$ representing a tendency towards alignment.
4.1. THE VICSEK MODEL AND THE VIRIAL EXPANSION

...tials of the same general form.

(2) Significant differences result from potentials of the same form with slightly different characteristics.

Three alternate forms of $V_{ij}^A(r, \phi)$ will be analysed in order to compare how small variations in the same of $V_{ij}^A(r, \phi)$ changes the resulting equation of state and how the resulting virial equations of state compare to one another and to the numerically simulated Vicsek model.

\begin{align*}
V_{ij}^{(2)}(\phi) & = \zeta H(r_i - r_j) \left( 1 - \exp \left( -\frac{\phi^2}{\pi} \right) \right), \quad (4.6) \\
V_{ij}^{(3)}(\phi) & = \zeta H(r_i - r_j) \left( \frac{1}{10} (\phi^2 - \pi^2 + 10) \right), \quad (4.7) \\
V_{ij}^{(4)}(\phi) & = \begin{cases} \\
-\zeta H(r_i - r_j) \frac{\phi}{\pi} & \phi < 0 \\
\zeta H(r_i - r_j) \frac{\phi}{\pi} & \phi > 0 \end{cases} \quad (4.8)
\end{align*}

where $-\pi < \phi < \pi$

In the primary derivation pursued in this chapter, the potential for $V(r, \phi) = \zeta H(r_i - r_j) \sin^2 \left( \frac{\phi_i - \phi_j}{2} \right)$ given in equation (4.4) will be used. However, the detailed derivations for the alignment potentials in equations (4.6)-(4.8) may be found in Appendix A and their comparative forms can be seen in Fig. 4.3. The resultant equations of state of these potentials will be compared later in the chapter.
Figure 4.3: A set of similar alignment potentials which will be compared in order to determine whether they result in different results, and if so, which gives the best representation of Vicsek model behaviour. (a) $V_{ij}^{(1)}(\phi)$, from equation 4.4 (b) $V_{ij}^{(2)}(\phi)$, from equation (4.6) (c) $V_{ij}^{(3)}(\phi)$, from equation (4.8) (d) $V_{ij}^{(4)}(\phi)$, from equation (4.8) at $\zeta = 1$ in all cases.
4.2 Deriving a Virial Equation of State for the Vicsek Model

Now that a set of potentials have been defined that will provide close agreement to the characteristics of the numerical Vicsek model [14], the virial expansion can be used in a similar fashion to Chapter 3 in order to find the virial coefficients and hence a virial equation of state and partition function for the Vicsek model.

As for Chapter 3:

\[
P_{\beta} = B_1 n - b_2 n^2 + O(3) + ... \quad (4.9)
\]

\[
Z_N = \frac{1}{N!} \frac{1}{(2\pi \hbar)^2N} \int_0^\infty dp_1 dp_2 ... dp_N |p_1||p_2|...|p_N| \exp \left( \frac{-\beta p^2}{2m} \right) \Xi_N \quad (4.10)
\]

where:

\[
\Xi_N = \int_0^A d^2x_1 d^2x_2 ... d^2x_N \int_{-\pi}^\pi d\phi_1 d\phi_2 ... d\phi_N \exp \left( -\beta H(x, \phi) \right) \quad (4.11)
\]

Substituting \( H(x, \phi) \) and converting to polar coordinates in this case leads to the equation:

\[
\Xi_N = \int_0^A dr_1 dr_2 ... dr_N \int_{-\pi}^\pi d\phi_1 d\phi_2 ... d\phi_N \int_{-\pi}^\pi d\theta_1 d\theta_2 ... d\theta_N \exp \left( -\zeta \beta H(r_i - r_j, \phi_i - \phi_j) \right) \quad (4.12)
\]

Since the virial expansion need only be solved to 2nd order in this case, \( \Xi_1 \) and \( \Xi_2 \) can be considered distinctly from one another.

For \( \Xi_1 \) this means that:

\[
\Xi_1 = \int_0^L dr_1 \int_{-\pi}^\pi d\phi_1 \int_{-\pi}^\pi d\theta_1 r_1. \quad (4.14)
\]
which is, trivially,

\[ \Xi_1 = 2\pi^2 L^2 = 2\pi A. \] (4.15)

For \( \Xi_2 \) the situation is a little more complicated. \( \Xi_2 \) may be written:

\[ \Xi_2 = \int_0^L \int_0^L \int_{-\pi}^\pi \int_{-\pi}^\pi d\theta_1 d\theta_2 \int_{-\pi}^\pi \int_{-\pi}^\pi d\phi_1 d\phi_2 \]
\[ \times \ r_1 r_2 \exp \left( -\zeta \beta H (r_1 - r_2) \sin^2 \left( \frac{\phi_1 - \phi_2}{2} \right) \right) \] (4.16)

It is convenient in this situation to change to centre of mass coordinates by setting:

\[ r = \frac{r_1 + r_2}{2} \quad \phi = \frac{\phi_1 + \phi_2}{2} \] (4.17)
\[ r_{12} = r_1 - r_2 \quad \phi_{12} = \phi_1 - \phi_2 \] (4.18)

which yields:

\[ \Xi_2 = 4\pi^2 \int_0^L \int_0^L dr dr_{12} \int_{-\pi}^\pi d\phi d\phi_{12} \]
\[ \times \ \left( r^2 - \frac{1}{4} r_{12}^2 \right) \exp \left( -\zeta \beta H (r_{12}) \sin^2 \left( \frac{\phi_{12}}{2} \right) \right) \] (4.19)
4.2. DERIVING A VIRIAL EQUATION OF STATE FOR THE VICSEK MODEL

It is important to remember that the step function \( H(r_{12}) \) is a simple discontinuous function where:

\[
H(r_{12}) = 1, \quad r_{12} < R
\]

\[
H(r_{12}) = 0, \quad R < r_{12} < L
\]

(4.20) \hspace{1cm} (4.21)

this means that the \( r \) dependence of equation (4.19) can be greatly simplified by just splitting the integral into two components. One portion where \( H(r_{12}) = 1 \) and the other where \( H(r_{12}) = 0 \).

\[
\Xi_2 = \frac{8\pi^3}{3} \int_0^L dr \int_{-\pi}^\pi d\phi_{12} \times \left[ \int_0^R dr_{12} (r^2 - r_{12}^2) \exp \left( -\zeta \beta \sin^2 \left( \frac{\phi_{12}}{2} \right) \right) + \int_R^L dr_{12} (r^2 - \frac{1}{4} r_{12}^2) \right]
\]

(4.22)

where \( R \) is the length scale over which the alignment potential interacts.

With the exponential dependence for \( r_{12} \) eliminated it is now relatively straightforward to solve the integrals in \( r \) and \( r_{12} \).

\[
\Xi_2 = \frac{8\pi^3}{3} \int_{-\pi}^\pi d\phi_{12} \left[ \frac{1}{12} (4L^3 R - R^3 L) \left( \exp \left( -\zeta \beta \sin^2 \left( \frac{\phi_{12}}{2} \right) \right) - 1 \right) + \frac{L^4}{4} \right]
\]

(4.23)

leaving only the integral over relative alignment angle, \( \phi_{12} \). This may be simplified using the identity \( \sin^2 \left( \frac{\phi}{2} \right) = \frac{1}{2} - \frac{\cos(\phi)}{2} \),

\[
\Xi_2 = \frac{8\pi^3}{3} \int_{-\pi}^\pi d\phi_{12} \left[ \frac{1}{12} (4L^3 R - R^3 L) \left( \exp \left( -\zeta \beta \frac{1}{2} \exp \left( \frac{\zeta \beta}{2} \cos(\phi) \right) \right) - 1 \right) + \frac{L^4}{4} \right]
\]

(4.24)
which allows the integral to be solved using the definition for a modified Bessel function:

\[
\int_{-\pi}^{\pi} \exp \left( \frac{\zeta \beta}{2} \cos(\phi) \right) = 2\pi I_0 \left( \frac{\zeta \beta}{2} \right),
\]

(4.25)
to yield

\[
\Xi_2 = 16\pi^4 \left[ \frac{1}{12} (4L^3R - R^3L) \left( \exp \left( -\frac{\zeta \beta}{2} \right) I_0 \left( \frac{\zeta \beta}{2} \right) - 1 \right) + \frac{L^4}{4} \right].
\]

(4.26)
Now with,

\[
\begin{align*}
b_1 &= 1, \quad (4.27) \\
b_2 &= \frac{1}{2A} (\Xi_2 - \Xi_1^2), \quad (4.28)
\end{align*}
\]

and

\[
\begin{align*}
\Xi_1 &= 2\pi^2 L^2, \quad (4.29) \\
\Xi_2 &= 16\pi^4 \left[ \frac{1}{12} (4L^3R - R^3L) \left( \exp \left( -\frac{\zeta \beta}{2} \right) I_0 \left( \frac{\zeta \beta}{2} \right) - 1 \right) + \frac{L^4}{4} \right]. \quad (4.30)
\end{align*}
\]

the series terms \(b_1\) and \(b_2\) may be written:

\[
\begin{align*}
b_1 &= 1, \quad (4.31) \\
b_2 &= 16\pi^4 A \left[ \frac{1}{12} \left( \frac{4R}{L} - \frac{R^3}{L^3} \right) \left( \exp \left( -\frac{\zeta \beta}{2} \right) I_0 \left( \frac{\zeta \beta}{2} \right) - 1 \right) \right]. \quad (4.32)
\end{align*}
\]

Equation (4.9) may then be used in order to find the equation of state:
4.2. DERIVING A VIRIAL EQUATION OF STATE FOR THE VICSEK MODEL

\[
P_\beta = n + n^2 16\pi^4 A \left( \frac{1}{12} \left( \frac{4R}{L} - \frac{R^3}{L^3} \right) - 1 - \exp \left( -\frac{\zeta_\beta}{2} \right) J_0 \left( \frac{\zeta_\beta}{2} \right) \right),
\]
\quad (4.33)

and equation (4.10) may be used to find the partition function:

\[
Z = 1 + \lambda \frac{1}{(2\pi\hbar)^2} \frac{2m}{\beta} (2\pi^2 L^2) + \lambda^2 \frac{1}{(2\pi\hbar)^4} \frac{A^2}{2} \left( \frac{16\pi^4}{12} (4L^3 R - R^3 L) \left( \exp \left( -\frac{\zeta_\beta}{2} \right) J_0 \left( \frac{\zeta_\beta}{2} \right) - 1 \right) + \frac{\pi}{2} L^4 \right).
\quad (4.34)

Returning to the other three systems specified by equations (4.6) - (4.8), the resultant virial equations of state are given by:

\[
P_\beta = n + n^2 16\pi^4 A \left[ \frac{1}{4} - \frac{1}{6\pi} \left( \frac{R}{L} - \frac{R^3}{L^3} \right) \left( e^{\zeta_\beta} \frac{4}{3\pi} e^{-\zeta_\beta} \sqrt{10\pi\zeta_\beta} \text{Erf} \left( \frac{\pi}{\sqrt{10\zeta_\beta}} \right) - 2\pi \right) \right]
\quad (4.35)
\]
\[
P_\beta = n + n^2 16\pi^4 A \left[ \frac{1}{4} - \frac{1}{6\pi} \left( \frac{R}{L} - \frac{R^3}{L^3} \right) \left( 2\pi \zeta_\beta \left( \frac{1}{2} \text{Erf} (\sqrt{\pi}) - 1 \right) \right) \right]
\quad (4.36)
\]
\[
P_\beta = n + n^2 16\pi^4 A \left[ \frac{1}{4} - \frac{1}{6\pi} \left( \frac{R}{L} - \frac{R^3}{L^3} \right) \left( \frac{1}{\zeta_\beta} \left( e^{-\zeta_\beta} - \zeta_\beta - 1 \right) \right) \right]
\quad (4.37)

The full derivation for these systems may be found in Appendix A.

