Abstract

It is well known that Onsager theory on hard rod system predicts that the system exhibits an isotropic-nematic phase transition at a critical density. Previous works by Viellard-Baron [1], Frenkel [2], Sheng [3], Foulaadvand [4], by Monte Carlo simulation or molecular dynamics studies of hard ellipse systems, all show similar results. The approach we adopt in this thesis is through molecular dynamics simulation of NVEP ensemble of 900 hard ellipses in a two dimensional box with periodic boundary conditions, the only interactions between ellipses being through hard collisions. We demonstrate results on thermodynamic properties such as linear speed and angular velocity distributions to show that our system is stabilized. Our results show that the system transits from isotropic fluid to nematic phase to solid phase as density increases for aspect ratio 4 and 6 and transits from isotropic phase to solid phase for aspect ratio 2.
A Molecular Dynamics Study of Systems of Hard Ellipses

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by
Amulya Vanga

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Thesis written by
Amulya Vanga
B.Sc. (Honors) University of Delhi, 2013
M.Sc. Kent State University, 2017

Approved by

XIAOYU ZHENG , Advisor
ANDREW TONGE , Chair, Department of Mathematics
JAMES L. BLANK , Dean, College of Arts and Sciences
“Give me a lever long enough and a fulcrum on which to place it, and I shall move the world.”

Archimedes
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Chapter 1

INTRODUCTION

Liquid crystals, as their name suggests, are materials whose properties are described as between those of a liquid phase and solid or crystalline phase. For example, a liquid crystal substance may flow like a liquid, while its molecules may orient in a crystal-like way.

There are various in-between phases of a liquid crystal, and they are characterized by their molecular ordering. Many parameters are used to distinguish the liquid crystal structures, most common of which are positional and orientational ordering and short and long range order. The presence of positional ordering indicates that the molecules in a liquid crystals are arranged in some sort of ordered lattice. A presence of orientational ordering indicates that the molecules more or less point in the same direction.

Short range order means that the molecules of the substance only share meaningful positional or orientational ordering with the molecules within its immediate surrounding, typically only one or two molecules range. Meanwhile, long range order means that a molecule shares positional and orientational order with molecules that are located at a large distance from itself.

The most common phases of a liquid crystal are the nematic and the isotropic phase. In the nematic phase, the molecules have no positional order but have strong long range orientational ordering typically with alignment along the longer axis. The isotropic phase, on the other hand, is characterized by no positional and orientational ordering.
Studies about liquid crystals are categorized based on whether the substance is thermotropic or lyotropic. A thermotropic liquid crystal will change its phase from nematic to isotropic or vice versa when the temperature of the substance is changed. Increasing the temperature typically results in an isotropic phase, while decreasing the temperature usually results in a nematic phase. On the other hand, the phase of a lyotropic liquid crystal depends on the density or number of molecules present per cubic volume of the substance. A liquid crystal with low density usually exhibits isotropic order while a high density system exhibits nematic order. This work focuses exclusively on lyotropic liquid crystals. The density at which a system transitions from the nematic phase to isotropic is the focus of many theories, and chief among them is the Onsager theory of liquid crystals.

Onsager theory, proposed by Lars Onsager [5], predicts the critical density at which a lyotropic liquid crystal transitions from an isotropic fluid to a nematic liquid crystal phase. To paraphrase the analysis put forth by Xiao and Sheng [3] on Onsager theory, the free energy of an NVT ensemble (an ensemble that depends on the number of particles $N$, the volume $V$, and the thermodynamical temperature $T$ of the system) to the first order can be expressed as

$$F = Nk_B T \left( \ln(\rho \eta \lambda^3) + \int d\omega f(\omega) \ln f(\omega) - \frac{\eta}{2} \int \int d\omega_1 d\omega_2 \beta_1(\omega_1, \omega_2)f(\omega_1)f(\omega_2) \right),$$

where $F$ denotes the free energy, $k_B$ the Boltzmann constant, $\eta$ the number density, $f$ the angular distribution function, $\omega$ the solid angle, $\beta_1$ the second virial coefficient and $\rho$ is a dimensionless constant and $\lambda$ is the thermal wavelength.

The free energy is minimized to obtain the orientational distribution function $f(\omega)$ of the molecules at any given density $\eta$. In two dimensions, Onsager theory qualitatively predicts the second order isotropic-nematic phase transition.