Fig. 4.4 shows \( P \) vs \( \beta \) plotted for all 4 different alignment potentials, and it can be seen that the shape and nature of the \( P-\beta \) relationship is remarkably similar for each of the different alignment potentials, with each showing the classic characteristics of exponential decay. This is due primarily to the presence of an overall division by \( \beta \) which causes the classic \( \frac{1}{x} \) decay profile. The differences lie primarily in the scaling of pressure with respect to \( \beta \), since although all potential forms display this exponential decay, there is some small variation in the numerical values of pressure for any given \( \beta \). This is obviously expected, since the alignment potentials are not identical, but the fact that small changes in the form
of the potential only result in minor changes in the relationships between thermodynamic variables is comforting, as it means that any potential with a similar form can be selected as the basis for this type of model, and it allows for the selection of a potential which is the most mathematically simple to work with.

Figure 4.4: Plots of the pressure vs $\beta$ for the different 4 potential forms. Due to the dominance of an overall $\frac{1}{\beta}$ in the equation of state all the relationships are remarkably similar and in fact it is difficult on any realistic scale to tell them apart. The relationships between $P$ and $\beta$ are plotted for: $\sin^2$ potential form (black), Gaussian potential form (blue), quadratic potential form (red) and triangular potential form (green)

When the relationship between pressure and interaction length, $R$, is examined and plotted, as is seen in Fig. 4.5 the result is quite interesting. As $R$ increases with respect to the box size, $L$, the pressure of the flocking gas initially rises quite rapidly, but as $\frac{R}{L} \to 1$, the rate of increase begins decreasing and the curve begins to flatten. Intuitively, this makes sense, since it would expected that as the interaction range increases, the number of boids within interaction range of one another increases, and the number of boids moving in a correlated fashion increases, which could lead to increased pressure at the boundary. However, as $\frac{R}{L} \to 1$ the interactions within the system will reach a saturation
4.3 NUMERICAL COMPARISON

point, increasing the range more won’t increase the amount of correlation between boids if they are all already correlated. Hence this would lead to a flattening of the curve at the upper values of $R$. This provides a firm prediction, based on the virial equation of state, about how the interaction length effects the pressure which will be useful for comparison to a computational Vicsek system.

It can also be seen that all four potentials give remarkably similar relationships for $P$ vs $R$, much in the same way as the $P$ vs $\beta$ relationship. This is primarily due to the fact that all of these potentials result in an equation of state dominated by the same polynomial of the form $\frac{\beta^3}{\gamma^3}$. Taken over all space, this results in a classic cubic shape when pressure is plotted against $R$, however, since $R$ is a length in circular coordinates, it is always positive, and since interaction length only makes sense for $R < L$, only part of the the cubic is relevant to the system being analysed here, and it is this region which is shown in Fig. 4.5.

4.3 Numerical Comparison

As in Chapter 2 the results of the analytically derived virial equation of state can now be compared to a numerical simulation in order to test the veracity of this method. In this case however, the numerical model will be a Vicsek-like model governed by the equations of motion:

$$r_i(t + \Delta t) = r_i(t) + v_i \Delta t,$$  \hspace{2cm} (4.38)

$$\theta_i(t + \Delta t) = \langle \theta_j(t) \rangle_r + \Delta \theta.$$  \hspace{2cm} (4.39)

These simulations were performed over 100000 time steps and each set of parameters was simulated for an ensemble of 25 runs in order to account for the random nature of the symmetric breaking in the model. The ensemble average of each of the key parameters was
Figure 4.5: Plots for the 4 different interaction potentials display extremely similar behaviour for pressure vs interaction length, with some slight variation in the value of the maximum pressure. Relationships between $P$ and $R$ are shown for: $\sin^2$ potential form (black), Gaussian potential form (blue) quadratic potential form (red) and triangular potential form (green).
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then calculated. Each simulation was performed with 200 boids placed in a box of width \( W = 10 \) and total area of \( A = 100 \). As in Vicsek’s early models, the speed of the particles was fixed with a value \( |v| = 1 \) and each particle has the same mass weighting of \( m = 1 \).

Initially, the boids were distributed randomly with equal probability of spawning at any point within the box. Additionally, the velocity direction of the particles was randomized such that each particle has an equal probability of starting with any alignment. After the simulation begins, the subsequent motion is completely dependent upon the equations of motion specified in equations (4.38) - (4.39) and the boundaries of the box are periodic in nature.

The first simulation performed involved measuring the pressure generated by the flock against the boundaries, and how this was related to the temperature. The pressure exerted by the flock was measured using the same approach as in Chapter 3 which is a modification of the standard kinetic theory method of measuring a pressure for a 3D transformed to calculate the pressure on the 1D boundaries of a 2D system.

\[
P_{sim} = \frac{Nm_v^2_{rms}}{2A} \tag{4.40}
\]

which reduces to, for the system considered here:

\[
P_{sim} = \frac{N}{200} \tag{4.41}
\]

The temperature of the flock is then derived using the ideal gas law to obtain \( Nk_B T = \frac{Nm_v^2_{rms}}{2A} \) and hence:

\[
T_{sim} = \frac{mv^2_{rms}}{2k_B} \tag{4.42}
\]

Where \( \beta = \frac{1}{k_BT} \) is measured, rather than the temperature directly.
\[ \beta = \frac{2}{mv_{rms}^2} \]  

(4.43)

In kinetic theory, the temperature, and hence $\beta$ is a function of the average speed of the particles in the gas. Therefore, by measuring the speed of the boids in the flock, the temperature of the flock can be determined in the simulation. In order to vary the temperature of the flock, the fixed speed of the boids in the flock was varied between $v = 0$ and $v = 2$ in increments of $\Delta v = 0.2$ for each ensemble.

The virial equation of state predicts a rapidly decaying in pressure $\beta$ primarily due to the inverse exponential term $\exp\left(-\frac{\beta}{2}\right)$ as well as the presence of an overall division by $\beta$, and this can be seen in Fig. 4.6 where the red line denotes the analytically derived data. When pressure is plotted against $\beta$ in the numerical case, shown as the blue dots in Fig. 4.6, this is exactly the behaviour observed. Due to the somewhat crude fashion in which pressure is measured, there are some differences in the overall scaling when comparing the numerical and analytical results, but these differences are relatively small, and the overall behaviour - with pressure decaying rapidly as $\beta$ increases - is very much the same in both cases.

However, this isn’t an especially interesting result. In kinetic theory, temperature is simply a measure of the average speed of the particles in a gas. In a hotter gas, the particles are faster, and hence travel further per unit time. Obviously then, in almost any conceivable gas, pressure will decline rapidly with increasing $\beta$. The fact that both models bear this out and compare well with one another is encouraging, but not at all surprising.

A far more interesting comparison lies in comparing the behaviour of pressure against interaction length. As the interaction length increases, it is clear that the flocking gas will become more correlated, up to a point where all particles are correlated. After that point,
Figure 4.6: Theoretical plot of pressure vs $\beta$ based on the virial equation of state for $R=1$ and $A=100$ (red line) compared to computational data of pressure vs $\beta$ from a simulated Vicsek model ensemble for $R=1$ and $A=100$ (blue dots).
increasing the interaction scale further won’t create any further correlation. However, since the particles have a fixed speed of $v$ regardless of whether their motion is correlated or uncorrelated, it should not be taken for granted that this will necessarily mean that pressure increases with interaction length. However, the virial expansion above makes a very clear prediction about the nature of the pressure vs interaction length curve. As $R$ increases from 0, pressure initially increases rapidly with interaction length, however as $\frac{R}{L} \to 1$ the rate of increase of pressure with respect to interaction length decreases, resulting in a flattening of the curve, most likely due to the system becoming saturated with correlation. This can be observed as the red line in Fig. 4.7.

This was simulated computationally by altering $R$ between 0 and 5.65. The reason for this is because for a square system of width $W = 10$ and area $A = 100$ the equivalent area circular system has a radius of $R = 5.65$ as noted in Fig. 3.3 in Chapter 3. Due to the fact that the interaction scale was infinite in Chapter 3, the consideration of equivalent system sizes was less important, however, in this case it is vitally important since many important quantities are dependent upon the interaction length. Therefore, it only makes sense for comparison to the virial system to analyse interaction lengths up to a maximum of $R = 5.65$. This is done for a fixed $v = 1$ as in the original Vicsek system and the results can be seen as the blue dots in Fig. 4.7.

It can clearly be seen that the computational system follows almost exactly the same pressure vs interaction length profile as the virial equation of state predicts. This is particularly true for $R > 0.5$ since as $R \to 0$ there are some divergences in behaviour which can be observed. For the virial equation of state, at the limit where $R \to 0$, the pressure generated by the flock drops to a very low value, a quick perusal of equation (4.33) shows this value to be $\frac{N}{4} = 2$. In contrast, for the computational simulation of the Vicsek model, the pressure appears to baseline to a value of around 35–40 units at this lower limit.

A possible explanation for this is that virial expansion does not explicitly take into account a fixed value of $v = \text{constant}$ but rather is based on an integration over all of momentum
space. This means that the flock modelled analytically would be ‘allowed’ to be stationary, and this may explain why when $R \to 0$, the pressure, $P$ drops to a far lower value than in the basic computational Vicsek model. In the analytically derived case, in the absence of interactions, the flock may tend to a stationary state generating very little motion and hence very little pressure. However, in the computational Vicsek model, the velocity is fixed to a constant value, even when no interactions are occurring, and this will result in some minimum fixed velocity which corresponds to a non-zero base pressure, because there will always be some boids colliding with the boundaries of the system.

![Figure 4.7: Theoretical plot of pressure vs interaction length based on the virial equation of state (red line) compared to computational data for pressure vs interaction length from a simulated Vicsek model ensemble (blue dots).](image)

So despite some minor discrepancies in the very low interaction length limit, the behaviour of the analytically derived curved closely matches that from the computational Vicsek system. Considering some of the approximations made, such as comparing systems of $2 \times 10^4$
different shapes (circular and square), the approximation of Vicsek’s interaction region as a $\sin^2$ potential and the simplistic way in which pressure is measured computational it is quite impressive how accurate the computational and analytical results match one another. This points to how robust the model seems to be, and could be indicative of a general result whereby all self-propelled systems governed by a simple alignment potential of range $R$ and no cohesion force obey a similar pressure vs interaction length relationship. However, at this stage this is mere speculation, and a number of quite contrasting systems would need to be tested to determine if this hypothesis is correct.

4.4 Order, Disorder and Phase Transitions in the Vicsek Gas Model

One of the primary motivations in developing a statistical mechanical gas model of flocking is that such a model gives access to a number of important thermodynamic quantities which can be difficult to analyse computationally. Amongst these are pressure and temperature which can be explored by reference to the virial equation of state, but others including the total energy of the system, the entropy and the specific heat capacity are best derived through the use of the partition function, expressed in equation (4.34). Perhaps the most interesting of these are the internal energy, $U$, which gives a measure of the energy of the system, the entropy, $S$, which gives a measure of the disorder of the system and specific heat, $C_V$, which can be used to determine the locations of any phase transitions that occur in the system. All three of these quantities can be related to the partition function, as shown below:
The internal energy, $U$, defines the total amount of energy contained within the thermodynamic system, in our case a flock of boids constrained by some boundary. Naturally, the total energy of the system is expected to increase with temperature, but the exact functional form is not known. Additionally, discontinuities or variations in the internal energy can provide important information about the phases and phase transitions of the system across the full range of temperature.

Taking the derivative of the internal energy with respect to $\beta$ as in equation (4.46) yields the specific heat capacity $C_V$. The behaviour of $C_V$ with respect to $\beta$ provides information about the nature of the phases and phase transitions present in a thermodynamic system. At the location of a phase transition, $C_V$ with respect to $\beta$ spikes rapidly, either discontinuously or to a continuous peak. This can mean that their is a sudden kink that makes the function non-analytic, a sudden rise on either side of the critical point to a well defined peak or a rapid divergence of the two values of specific heat on either side of the critical point. This indicates a breakdown in the model for specific heat at the critical point, but also indicates that the heat energy entering the system is no longer simply raising the temperature, but is rather going into changing the system from one configuration to another. On either side of the phase transition, $C_V$ is generally analytic and gives the behaviour of the heat capacity for the two different phases on either side of the phase transition. Thus $C_V$ provides a very useful tool for finding the location of phase transitions in parameter space and it is this application of $C_V$ that will be used to look for possible phase transitions in the flocking system derived here.
To fully understand this set of thermodynamic variables however, their remains one unknown that still needs to be considered, the fugacity, $\lambda$. This may be found by consideration of the relationship between boid number $N$ the partition function $Z$ and the fugacity $\lambda$. Note that the full derivation of this is a little lengthy for the main text, but is presented in Appendix B. Beginning with:

$$N = \lambda \left( \frac{\partial \ln(Z)}{\partial \lambda} \right). \quad (4.47)$$

A quadratic function may be found in $\lambda$,

$$2\lambda^2 \left( Z_2 - \frac{Z_1^2}{2} \right) + \lambda Z_1 - N = 0, \quad (4.48)$$

and solved using the quadratic equation to yield,

$$\lambda = \left( \frac{-1 + \sqrt{1 + 4N \left( \frac{Z_1}{2} \right) - 1}}{2 \left( \frac{Z_1}{2} \right) - 1} \right) \frac{A_Q}{\Xi_1}, \quad (4.49)$$

Note that the positive root is taken here as a complex or negative value of fugacity is nonsensical.

With an expression for $\lambda$ now in hand, one can return to the partition function expressed in equation (4.34). With fugacity now written in terms of $A_Q$ it makes sense to write the partition function in terms of $A_Q$ for consistency, where $A_Q = \left( \frac{1}{(2\pi\hbar)^2} \frac{2m}{\beta} \right)^{-1}$. This allows the partition function to be simplified to:
4.4. ORDER, DISORDER AND PHASE TRANSITIONS IN THE VICSEK GAS MODEL

\[ Z = 1 + \lambda \frac{2\pi A}{A_Q} + \lambda^2 A^2 \frac{16\pi^4}{2A_Q^2} \left( \frac{4L^3 R - R^3 L}{12} \right) \left( \exp \left( -\frac{\zeta_\beta}{2} \right) I_0 \left( \frac{\zeta_\beta}{2} \right) - 1 \right) + \frac{\pi}{2} L^4 \). \]  

(4.50)

The first question that needs to be considered when plotting this set of thermodynamic variables is the range of temperatures over which interesting behaviour is likely to be observed. As noted in Chapter 3 one must remember that the temperature associated with a flock is not physical in the same sense as that of a gas, as the interaction strengths associated with alignment are scaled for convenience as there is no quantitative or experimental value associated with the desire for a boid to follow its neighbours. By defining a step function of magnitude 1 and setting \( \zeta = 1 \) as the coefficient of the alignment potential, the depth of the potential well which is producing the tendency for aligned behaviour is approximately \( U = 1 \). This means that roughly speaking, a thermal energy of \( k_B T >> 1 \) is required to completely disrupt the correlated alignment behaviour of the flock, whilst at thermal energies of \( k_B T << 1 \) one would expect to observe the flock in its lowest energy state, corresponding to completely correlated flocking behaviour. This means that any phase transition between ordered and disorder behaviour is likely to occur around \( k_B T = 1 \), and a sensible range of values to look for this behaviour would be for \( 0.1 < k_B T < 10 \). For increased certainty, the plots will be extended out to \( 10^{-4} < k_B T < 10^4 \) and plotted logarithmically to highlight any signal which could be indicative of a phase transition.

The internal energy of the system, \( U \), may now be calculated from the partition function using equation (4.44). Due the complexity of the resulting functional form, the result is somewhat too cumbersome to express here, but may be found in Appendix C. Instead \( U \) can be plotted against \( k_B T \), which is more insightful than examining the expression directly. However, before generating such a plot there is still the slightly troublesome
fugacity and $A_Q$ terms to be dealt with. $A_Q$ can be eliminated from the equation for internal energy, and subsequently specific heat by defining a new term $\lambda_e = \lambda A_Q$. This new term can be referred to as the effective fugacity. This quite tidily allows the quantum area dependence of $\lambda$ from equation (4.49) to cancel with the various $A_Q^{-1}$ terms that always appear alongside fugacity as shown in Appendix C. It also has the added bonus that the effective fugacity, $\lambda_e$ is relatively constant for all temperatures and at all interaction lengths, which is shown in Fig. 4.8. This is with the exception of a small kink which appears at approximately $k_B T = 1$. The size of this kink is dependent on the interaction length, and causes the value for $\lambda_e$ to split for $k_B T < 1$. However, the magnitude of this splitting is extremely small, even for the maximum value of interaction length $\frac{R}{L} = 1$, and for the purposes of this analysis $\lambda_e = 0.00015$ can be considered constant. However, the mere presence of this kink may be indicative of interesting behaviour happening around $k_B T = 1$.

![Figure 4.8](image_url)

**Figure 4.8:** The effective fugacity $\lambda_e$ plotted against $k_B T$ for various values of interaction scales $\frac{R}{L}$, specifically $\frac{R}{L} = 0$ (black), $\frac{R}{L} = 0.2$ (green), $\frac{R}{L} = 0.4$ (red), $\frac{R}{L} = 0.6$ (blue), $\frac{R}{L} = 0.8$ (indigo) and $\frac{R}{L} = 1$ (purple). Note that despite the presence of small kink in $\lambda_e$, the size of which depends on the interaction scale $\frac{R}{L}$ that $\lambda_e = 0.00015$ is effectively constant to within $\pm 5\%$ of the total value of fugacity for all interaction length scales.
4.4. ORDER, DISORDER AND PHASE TRANSITIONS IN THE VICSEK GAS MODEL

With the fugacity and the quantum area dealt with, the internal energy can now be plotted straightforwardly as shown in Fig. 4.9. The first thing to note is that the relationship between temperature and energy is almost perfectly linear (Fig. 4.9 is plotted on a Log scale in $k_B T$ for consistency with later plots). At $\frac{R}{T} = 0$ this is to be expected, since this is exactly the relationship obeyed by a non interacting ideal gas at this interaction range. However, as $\frac{R}{T}$ is increased, there is no discernible change in the shape of the internal energy curve at these scales. It perhaps requires a little more thought, but this again makes sense. As temperature is increased, the boids will be jostled about randomly. At low temperatures they will merely be jostled about within the potential well, and at higher temperatures they will be jostled such that they can escape the potential well enforcing alignment. Since the alignment potential considered here is classic, smooth and continuous, it makes no difference whether the boid is being jostled within the well or at energies well above those of the potential well, the behaviour of energy as temperature is increased will remain linear.

What one might expect to see however is a kink or jump in the internal energy with respect to $k_B T$ when $k_B T$ is approximately the same magnitude as the depth of the potential well. This would come about due to the random thermal energies being just high enough that some particles would be jostled out of the ordered phase while some would remain bound by the alignment potential. Basically, this would signify a phase transition from the ordered to the disordered phase as the thermal energy $k_B T$ increased. Observing Fig. 4.9 it is not immediately obvious that any phase transition is occurring as the curve looks relatively smooth for all interaction scales. This is not a particularly surprising result as the kinetic energy of the individual particles would likely drown out any small signal from a phase transition based on the interactions between particles. This is one reason why the specific heat is such a useful quantity. Being the derivative of the internal energy, the specific heat eliminates the primarily linear increase in energy from simple kinetic motion, allowing any discontinuities or sudden changes in gradient to be observed. Thus it makes sense to analyse the specific heat to see if their is any interesting behaviour in the system which is not evident from a simple observation of the energy.

It is turning to the specific heat, which can be derived from the internal energy using
Figure 4.9: The fugacity $\lambda$ plotted against $k_B T$ for various values of interaction scales $\frac{R}{L}$, specifically $\frac{R}{L} = 0$ (black), $\frac{R}{L} = 0.2$ (green), $\frac{R}{L} = 0.4$ (red), $\frac{R}{L} = 0.6$ (blue), $\frac{R}{L} = 0.8$ (indigo) and $\frac{R}{L} = 1$ (purple). Note that the curve shows a linear relationship between internal energy and temperature, and that changes to the interaction length, $\frac{R}{L}$ make no discernible difference to the shape or gradient of the curve.
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equation (4.45), that reveals the phase transition in all of its glory. Again the specific mathematical form of \( C_V \) is not shown here but may be found in Appendix C. In Fig. 4.10 where \( C_V \) is plotted against \( k_B T \) the shape of the \( C_V \) curve instantly displays the clear signature of a phase transition. \( C_V \) also reveals a number of things about the nature of the phase transition that the internal energy alone does not. Firstly, although the phase transition is not instantaneous, and rather exists over some range of \( k_B T \) where \( 0.05 < k_B < 10 \) the peak of the \( C_V \) curve will give a value for the critical temperature, where the system is neither primarily in one phase nor the other. In keeping with the rest of this section, the critical point will be referred to in units of \( k_B T \), rather than \( T \) alone, and this value turns out to be about \( k_B T_c = 0.3 \) as can be seen from Fig. 4.10. This is interesting, as the rough analysis expressed earlier indicated that \( k_B T = 1 \) would be the value required for the energy of the thermal fluctuations to offset the tendency of the boids towards alignment due to the alignment potential. However, it must be remembered that in order to induce a phase transition from the ordered state at low \( T \), to the disordered state at high \( T \), it is not required that the thermal energy, \( k_B T \), be greater than the magnitude of the alignment potential expressed in equation (4.4), rather it is only required that the thermal fluctuations disrupt the alignment tendency enough that the motion of the flocking system as a whole is no longer correlated. Thus, although it would be expected that the phase transition will occur in the order of unity, it is not surprising that the value is actually somewhat less than this, as the thermal fluctuations do not need to totally overcome the alignment potential in order to disrupt the alignment of the boids enough to induce a phase transition to a disordered state.