Onsager theory makes several omissions and approximations that often hinder accurate predictions. The first approximation the theory makes is that only steric repulsive interactions affect the system, thus disregarding the dependance of the systems on temperature. Furthermore, the theory assumes that short range order does not play a role in the theory. The theory is intended for molecules of very large aspect ratios, while the theory is considered to be unreliable in its prediction of phase transition for smaller aspect ratios.
The study of liquid crystals in nature is often incomplete and unreliable, as many properties of the substance, such as velocity and energy of the molecules, cannot be determined. For this reason, to gain meaningful and data rich insight of liquid crystals, one must rely heavily on computer simulations. Over the years, extensive algorithms have been generated that account for all physical properties of the substance, leaving little room for observational error.

When deciding how best to construct the algorithm from which the data is to be analyzed, one must choose between the Monte Carlo simulation and molecular dynamics. Both simulations have different approaches and have a wide range of advantages. Molecular dynamics is essential if one wishes to study structural and thermodynamic properties of molecules in contact. An obvious advantage of Monte Carlo methods is the ease with which one may study different statistical models.


In a Monte-Carlo simulation of NVT ensemble, particles are chosen at random to be randomly displaced, and if the movement causes an overlap with the other particles, then the move is disregarded. If there is no overlap, then the move is accepted with certain probability and the process is repeated [6].

Viellard-Baron [1] used Monte Carlo simulations on systems of 170 hard ellipses to study the properties of a two dimensional system of hard ellipses whose aspect ratio equals 6. This system was chosen because its properties most closely resemble the properties one may expect from a nematic liquid crystal whose molecules interact with steric forces dominantly. He showed that the system exhibits a first order isotropic-nematic phase transition followed by a first order nematic-solid transition as density increases.

Cuesta and Frenkel [2] conducted constant pressure Monte-Carlo simulations for a system of about 200 hard ellipses with aspect ratios 2, 4 and 6 in a nearly squared box. The system with aspect ratio 2 exhibits a first order isotropic-solid transition as density increases. The system with aspect ratio 4 exhibits a first order isotropic-nematic and a first
order nematic-solid transition. The system with aspect ratio 6 appears to have second order isotropic-nematic and a first order nematic-solid transition.

Molecular dynamics is a simulation method developed to study the physical movement of molecules [6]. The particles of the system are allowed to interact with each other, and the trajectories and forces acting on the particles are calculated using Newton’s Laws of Motion [7].

Foulaadvand and Yarifard [4] performed molecular dynamics with a system of hard ellipses with aspect ratio 2. The main focus of the work was the nontrivial dynamic properties of the system, for example, the existence of three regimes in the temporal behavior of the angular mean-square displacement.

Xiao and Sheng [3] generalized the Onsager theory of liquid crystals in two dimensions. They showed that by performing molecular dynamics on molecules composed of linked hard disks with different aspect ratios, the generalized theory was improved, and its prediction of the transition density agreed well with the simulation results. Molecular dynamics further yielded evidence of hexagonal order for molecules with certain aspect ratios, indicating an intermediate hexagonal phase before solidifying at higher densities.

In this thesis, we study the behavior of the system of hard ellipses in a microcanonical ensemble via molecular dynamics. This means that the total energy of the system remains constant throughout the process. Although there exist many works on this very similar topic, it is our intention to develop a sound molecular dynamics model that can also be easily extended to arbitrary aspect ratios, to higher dimension and maybe to other particle shapes.

Also known as an NVEP ensemble, this statistical model represents the possible states of a system when in equilibrium, where \( N \), the number of molecules in the system, \( V \), the volume of the system, \( E \), the energy of the system and \( P \), the linear momentum, are the principle variables of the system.

We introduce the molecular dynamics simulation details of the system in Chapter 2 and present the results generated by the algorithm in Chapter 3 and conclude in Chapter 4.
Chapter 2

SIMULATION METHOD

To study the properties of liquid crystals, a comprehensive study of the properties of its molecules must be made. Fig. 2.1 shows 5CB, which is a nematic liquid crystal with the chemical formula $C_{18}H_{19}N$. Ellipses closely resemble the shape of the molecules of liquid crystals and may be used in the simulations to accurately reflect the behavior of liquid crystals.