Another interesting observation is that varying the value of the interaction scale \( \frac{R}{L} \) does not change the location of the phase transition. This however, makes sense, since varying the interaction scale does not change the strength of the energy binding individual particles into alignment with one another. However, increasing the interaction scale does increase the number of particle to particle interactions occurring and at \( \frac{R}{L} = 1 \) it is expected that every particle in the system is interacting with every other particle. Increasing the number of interactions, without increasing the strength of each individual interactions means that
although the location of the phase transition in $k_B T$ is unchanged, the peak in $C_V$ at the phase transition increases in magnitude, meaning the phase transition becomes more pronounced. Essentially in the case where $\frac{R}{L} = 1$ the ordered phase is far more ordered than in the ordered phase for say $\frac{R}{L} = 0.2$ meaning that the change in heat capacity near the phase transition is much greater. This will be further demonstrated when the entropy of the system is considered. In the absence of interactions, the flock is always in the disordered state and hence no phase transition occurs which is indicated by the lack of a corresponding peak in $C_V$, rather, as Fig. 4.10 demonstrates the value of $C_V$ for $\frac{R}{L} = 0$ is constant at $C_V = 2$ throughout (see the black line). This rather encouragingly coincides with the result for a non interacting ideal gas in $2D$ which has $C_V = \frac{N}{V} k_B$.

Figure 4.10: The specific heat $C_V$ plotted against $k_B T$ for various values of interaction scales $\frac{R}{L}$, specifically $\frac{R}{L} = 0$ (black), $\frac{R}{L} = 0.2$ (green), $\frac{R}{L} = 0.4$ (red), $\frac{R}{L} = 0.6$ (blue), $\frac{R}{L} = 0.8$ (indigo) and $\frac{R}{L} = 1$ (purple). The critical temperature can be determined as $k_B T_c = 0.3$ from the peak values of the $C_V$ curve. Note that the length of the interaction scale $\frac{R}{L}$ does not change the location of the phase transition, only how pronounced the phase transition is.

Finally, the behaviour of $C_V$ reveals something about the nature of the phase transition.
Specifically, it shows that the phase transition in specific heat is continuous due to the lack of mathematical discontinuities in $C_V$ and $U$. Although there is a sharp increase in $C_V$ on either side of the critical temperature, there is no divergence, and the specific heat forms a smooth peak. Now it should be remembered at this juncture that this model is not an exact replica of the Vicsek model solved analytically, as some alterations were made to the alignment potential in order to make it suitable for this treatment. However, for a Vicsek-like model with the inter-particle alignment potential being approximated as in equation (4.4) it does appear as though the phase transition is continuous. This could be of interest due to the debate over the nature of the phase transition between order and disorder in the Vicsek model, which has continued for some time [14, 27, 33, 34, 28, 32].

The behaviour of entropy will be the final thermodynamic variable examined in this thesis, due to its relationship with stochastic noise as implemented in most computational flocking models. Entropy is even more straightforward to calculate due to the fact that fugacity need not be held constant in the differentiation. Thus the constant $\lambda_e$ may be substituted directly into the partition function, removing $A_Q$ from consideration from the outset.

\[
Z = 1 + \lambda_e (2\pi A) + \lambda_e^2 A^2 \left( \frac{16\pi^4}{12} (4L^3R - R^3L) \right) \left( \exp \left( -\frac{\zeta \beta}{2} \right) I_0 \left( \frac{\zeta \beta}{2} \right) - 1 \right) + \frac{\pi}{2} L^4 \right).
\]

(4.51)

with:

\[
\lambda_e = \left( \frac{-1 + \sqrt{1 + 4N \left( \frac{\Xi}{\Xi_1} - 1 \right)}}{2 \left( \frac{\Xi}{\Xi_1} - 1 \right)} \right) \frac{1}{\Xi_1}.
\]

(4.52)

This allows a relationship between entropy and temperature to be found using equation (4.46). Entropy is usually considered a measure of disorder in the system and as such, it is particularly useful for measuring the quantitative differences between the ordered and
disordered motion in a gas system. Once again the functional form of entropy will not be expressed here but can be found in Appendix C, while the relationship between entropy and $k_BT$ is examined graphically in Fig. 4.11.

Again a kink can be observed about the critical temperature $k_BT_c$ with the entropy reaching a maximal value in the high temperature phase for all interaction scales $\frac{R}{L}$. This means that regardless of the interaction length in the system, in the disordered state the level of disorder is exactly the same. This makes sense, since if the thermal fluctuations are large enough to completely disorder the system, it doesn’t matter how long the interaction scale is. A completely disordered system is maximally disordered, regardless of the interaction length. Another interesting aspect is that the level of disorder reaches its maximum value at $k_BT \approx 1$ in all cases, which is significantly above the critical point of $k_BT_C = 0.3$ but corresponds to the point where the magnitude of the average thermal fluctuations is exactly equal to the magnitude of the potentials inducing alignment in the flock. Thus it can be said that the thermal fluctuations needed to induce a transition from order to disorder are substantially lower than the potential inducing alignment of the boids, but the level of thermal fluctuations required to generate a completely disordered system is equal to the magnitude of the alignment inducing potentials.

Just as interesting is the behaviour of entropy where $T < T_c$. Firstly Fig. 4.11 shows that the length of the kink is directly related to the interaction scale with higher interaction scales showing exponential behaviour in $S$ which starts far below the critical point, whilst lower values of $\frac{R}{L}$ exhibit this behaviour only very near the critical point. This comes back to the point which was eluded to briefly when discussing specific heat. In the ordered phase, the total disorder of the system, measured by entropy, is far lower for high values of $\frac{R}{L}$. This is due to the fact that although all values of $\frac{R}{L}$ exhibit some kind of ordered phase, this ordered phase becomes far more extensive as $\frac{R}{L}$ is increased, and in the limit where $\frac{R}{L} = 1$ virtually every particle in the system should be correlated with every other particle at very low $T$. 

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4.4. ORDER, DISORDER AND PHASE TRANSITIONS IN THE VICSEK GAS MODEL

Figure 4.11: Entropy, $S$, plotted against $k_B T$ for various values of interaction scales $\frac{R}{L}$, specifically $\frac{R}{L} = 0$ (black), $\frac{R}{L} = 0.2$ (green), $\frac{R}{L} = 0.4$ (red), $\frac{R}{L} = 0.6$ (blue), $\frac{R}{L} = 0.8$ (indigo) and $\frac{R}{L} = 1$ (purple). Note how the value and behaviour of the entropy curve in the ordered phase is strongly dependent on the interaction scale, whilst in the disordered phase all interaction scales tend to the same value of entropy, indicating a completely disordered system, regardless of the interaction length.
Now in the case where $\frac{R}{L}$ is smaller, increasing $k_B T$ does not change the overall order of the system much until the critical point, because even though the flock is in the more ordered phase, it is still relatively disordered compared to the ordered phase of flocks with a longer interaction scales. But in the long interaction scale limit where $\frac{R}{L} = 1$ and the motion of virtually every particle in the system is correlated with every other particle even a small increase in $T$ with result in an increase in entropy, since even jostling a single particle slightly out of the alignment will increase the overall disorder of the system. This is a very neat result which really illustrates the differences in the ordered phases in this Vicsek-like model for different interaction scales.

The discovery of the phase transition from order to disorder in an analytical Vicsek system derived completely independently of Vicsek’s original computational implementation presents a significant discovery, and a huge verification of the validity of this approach to modelling flocking. This phase transition is the key component of Vicsek’s original flocking model and the transition from disordered random motion to ordered correlated motion is one of the most important aspects of flocking behaviour. This verification whilst being an important validation of this analytic technique to studying flocking is also a further validation of the basic nature of phase transitions from disorder to order in directionally correlated flocking systems generally, and the Vicsek model specifically, as it shows that yet another method of deriving flocking behaviour gives the same general results. This verification is important, because this method of analysing flocking as a gas system opens up additionally information about the system through a number of thermodynamic variables that can be derived from the partition function. It is hoped that the information provided by these state variables will shed new light on some of the little understood aspects of flocking systems which are difficult to approach using other methods.

Furthermore, with the partition function and the equation of state derived, there is an almost limitless amount of information available. Although the internal energy, entropy and specific heat are explored here, a number of other thermodynamic variables could provide further information about the system, such as the enthalpy, energy density, free energy,
and quantities like the expected number of boids for different flocking configurations. The work done thus far has only just scratched the surface of what is possible, and it is hoped that others will be able to use this as a launching pad in future to further extend this novel technique for looking at flocking systems, and provide another approach on top of the typical hydrodynamic and computational methods which are currently most prevalent in the field.

4.5 Discussion and Limitations

The effectiveness of the virial expansion in modelling a Vicsek-like flocking system has been established by comparing the relationships predicted by the analytical virial equation of state to those observed from a typical computational Vicsek flocking system. The predictions made by the virial equation of state were found to qualitatively and in some cases quantitatively match with quite good accuracy, the results obtained from a typical computational Vicsek flocking system.

In particular the same qualitative relationships were established for pressure vs interaction length and pressure vs temperature ($\beta$), which are key thermodynamic variables. Although the exponential decay of $P$ vs $\beta$ was naturally expected, it was not clear how pressure and interaction length would relate to one another, and the resulting agreement of the analytic virial based result with the computational model was very strong confirmation of the veracity of this approach to modelling a Vicsek flocking systems - and furthermore, flocking systems in general.

It was further established that changes in the mathematical form of the potential which still resulted in a similarly shaped potential well centered on a relative angle $\phi_{ij} = 0$ resulted in only very minor changes in the final form of the equation of state and the partition function. This demonstrates the stability and robustness of the model, as small changes in the initial potential are unlikely to give widely varying results, and hence, this allows some freedom in the choice of the mathematical form of the potential so that the
problem can be made simpler by making a sensible choice of governing alignment interaction.

Finally the thermodynamic variables internal energy, specific heat and entropy were derived from the partition function behaviour of the were analysed against temperature in order to obtain information about the phases and phase transitions which are exhibited by this system. The behaviour of these thermodynamic variables revealed the existence of two distinct phases in this Vicsek-like system independently of any computational model. An ordered phase at low temperatures where the motion of the boids is correlated based on the alignment tendency written into the equations governing their motion and a disordered phase at high temperatures, where random thermal fluctuations have overcome this alignment tendency and the motion of the flock is completely disordered. Between these two distinct regions of phase space lies the phase transition between order and disorder much like in Vicsek’s original computational system [14]. This is the first time that the phase transition between order and disorder in a system of this type has been derived in this way, and the natural way in which this behaviour falls out of this analytical framework is an encouraging sign for the validity and usefulness of studying flocking systems using this technique.
5.1 Hard-Core and Soft-Core Free Space Flocking

In Chapter 2, two different models of flocking were explored in free space, in order to determine whether the flocking behaviour that has previously been seen in periodic boundary conditions by T. Vicsek, and later by Y. Tu would also be displayed in the absence of these constraining boundary conditions. Additionally, two contrasting models, one based on the Lennard-Jones potential, and the other based on the Morse potential were chosen in order to compare the differences of the resulting flocking behaviour produced by a mode based on a hard-core cohesion potential and a soft core cohesion potential.

It was demonstrated that both a hard-core and soft-core potential generate phases of the same key forms, namely, moving liquid, moving solid, stationary liquid and stationary solid, in the absence of boundary conditions. This indicates that potentials with the same key features of close range repulsion, a medium range attraction, and no interaction at long range will result in the self-organising behaviour that gives rise to these different phases.

In particular, the analysis focused on the transition between the single flock state and the
multi flock state, and how the difference between hard-core and soft-core potential types affected the nature of this transition. Indeed it was shown that, in both cases a transition between a single cohesive flock and multiple non-interacting flocks is observed as initial density is decreased, however, the breakdown modes in both cases were shown to be substantially different. Whereas the soft-core Morse potential based flock resulted in a distinctive train like splitting parallel to the direction of motion, the hard-core Lennard-Jones based flock transitioned from the single to multi flock state via splitting perpendicular to the line of motion.

It was also observed that the two different potential types generate flocking formations and structures which are quite distinct from one another. Notably, a hard-core model produces a distinctive wavefront flock, reminiscent of the kind of flocks produced by wildebeest as they move across a well-grassed plain to graze. In the case of the soft-core potential, however, the shape of the resultant flock is the more typical teardrop shape often observed in small bird flocks and fish schools. It is hoped that deeper analysis of these two different types of flocks will in the future bring us closer to understanding why different species of animals display such different formations while still demonstrating the same universal flocking behaviours.

It is also hoped that these two flocking models can be extended into 3D in order to explore a wider range of realistic flocking behaviours in the dimensionality that many real flocks occur in. Thus far, we have made comparisons between our models and some 2D flocks (wildebeest, bacteria), but have had to extrapolate to 3D in order to make some other comparisons (fish, birds). It is hoped that in future, these models can be extended to 3D in order to confirm that these behaviours hold in that dimensionality, or if they do not, to explore the new behaviours exhibited.

Beyond this, it is hoped that the models developed here may form a basis for future investigations into predator-prey relationships, and how the nature of the potential used effects how the predator and prey interact. Just as the nature of the potential (hard-core
or soft-core) effects the bulk properties and structure of single-species flocks, it would be intriguing to compare the different effects a hard-core or soft-core flocking model would introduce into bi-species or multi-species interactions, including the relationship between predators and prey which has recently become a popular area of flocking research.

5.2 Flocking as a Simple Gas

In Chapter 3 a methodology was established for analytically deriving the gas equation of state for a simple flocking system using a virial expansion approach. It is hoped that this approach will compare favourably to both the individual-based and fluid-based approaches of analysing flocking systems. Reducing flocking phenomena to a gas equation of state allows simple quantities such as pressure and temperature to be investigated in a relatively straightforward manner and also opens up new avenues to looking at other potentially interesting quantities such as entropy, free energy, the partition function and others and what these mean in the context of flocking behaviour. The real power of this new approach lies in the number of thermodynamic quantities which it could shed light on, which are more difficult, or impossible to calculate currently using the two most popular types of flocking model.

In Chapter 4 the methods used for solving a simple flocking system analytically were applied in order to generate an equation of state for the well-known Vicsek model. Relationships between pressure, temperature and density were established from the virial equations of state which could then be compared to the same quantities in computational simulations of the Vicsek model. The similarities between the relationships obtained using these semi-analytic method versus the results obtained by the established simulation methods in Chapter 4 confirmed the efficacy and accuracy of the new gas based method of modelling flocking behaviour.

Thus far however, the comparison between the gas model approach proposed in Chapter
5.2. FLOCKING AS A SIMPLE GAS

3 and the established IBMs has only been performed for two models. One being and somewhat simplistic toy model and the other being the well-understood vicsek model. Significantly, this means that the veracity of the gas model has been established for a model which includes only an enforced alignment and also a model which includes an attractive/repulsive component. Although this covers two of the most important families of IBMs which have been used in the physics literature, additional test cases are required to ensure that a gas-model based approach is both accurate and useful in deriving and interpreting the behaviour of flocking systems.

The use of the virial expansion approach to deriving flocking equations of state also provides a neat avenue to determining the partition function of a flocking system. The partition function, $Z$, provides a gateway to a whole family of other statistical variables which are encoded within it and can be calculated using statistical mechanics techniques. Some of the quantities which can be calculated through the partition function include (but are not limited to) the energy, energy variance, specific heat, free energy and entropy of a given flocking system.

Of particular interest in the specific heat, $C_V$ and the entropy, $S$. The specific heat can be used to locate phase transitions in a system as sharp changes in specific heat signify the existence of a phase transition. In Chapter 4 it was shown that for a Vicsek system, the change in phase between ordered and disordered states can be independently derived using the virial expansion and the specific location of the critical point can be found. This is the first time that the phase transition in the Vicsek model has been independently reproduced using a method such as this. The entropy was also shown to be a useful quantity in the analysis of the behaviour of the flock in the ordered and disordered phase. Specifically, it was used to shown that their exist interaction length dependent changes in the overall order of the ordered phase, but that in the disordered phase, the entropy is a maximum, regardless of interaction length.

However, due to time constraints, the analysis and comparisons we achieved were some-
what restricted and it is hoped that in future, with the efficacy of the gas model approach confirmed, other key thermodynamic properties of a flock can be explored, including entropy and free energy, which are more difficult to investigate using conventional approaches. Whilst it would be premature to predict what exactly changes in these quantities might mean in the context of a flocking system, it would seem very likely that such quantities, given their great importance to other thermodynamic phenomena, would provide key information about a flocking system, and knowledge of how such quantities behave in a flocking system would inevitably lead to a deeper understanding of the overall behaviour of these intricate systems.

Finally, the models compared to our analytic results thus far have all been IBMs. There is another family of flocking models that exist, hydrodynamic flocking models. It is important that the results derived using both hydrodynamic and gas-based models of flocking are consistent with one another in regimes where both are applicable. Confirming that this is the case would firmly establish gas-based equation of state models as a third independent approach to measuring and modelling some of the important thermodynamic variables which play a major role in many complex systems - including flocking.

It is hoped that the work done in Chapters 3 and 4, modelling flocking as a virial gas will form the basis for future models using the same methodology. The model presented here was designed as a template, first demonstrating a simple non-local model which can be solved analytically to generate ordered behaviour in a system of self-propelled particles and then using a similar methodology to generate a gas equation of state semi-analytically for the well known Vicsek model. Now that this methodology has been demonstrated both analytically and semi-analytically, and shown to open up some novel and interesting new insights and information into flocking behaviour, it is hoped that in future this technique can be used as a template by other flocking researchers to examine other interesting and more complex flocking models.

Much like the fluid dynamical models of flocking can now be researched hand in hand
5.3. STATE OF PLAY

with the original individual based models, it is hoped that virial gas models of flocking can also fill a similar role, opening the door for investigating quantities and properties of flocks which have hitherto been largely unexplored. These include quantities such as the equation of state, partition function, pressure, entropy, temperature and total energy, all of which could give important insights into the properties of a flock. Considering how fundamental and important the information these quantities convey about a gas system is, there is good reason to believe that these quantities will prove to be equally important and useful in the investigation of analogous flocking systems.

5.3 State of Play

Modelling flocking from a physics perspective is a constant battle between complexity and simplicity. As physicists, the innate desire is to find the simplest possible model which captures the fundamental elements of flocking - elements such as cohesion, alignment, collision avoidance, coherent, ordered motion and the presence of spontaneous breakings of symmetry - which are essential for a flock to exist, and are globally present in all examples of flocking.

However, at its heart, flocking is not a simple phenomena. A flock is a complex, many-bodied system and despite the fact that very simple models can describe many of the fundamental and universal properties of flocking, there are other aspects of flocking behaviour that cannot be fully understood using only the simplest forms of flocking models, characteristics such as edge effects or specific types of phases which can only be studied and observed using more complex modelling techniques.

The early years of flocking research were dominated by analysis of the Vicsek model, and elegant example of simplicity which was able to capture some of the most universal aspects of flocking behaviour, including phase transitions from disorder to order, and from a single coherent flock to several independently evolving flocks. The Vicsek model is a
case study in how behaviour which appears complex, need not be described with particularly complex equations. Furthermore, Vicsek’s model has stood the test of time, and it still remains a cornerstone of flocking research today, which much discussion about the nature of the different phase transitions continuing, and several modification to the theory to make it more effective at describing real flocks - at the cost of additional complexity.

Therein lies one of the key difficulties with deriving any flocking model. When describing a complex system - such as a flock - the range of applicability for a given model is often inverse proportional to its simplicity. Whilst the Vicsek model is able to capture many of the universal, core behaviours of flocking, it is only applicable to describing the bulk properties of real flocks, as it neglects edge effects due to the presence of periodic boundary conditions, and lacking some sort of cohesive force the natural propensity of boids in a flock to cluster together is lost. The simplicity of the Vicsek model, for all its beauty and power, has a cost, and that cost is that although it illustrates the fundamental characteristics of flocking so well, it cannot capture some of the more novel aspects of a flock, things such as vortex formation in bacteria, the dynamics associated with the edge of a flock, the nature of flocks moving through free space or effects such as line of sight considerations.

In recent years, there has been more attempts towards modelling some of the more complex characteristics and manifestations of flocking behaviour. One such example of this is vortex formation displayed by some amoeba and bacterium species such as Dictyostelium, Daphnia and E.coli. The vortex phase is a special case of the stationary liquid phase, whereby the centre of mass of the flock is stationary, but their is a net rotation about that centre of mass. This phase is of particular interest because it is seen in reality in a number of bacteria species, and because of the size of these systems, they are more readily amenable to experimental analysis than larger flocking systems. Furthermore, the vortex phase is a particularly special form of flocking because it represents ordered motion in the rotational frame, something not seen in most other examples of flocking behaviour, which are generally ordered in a more simple spatial frame. Finally, the vortex phase is particularly fragile to noise and sensitive to potential types and one of the more difficult
phases to model computationally. To-date it has only been observed in soft-core flocking models.

Another example of more complex, higher-order systems being studied in flocking literature recently include the predator-prey systems modelled by S-H. Lee, who has looked at how members of a flock respond to the presence of boids that interact repulsively - predator boids - and how different angles of attack change the way the flock responds to these predators. Additionally, other authors have looked at a number of complex flocking phenomena such as the speed and nature of information flow through a flock, and how that effects the nature of a flock's response to external threats or obstacles, and also how different flock shapes and formations effect the energy economics of a flock and how these energy considerations may be used to understand why flocks form, and whether flocking confers an overall aerodynamic benefit, or an overall aerodynamic deficit to its constituents.

Finally, the STARFLAG project, which is the first attempt at measuring macroscopic flocks experimentally continues in Rome and has resulted in several papers to date and is highly likely to result in many more as time goes by. The results of these experiments are of vital importance to theorists in this field as experiment has lagged well behind theory for some time, resulting in a plethora of different flocking models but few experimental results with which to compare against. As more detailed and accurate results come out of STARFLAG it should have the effect of giving more constraints to the types of models which are observed in reality, and give improved guidance and direction to theorist working in the field as to what sorts of models are appropriate for modelling what sorts of flocks.

It is hoped that this thesis provides a contribution to the overall understanding of this field by advancing our understanding of a wide range of universal flocking characteristics using the models presented in chapter 2, as well as outlining a novel approach to studying flocking in Chapters 3 and 4 which could open up new avenues and physics analogous to help build our understanding of this phenomena.
5.4 Future Directions in Flocking Research

In the near future, it is expected that flocking researchers will continue to refine and build on some of the relatively simple individual-based models in order to achieve a deeper, broader and more accurate representation of flocking in the real world. This is particularly important at this point in time, as STARFLAG is now fully operational and is beginning to deliver experimental measurements of real macroscopic flocking parameters for the first time. This means that, for the first time, there is experimental measurements for simple bird flocking behaviour (in this case starling flocks) of the kind that many of these models are attempting to simulate. In the near future, it may finally be possible, based on these new experimental results, to gain a much better understanding of the types of theoretical interactions, which result in quantitatively realistic flocking behaviour, as opposed to simply qualitatively realistic behaviour.

Another avenue of research involves investigating the dynamical properties of a flocking system, rather than simply looking at the bulk properties of a flocking systems. This means looking at things like the formation and dissipation of flocks, how different flocks can merge with one another to create a larger flock or breakdown into two smaller flocks. Basically any time-dependent behaviour which changes the overall properties of the flocking system.

In Chapters 3 and 4 an entirely new approach to modelling flocking as a virial gas was introduced, and it is hoped that this approach can be further developed in the future, in order to investigate a wider range of flocking models. To date, only two families of flocking models have gained wide acceptance, simple individual-based models and hydrodynamic models. It is hoped that the approach introduced in Chapter 3 can add a third angle of attack for analysing flocking systems, and also encourage other researchers to think of other novel ways of approaching flocking phenomena. It may be that there are more accurate and analytical techniques out there which can be used to extract interesting information
about flocking behaviour, and adding new tools to the current toolset of flocking analysis techniques will be a big part of future flocking research.

One recent avenue of flocking research is looking at how flocking models can be used to help determine how different predator strategies arise in nature. For instance, are these predatory strategies a result of complex thought on the part of the predator, or do they arise naturally out of simple feedback effects between members of two different groups (predator and prey groups) following very simple laws that can be encapsulated in hard or soft-core potentials as we have done in Chapter 2. For instance, when a pride of lions hunt, they exhibit some hunting techniques that appear quite sophisticated, however, it is possible that some of these hunting strategies, particularly ones that appear once the predator and prey have begun interacting, occur simply through the feedback of interactions between individual lions and other lions in the pride, and also with the prey flock. Likewise the prey flock will respond to the predators hunting strategy as a result of 2nd-order feedback and so on, and it is important to observe how well these feedback effects explain the behaviours of interacting predator-prey flocks, and how the type of potential selected changes these large scale behaviours. For example, it could be that a hard-core potential accurately simulates the interplay between lions and wildebeest while a soft-core potential more accurately simulates the behaviour of dolphins hunting a school of fish. These remain open questions which could potential bring new insights into flocking behaviour once they are investigated.

The literature so far on such systems has barely scratched the surface on what sorts of questions can be asked, and these multi-species flocking systems are certain to be an area of far more robust investigation in the future. In a broader context, it may be possible to model a whole basic ecosystem, based on the fundamental premises of flocking behaviour. The Serengeti, to provide one specific instance, is populated by a large number of herding species, such as wildebeest, zebra, elephants and rhinoceros, which all interact with one another, as well as herds of other species and predators. In the context of flocking, this could be modelled much like a gas system containing multiple species of gas with differing
interaction characteristics. The possibilities are endless.

Perhaps the holy grail of flocking research however, would a model robust enough that it can simulate the fundamental flocking characteristics of any flocking species simply by altering a small number of free parameters. A model which can replicate the behaviour of flocking species ranging from tiny bacteria, through flocks of birds, schools of fish and herds of wildebeest. In such a model, it would be possible to specify different regions of parameter space which represent the flocking behaviour of all these different species, and in some sense provide a 'Grand Theory of Flocking'. Right now however, the field is still very much in its infancy, and there is still much exciting and fascinating research to be performed before such a point could conceivably be reached.

5.5 Final Remarks

The world of flocking is the world of the very small, and the very large. From the smallest of creatures, such as bacteria and amoeba, to the very largest, such as whales and elephants, this fascinating phenomena of emergent order can be observed on every scale. Every rock unturned and every nook investigated reveals new examples of this kind of complex, ordered behaviour in the natural world. Flocking is the story of order arising from chaos and of the simple, fundamental interactions which lead to an abundance beautiful complexity of the world we see around us. To understand the nature of flocking is to understand something deeply profound and universal about the nature of the world we live in, and that alone makes it a worthwhile and exciting avenue of research.

The author hopes that you have enjoyed this journey through the many and varied aspects of flocking behaviour, and that this work has illustrated some of the awe and wonder associated with the study of these fascinating and unique systems which are observed in all environments, on all lengths scales, all over the biological world. This is a huge part of what makes flocking such a fascinating area of study, for all the myriad different forms,
5.5. FINAL REMARKS

formations and behaviours exhibited by types of social creatures, there are sets of fundamental underlying interactions which link them all, independent of species. It is this ubiquity, this universality, that is the beauty, and the power, of understanding flocking.

This is a very exciting time to be working in the field of self-organising behaviour, with the existence of a number important, unanswered questions and a number of new applications on the horizon in a wide range of fields from military robotics to public transport to medicine. In the past few years, the field has been sitting on the cusp of some very important developments, from the first experimental results coming out of STARFLAG, to novel types of research looking at information flow in flocking systems, the interaction of predators and prey, and even the energy economics associated with flocking behaviour. It has been an honor and a privilege to have undertaken research in this field of study.
REFERENCES


From Chapter 4, there exist 3 alternative angular potential which express the behaviour of the Vicsek model. These are given by equations (4.6-4.8) but are reproduced below for convenience.

\begin{align*}
V_{ij}^{(2)}(r, \phi) &= \zeta H(r_i - r_j) \left( 1 - \exp \left( -\frac{\phi^2}{\pi} \right) \right), \quad (A.1) \\
V_{ij}^{(3)}(r, \phi) &= \zeta H(r_i - r_j) \left( \frac{1}{10} (\phi^2 - \pi^2 + 10) \right), \quad (A.2) \\
V_{ij}^{(4)}(r, \phi) &= \begin{cases} \\
-\zeta H(r_i - r_j) \frac{\phi}{\pi} & \phi < 0 \\
\zeta H(r_i - r_j) \frac{\phi}{\pi} & \phi > 0 \\
\end{cases} \quad (A.3)
\end{align*}

where $-\pi < \phi < \pi$.

Since the $R$ dependence of the model remains the same, and the integration over the angular dependent portion of the potential occurs last, the derivation for these different potentials only diverges at equation (4.23):

\begin{equation}
\Xi_2 = 8\pi^3 \left[ \int_{-\pi}^{\pi} d\phi_{12} \frac{1}{12} (4L^3 R - R^3 L) \left( \exp \left( -\zeta \beta \sin^2 \left( \frac{\phi_{12}}{2} \right) \right) - 1 \right) + \frac{L^4}{4} \right], \quad (A.4)
\end{equation}
which can be generalised such that:

\[
\Xi_2 = 8\pi^3 \left[ \int_{-\pi}^{\pi} d\phi_12 \left( \frac{1}{12} (4L^3R - R^3L) \left( \exp \left( -\frac{\zeta \beta \phi}{10} \right) - 1 \right) \right) + \frac{L^4}{4} \right], \quad (A.5)
\]

where \( f(\phi) = V_{ij}^2(\phi), V_{i1}^2(\phi), V_{ij}^2(\phi) \) with \( H(r_i, r_j) = 1 \).

These can now be considered on a case by case basis.

A.1 Quadratic Potential \((V_{ij}^{(2)}(\phi))\)

Beginning with the substitution of \( f(x) = V_{ij}^{(2)}(\phi) \)

\[
\Xi_2 = 8\pi^3 \left[ \int_{-\pi}^{\pi} d\phi_12 \left[ \frac{1}{12} (4L^3R - R^3L) \left( \exp \left( -\frac{\zeta \beta \phi^2}{10} (\phi^2 - \pi^2 + 10) \right) - 1 \right) \right] + \frac{L^4}{4} \right], \quad (A.6)
\]

which can be simplified to:

\[
\Xi_2 = 8\pi^3 \left[ \frac{1}{12} (4L^3R - R^3L) e^{\zeta \beta \frac{\pi^2}{10}} e^{-\zeta \beta} \int_{-\pi}^{\pi} d\phi_12 \left( \exp \left( -\frac{\zeta \beta \phi^2}{10} \right) - 1 \right) + \frac{L^4}{4} \right], \quad (A.7)
\]

and then integrated by \( \phi \) to obtain the result:

\[
\Xi_2 = 8\pi^3 \left[ \frac{1}{12} (4L^3R - R^3L) \left( e^{\zeta \beta \frac{\pi^2}{10}} e^{-\zeta \beta} \sqrt{10\pi \zeta \beta} \text{Erf} \left( \frac{\pi}{\sqrt{10\zeta \beta}} \right) - 2\pi \right) + 2\pi \frac{L^4}{4} \right]. \quad (A.8)
\]

\( \Xi_1 \) remains unchanged from the case in Chapter 4:

\[
\Xi_1 = 2\pi^2 A, \quad (A.9)
\]
leading, as a result of equation (4.28), to:

\[ b_2 = \frac{16\pi^4}{A} \left[ \frac{1}{8\pi} \left( \frac{4R}{L} - \frac{R^3}{L^3} \right) \left( e^{\xi\beta} \frac{\phi^2}{\pi} e^{-\xi\beta} \sqrt{10\pi\xi\beta} \text{Erf} \left( \frac{\pi}{\sqrt{10\xi\beta}} \right) - 2\pi \right) \right]. \quad (A.10) \]

and hence, with \( B_2 = -b_1 \):

\[ B_2 = \frac{16\pi^4}{A} \left[ -\frac{1}{8\pi} \left( \frac{4R}{L} - \frac{R^3}{L^3} \right) \left( e^{\xi\beta} \frac{\phi^2}{\pi} e^{-\xi\beta} \sqrt{10\pi\xi\beta} \text{Erf} \left( \frac{\pi}{\sqrt{10\xi\beta}} \right) - 2\pi \right) \right]. \quad (A.11) \]

Allowing the equation of state to be written using equation (4.9) as:

\[ P_\beta = n + n^2 \frac{16\pi^4}{A} \left[ -\frac{1}{8\pi} \left( \frac{4R}{L} - \frac{R^3}{L^3} \right) \left( e^{\xi\beta} \frac{\phi^2}{\pi} e^{-\xi\beta} \sqrt{10\pi\xi\beta} \text{Erf} \left( \frac{\pi}{\sqrt{10\xi\beta}} \right) - 2\pi \right) \right] \quad (A.12) \]

which matches equation (4.35) in Chapter 4.

### A.2 Gaussian Potential \( (V_{ij}^{(3)}(\phi)) \)

Beginning by substituting \( f(x) = V_{ij}^{(3)}(\phi) \)

\[ \Xi_2 = 8\pi^3 \left[ \int_{-\pi}^{\pi} d\phi_{12} \frac{1}{12} \left( 4L^3 R - R^3 L \right) \left( \exp \left[ -\xi\beta \left( 1 - \exp \left( \frac{\phi^2}{\pi} \right) \right) \right] - 1 \right) + \frac{L^4}{4} \right] \quad (A.13) \]

it can be seen that the complication here is the exponential of an exponential within the integration. If the assumption that \( \xi\beta << 1 \) is made, a Taylor expansion about \( \beta\xi \) may be used:

\[ \exp \left[ -\xi\beta \left( 1 - \exp \left( \frac{\phi^2}{\pi} \right) \right) \right] = 1 - \xi\beta \left( 1 - \exp \left( \frac{\phi^2}{\pi} \right) \right), \quad (A.14) \]
With the expansion truncated to first order, as in chapter 3:

$$
\Xi_2 = 8\pi^3 \left[ \int_{-\pi}^{\pi} d\phi_{12} \frac{1}{12} (4L^3 R - R^3 L) \left( \zeta \beta \exp \left( \frac{\phi^2}{\pi} \right) - 1 \right) + \frac{L^4}{4} \right], \quad (A.15)
$$

which after integration by $\phi$ becomes:

$$
\Xi_2 = 8\pi^3 \left[ \frac{1}{12} (4L^3 R - R^3 L) \left( 2\pi \zeta \beta \left( \frac{1}{2} \text{erf}(\sqrt{\pi}) - 1 \right) \right) + 2\pi \frac{L^4}{4} \right]. \quad (A.16)
$$

From equation (4.28) this allows it to be shown that:

$$
b_2 = \frac{16\pi^4}{A} \left[ \frac{1}{12} \left( \frac{4R}{L} - \frac{R^3}{L^3} \right) \left( 2\pi \zeta \beta \left( \frac{1}{2} \text{erf}(\sqrt{\pi}) - 1 \right) \right) \right], \quad (A.17)
$$

leading to:

$$
B_2 = \frac{16\pi^4}{A} \left[ - \frac{1}{12} \left( \frac{4R}{L} - \frac{R^3}{L^3} \right) \left( 2\pi \zeta \beta \left( \frac{1}{2} \text{erf}(\sqrt{\pi}) - 1 \right) \right) \right] \quad (A.18)
$$

and ultimately, from equation (4.6) a virial equation of state:

$$
P_\beta = n + n^2 \frac{16\pi^4}{A} \left[ - \frac{1}{12} \left( \frac{4R}{L} - \frac{R^3}{L^3} \right) \left( 2\pi \zeta \beta \left( \frac{1}{2} \text{erf}(\sqrt{\pi}) - 1 \right) \right) \right]. \quad (A.19)
$$

Which matches equation (4.36) of Chapter 4.
A.3 Triangular Potential \( (V_{ij}^{(4)}(\phi)) \)

Beginning with the substitution of \( f(x) = V_{ij}^{(4)}(\phi)(\phi) \) and splitting the integral in half, due to the discontinuity, yields:

\[
\Xi_2 = 8\pi^3 (4L^3 R - R^3 L) \times \left[ \left( \int_{-\pi}^{0} d\phi \frac{1}{12} \left( \exp \left( \frac{\zeta \beta}{\pi} \phi \right) - 1 \right) \frac{L^4}{4} \right) + \left( \int_{0}^{\pi} d\phi \frac{1}{12} \left( \exp \left( -\frac{\zeta \beta}{\pi} \phi \right) - 1 \right) \frac{L^4}{4} \right) \right],
\]

which by solving the integration over \( \phi \) is, rather straightforwardly:

\[
\Xi_2 = 8\pi^3 \left\{ \frac{1}{12} \left( 4L^3 R - R^3 L \right) \left[ \frac{2\pi}{\zeta \beta} e^{-\zeta \beta} (-\zeta \beta - 1) \right] + 2\pi \frac{L^4}{4} \right\},
\]

leading to (from equation (4.28)):

\[
b_2 = \frac{16\pi^4}{A} \left\{ \frac{1}{12} \left( \frac{4R}{L} - \frac{R^3}{L^3} \right) \left( \frac{1}{\zeta \beta} \left( e^{-\zeta \beta} - \zeta \beta - 1 \right) \right) \right\}
\]

and yielding:

\[
B_2 = \frac{16\pi^4}{A} \left\{ -\frac{1}{12} \left( \frac{4R}{L} - \frac{R^3}{L^3} \right) \left( \frac{1}{\zeta \beta} \left( e^{-\zeta \beta} - \zeta \beta - 1 \right) \right) \right\},
\]

and finally, from equation (4.9):

\[
P_{\beta} = n + n^2 \frac{16\pi^4}{A} \left\{ -\frac{1}{12} \left( \frac{4R}{L} - \frac{R^3}{L^3} \right) \left( \frac{1}{\zeta \beta} \left( e^{-\zeta \beta} - \zeta \beta - 1 \right) \right) \right\}.
\]

Which matches equation (4.37) in Chapter 4.
DERIVING THE EQUATION OF STATE FOR ALTERNATE POTENTIAL FORMS.
Beginning with the relationship between boid number, \( N \), the partition function, \( Z \), and the fugacity, \( \lambda \):

\[
N = \lambda \left( \frac{\partial \ln(Z)}{\partial \lambda} \right). \tag{B.1}
\]

\( \ln(Z) \) may be written as:

\[
\ln(Z) = \ln(1 + \lambda Z_1 + \lambda^2 Z_2), \tag{B.2}
\]

and since,

\[
\ln(1 + x) \approx x - \frac{x^2}{2}, \tag{B.3}
\]

then setting \( x = \lambda Z_1 + \lambda^2 Z_2 \) results in,

\[
\ln(Z) = \lambda Z_1 + \lambda^2 \left( Z_2 - \frac{Z_1^2}{2} \right). \tag{B.4}
\]
Calculating the fugacity for a system of indistinguishable particles.

Which means that,

\[ N = \lambda Z_1 + 2\lambda^2 \left( Z_2 - \frac{Z_1^2}{2} \right). \]  \hspace{1cm} (B.5)

This may be written as,

\[ 2\lambda^2 \left( Z_2 - \frac{Z_1^2}{2} \right) + \lambda Z_1 - N = 0 \]  \hspace{1cm} (B.6)

and solved using the quadratic equation in \( \lambda \) such that,

\[ \lambda = \frac{-Z_1 \pm \sqrt{Z_1^2 + 8N \left( Z_2 - \frac{Z_1^2}{2} \right)}}{4 \left( Z_2 - \frac{Z_1^2}{2} \right)} \]  \hspace{1cm} (B.7)

which, after some simple algebra, becomes:

\[ \lambda = \left( \frac{-1 \pm \sqrt{1 + 8N \left( \frac{Z_2}{Z_1^2} - \frac{1}{2} \right)}}{4 \left( \frac{Z_2}{Z_1^2} - \frac{1}{2} \right)} \right) \frac{1}{Z_1}. \]  \hspace{1cm} (B.8)

Substitution of,

\[ Z_1 = \Xi_1 A_Q, \]  \hspace{1cm} (B.9)
\[ Z_2 = \frac{1}{2} \Xi_2 A_Q^2, \]  \hspace{1cm} (B.10)

where \( A_Q = \left( \frac{1}{(2\pi\hbar)^2 \frac{2m}{\beta}} \right)^{-1} \) yields:

\[ \lambda = \left( \frac{-1 \pm \sqrt{1 + 4N \left( \frac{\Xi_2}{\Xi_1^2} - \frac{1}{2} \right)}}{2 \left( \frac{\Xi_2}{\Xi_1^2} - \frac{1}{2} \right)} \right) \frac{A_Q}{\Xi_1}. \]  \hspace{1cm} (B.11)
Now a negative or complex fugacity is not a sensible result, so the positive root is taken and the discriminant must be a positive quantity. Hence,

$$\lambda = \left( \frac{-1 + \sqrt{1 + 4N \left( \frac{\Xi}{\Xi_1} - 1 \right)}}{2 \left( \frac{\Xi}{\Xi_1} - \frac{1}{2} \right)} \right) A_Q \frac{\Xi}{\Xi_1}$$  (B.12)

and substituting for $X_1 = 2\pi A$ yields the result in equation (4.49) of Chapter 4.
Calculating the fugacity for a system of indistinguishable particles.
Appendix C includes the notebook used for calculating the forms of the internal energy, $U$, entropy, $S$, and the specific heat $C_V$ from the partition function derived in equation (4.34) of Chapter 4.

Due to the results for fugacity, $U$ and $C_V$ are calculated from the partition function where the effective fugacity discussed in Chapter 4 is held to be $\lambda_e = 0.00015$ and is represented by $f$. The constant portion of the quantum area is represented by $h = \left( \frac{1}{(2\pi \hbar)^2} \right)^{-1}$. Other constants are set to be $m = 1$, $A = 100$, $N = 200$. The functional forms for $U$ and $C_V$ are then derived using equations (4.44) - (4.46) and plotted for suitable values of $\beta$. Note also that the term $\Xi$ in the mathematica notebooks corresponds to $\Xi_2$, since $\Xi_1$ is trivial it is included directly as $\Xi_1 = 2\pi A$. 
The 2-particle configuration integral:

\[
\mathcal{E} = 16 \cdot (3.1415)^4 \left(1/12\right) \left(4 \cdot L^3 \cdot R - R^3 \cdot L\right) \left(\exp[-\beta/2] + \text{BesselI}[0, \beta/2] - 1\right) + 3.1415 \cdot L^4 / 2 \\
\mathcal{E} = 1558.3616027359212 \cdot \left(1.57075 \cdot L^4 + \frac{1}{12} \left(4 \cdot L^3 \cdot R - L \cdot R^3\right) \left(-1 + e^{-\beta/2} \cdot \text{BesselI}[0, \beta/2]\right)\right)
\]

The functional form for Internal Energy (U):

\[
U = -D \cdot \log \left(1 + \lambda \cdot \frac{A}{h \cdot \beta}\right) + \lambda^2 \cdot \frac{A}{\left(2 \cdot h^2 \cdot \beta^2\right)} \cdot \mathcal{E}, \beta
\]

\[
U = -\left(\frac{A \cdot \lambda}{h \cdot \beta^2} - \frac{1}{h^2 \cdot \beta^3}\right) \cdot 1558.3616027359212 \cdot A^2 \cdot \lambda^2 \cdot \left(1.57075 \cdot L^4 + \frac{1}{12} \left(4 \cdot L^3 \cdot R - L \cdot R^3\right) \left(-1 + e^{-\beta/2} \cdot \text{BesselI}[0, \beta/2]\right)\right) + \\
\frac{1}{h^2 \cdot \beta^2} \cdot \left(779.1808013679606 \cdot A^2 \cdot \lambda^2 \cdot \left(1.57075 \cdot L^4 + \frac{1}{12} \left(4 \cdot L^3 \cdot R - L \cdot R^3\right) \left(-1 + e^{-\beta/2} \cdot \text{BesselI}[0, \beta/2]\right)\right)\right)
\]

or after elimination of the quantum area (h) terms:

\[
U = -\left(\frac{A^2}{\beta} - 1/1558.3616027359212 \cdot A^2 \cdot \frac{1}{\beta}\right) \cdot 15270.75 \cdot L^4 + \frac{1}{12} \left(4 \cdot L^3 \cdot R - L \cdot R^3\right) \left(-1 + e^{-\beta/2} \cdot \text{BesselI}[0, \beta/2]\right) + 779.1808013679606 \cdot A^2 \cdot \frac{1}{\beta} \cdot \left(1.57075 \cdot L^4 + \frac{1}{12} \left(4 \cdot L^3 \cdot R - L \cdot R^3\right) \left(-1 + e^{-\beta/2} \cdot \text{BesselI}[0, \beta/2]\right)\right) \right)
\]

And in terms of \(k_B T\):

\[
U = -\left(\frac{A^2}{k_B T} - 1/1558.3616027359212 \cdot A^2 \cdot \frac{1}{(k_B T)}\right) \cdot 15270.75 \cdot L^4 + \frac{1}{12} \left(4 \cdot L^3 \cdot R - L \cdot R^3\right) \left(-1 + e^{-\beta/2} \cdot \text{BesselI}[0, \beta/2]\right) + 779.1808013679606 \cdot A^2 \cdot \frac{1}{(k_B T)} \cdot \left(1.57075 \cdot L^4 + \frac{1}{12} \left(4 \cdot L^3 \cdot R - L \cdot R^3\right) \left(-1 + e^{-\beta/2} \cdot \text{BesselI}[0, \beta/2]\right)\right) \right)
\]
\[ U = -\left( -A f \, kT - 1558.3616027359212 \cdot A^2 \, f^2 \, kT \right) \]
\[ \left( 1.57075 \cdot L^4 + \frac{1}{12} \left( 4 \, L^3 \, R \cdot L \, R \right) \left( -1 + e^{-\frac{1}{2} BesselI[0, \frac{1}{2}] + \frac{1}{2} e^{-\frac{\beta}{2}} BesselI[1, \frac{1}{2}] - 1 \right) \right) \]
\[ + \left( 1 + A \, f + 779.1808013679606 \cdot A^2 \, f^2 \right) \left( 1.57075 \cdot L^4 + \frac{1}{12} \left( 4 \, L^3 \, R \cdot L \, R \right) \left( -1 + e^{-\frac{1}{2} BesselI[0, \frac{1}{2}] + \frac{1}{2} e^{-\frac{\beta}{2}} BesselI[1, \frac{1}{2}] - 1 \right) \right) \]

The functional form for Specific Heat Capacity \((C_v)\):

\[ C_v = -\beta^2 \left( 779.1808013679606 \cdot A^2 \cdot f^2 \right) \]
\[ \left( 0.1 + \frac{1}{12} \left( 4 \, L^3 \, R \cdot L \, R \right) \left( -1 + e^{-\frac{1}{2} BesselI[0, \frac{1}{2}] + \frac{1}{2} e^{-\frac{\beta}{2}} BesselI[1, \frac{1}{2}] - 1 \right) \right) \]
\[ \left( \frac{1558.3616027359212 \cdot A^2 \cdot f^2}{\beta} \right) \]
\[ \left( 1.57075 \cdot L^4 + \frac{1}{12} \left( 4 \, L^3 \, R \cdot L \, R \right) \left( -1 + e^{-\frac{1}{2} BesselI[0, \frac{1}{2}] + \frac{1}{2} e^{-\frac{\beta}{2}} BesselI[1, \frac{1}{2}] - 1 \right) \right) \]
\[ + \left( 1 + A \, f + 779.1808013679606 \cdot A^2 \, f^2 \right) \left( 1.57075 \cdot L^4 + \frac{1}{12} \left( 4 \, L^3 \, R \cdot L \, R \right) \left( -1 + e^{-\frac{1}{2} BesselI[0, \frac{1}{2}] + \frac{1}{2} e^{-\frac{\beta}{2}} BesselI[1, \frac{1}{2}] - 1 \right) \right) \]

\[ + \frac{1}{2} e^{-\frac{1}{2} BesselI[0, \frac{1}{2}] + \frac{1}{2} e^{-\frac{\beta}{2}} BesselI[1, \frac{1}{2}] - 1 \}
\[ \frac{1}{8} e^{-\frac{1}{2} BesselI[0, \frac{1}{2}] + \frac{1}{2} e^{-\frac{\beta}{2}} BesselI[1, \frac{1}{2}] - 1 \}
\[ \left( 1 + A \, f + 779.1808013679606 \cdot A^2 \, f^2 \right) \left( 1.57075 \cdot L^4 + \frac{1}{12} \left( 4 \, L^3 \, R \cdot L \, R \right) \left( -1 + e^{-\frac{1}{2} BesselI[0, \frac{1}{2}] + \frac{1}{2} e^{-\frac{\beta}{2}} BesselI[1, \frac{1}{2}] - 1 \right) \right) \]

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and in terms of $k_B T$:

$$C_v = \frac{-1}{kT^2} \left( 779.1808013679606' A^2 f^2 \right.$$  

$$\left( 0. + \frac{1}{12} \left( 4 L^3 R - L R^3 \right) \left( -\frac{1}{2} e^{\frac{i}{2} \pi} \text{BesselI} \left[ 0, \frac{1}{2} kT \right] + \frac{1}{2} e^{\frac{i}{2} \pi} \text{BesselI} \left[ 1, \frac{1}{2} kT \right] \right) \right)$$  

$$\left( -A f kT - 1558.3616027359212' A^2 f^2 kT \left( 1.57075' L^4 + \frac{1}{12} \left( 4 L^3 R - L R^3 \right) \right) \right.$$

$$\left( -1 + e^{\frac{i}{2} \pi} \text{BesselI} \left[ 0, \frac{1}{2} kT \right] \right)^2$$

$$\left( A f kT^2 + 1558.3616027359212' A^2 f^2 kT \left( 1.57075' L^4 + \frac{1}{12} \left( 4 L^3 R - L R^3 \right) \right. \right.$$  

$$\left. \left( -1 + e^{\frac{i}{2} \pi} \text{BesselI} \left[ 0, \frac{1}{2} kT \right] \right)^2 \right) - 1558.3616027359212' A^2 f^2 kT$$

$$\left( 0. + \frac{1}{12} \left( 4 L^3 R - L R^3 \right) \left( -\frac{1}{2} e^{\frac{i}{2} \pi} \text{BesselI} \left[ 0, \frac{1}{2} kT \right] + \frac{1}{2} e^{\frac{i}{2} \pi} \text{BesselI} \left[ 1, \frac{1}{2} kT \right] \right) \right)$$  

$$\left( 64.9317334733005' A^2 f^2 \left( 4 L^3 R - L R^3 \right) \left( \frac{1}{4} e^{\frac{i}{2} \pi} \text{BesselI} \left[ 0, \frac{1}{2} kT \right] \right. \right.$$  

$$\left. \left( -\frac{1}{4} e^{\frac{i}{2} \pi} \text{BesselI} \left[ 1, \frac{1}{2} kT \right] + \frac{1}{8} e^{\frac{i}{2} \pi} \text{BesselI} \left[ 0, \frac{1}{2} kT \right] + \text{BesselI} \left[ 2, \frac{1}{2} kT \right] \right) \right)$$

$$\left( 1 + A f + 779.1808013679606' A^2 f^2 \left( 1.57075' L^4 + \frac{1}{12} \left( 4 L^3 R - L R^3 \right) \right. \right.$$  

$$\left. \left( -1 + e^{\frac{i}{2} \pi} \text{BesselI} \left[ 0, \frac{1}{2} kT \right] \right)^2 \right)$$

$$\left. \right)$$

The functional form for Entropy ($S$):

$$S = -(B^2) D \left( \frac{1}{B} \right) \log \left[ 1 + f \ast A + f \ast 2 \left( A^2 / 2 \right) \ast B \right] \beta, \beta$$
\[ S = -\beta^2 \left( \left( 779.1808013679606 \cdot A^2 \cdot f^2 \right) \left( 0. + \frac{1}{12} \left( 4 L^3 R - L R^3 \right) \left( -\frac{1}{2} e^{-\beta/2} \text{BesselI} \left( 0, \frac{\beta}{2} \right) + \frac{1}{2} e^{-\beta/2} \text{BesselI} \left[ 1, \frac{\beta}{2} \right] \right) \right)/\right) \]

\[ \beta \left( 1 + A f + 779.1808013679606 \cdot A^2 \cdot f^2 \left( 1.57075 \cdot L^4 + \frac{1}{12} \left( 4 L^3 R - L R^3 \right) \left( -1 + e^{-\beta/2} \text{BesselI} \left[ 0, \frac{\beta}{2} \right] \right) \right) \right) - \frac{1}{\beta^2} \log \left( 1 + A f + 779.1808013679606 \cdot A^2 \cdot f^2 \left( 1.57075 \cdot L^4 + \frac{1}{12} \left( 4 L^3 R - L R^3 \right) \left( -1 + e^{-\beta/2} \text{BesselI} \left[ 0, \frac{\beta}{2} \right] \right) \right) \right) \]

And in terms of \( k_B T \):

\[ S = -\frac{1}{kT^2} \left( \left( 779.1808013679606 \cdot A^2 \cdot f^2 \cdot kT \right) \left( 0. + \frac{1}{12} \left( 4 L^3 R - L R^3 \right) \left( -\frac{1}{2} e^{-\frac{1}{2} \cdot i \cdot \frac{k}{kT}} \text{BesselI} \left[ 0, \frac{1}{2} \cdot kT \right] + \frac{1}{2} e^{-\frac{1}{2} \cdot i \cdot \frac{k}{kT}} \text{BesselI} \left[ 1, \frac{1}{2} \cdot kT \right] \right) \right)/\right) \]

\[ \left( 1 + A f + 779.1808013679606 \cdot A^2 \cdot f^2 \left( 1.57075 \cdot L^4 + \frac{1}{12} \left( 4 L^3 R - L R^3 \right) \left( -1 + e^{-\beta/2} \text{BesselI} \left[ 0, \frac{\beta}{2} \right] \right) \right) \right) - kT^2 \log \left( 1 + A f + 779.1808013679606 \cdot A^2 \cdot f^2 \left( 1.57075 \cdot L^4 + \frac{1}{12} \left( 4 L^3 R - L R^3 \right) \left( -1 + e^{-\beta/2} \text{BesselI} \left[ 0, \frac{\beta}{2} \right] \right) \right) \right) \]
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