Some methods used within the algorithm have been explored in this section to help understand its construction. An over simplified pseudocode can be put as follows. The system is first initialized as described in Sec. 2.1. Once initialized, the system is advanced step by step through hard particle molecular dynamics; the system of ellipses is scanned for an overlap; and collision is detected using the back tracing method as described in 2.2.2. The system is advanced as many time steps as required until the system reaches equilibrium. The system may take anywhere from five thousand to five million time steps to stabilize. Data such as linear and angular momentum, angle and center from every ellipse is collected after the system has stabilized for 10,000 steps. Periodic boundary conditions are used to preserve the energy of the system, and cell linked lists are used to make computations efficient.

![Figure 2.1: 5CB, also know as 4-Cyano-4'-pentyphenyl.](image)
2.1 Initialization

Consider a fixed $L \times W$ sized simulation box that is divided into a triangular lattice. We choose the fundamental unit length $l_c = 1$ as the lattice size. All lengths are expressed in units of $l_c$. Suppose the system comprises $M \times N$ ellipses, each with a major axis length of $2a$ and a minor axis length of $2b$. An ellipse is centered at every grid point of the lattice as shown in Fig. 2.2. So the dimensions of the simulation box may be defined as

$$L \times W = 2Ml_c \times 2Nw,$$

where $w = \frac{l_c \sqrt{3}}{2AR}$.

The aspect ratio $AR$ describes the ratio of $a$ over $b$. If a system of aspect ratio $AR$ needs to be studied, then the value of $a$ is chosen from $(0,1)$ and so $b = \frac{a}{AR}$. Systems with $AR = 2, 4, \text{ and } 6$ have been studied in this thesis. Changing the values of $a$ and consequently $b$ changes the packing density $\eta$ of the system. So while the size of the ellipse is varied, the underlying triangular lattice remains unchanged. The packing density is defined as the ratio of the total area covered by the ellipses over the total area of the system and is given by

$$\eta = \frac{M \times N \pi ab}{L \times W}.$$

Figure 2.2: A triangular lattice is overlaid on an $L \times W$ grid and an ellipse with major axis length $2a$ and minor axis length $2b$ is centered at every grid point. The ellipses continue in all directions due to the implementation of periodic boundary conditions.
The highest density system one can study occurs when \( a = l_c = 1 \), so \( \eta = \frac{\pi}{2\sqrt{3}} \approx 0.9069 \). Every ellipse has a fixed mass \( m_i \) and moment of inertia \( I_i \), where

\[
m_i = \rho_c \pi ab, \quad (2.3)
\]

\[
I_i = m_i \frac{(a^2 + b^2)}{4}, \quad (2.4)
\]

and \( \rho_c \), the density of the particle is set to 1. Here, the moment of inertia \( I_i \) is about the \( z- \) axis through the center.

The ellipses are restricted in their movement to a two dimensional \( x - y \) plane. The ellipses of this frictionless system are assumed to be hard. That is, when they collide, they do not change their shape and they never overlap. This thesis will only analyze systems of 900 ellipses.

Initializing the system involves assigning every ellipse an initial angle \( \theta_i \), velocities \( u_i \) and \( v_i \) in the \( x \) and \( y \) direction respectively, and an angular velocity \( \omega_i \) for \( i = 1 \) to \( M \times N \). In this study, we choose the characteristic linear velocity as \( u_c = 1 \), and characteristic time is defined to be \( t_c = l_c/u_c = 1 \), and characteristic angular velocity is \( \omega_c = 1/t_c = 1 \). We assume that linear velocities and angular velocity are uniformly distributed in the range \((-1, 1)\). Taking a larger range of velocities results in a system of higher temperature. Note that the higher temperature does not affect the results, it only speeds up the dynamics. Once the system is initialized, these parameters ensure that every ellipse can traverse the \( x - y \) plane linearly as well as rotate along its major axis.
2.2 Hard Particle Molecular Dynamics

The system is advanced through hard molecular dynamics by time steps. At each time instance, every ellipse travels with its own linear and angular velocity before colliding with other ellipses. At every time step, every ellipse has its angle and center of mass updated using free flight dynamics. The algorithm then scans all the ellipses for overlap and, if no overlap is detected, the algorithm proceeds to the next time step. If an overlap between two ellipses is detected, a back tracing method is implemented and the time of collision is detected. The velocities of the colliding ellipses are updated using Conservation Laws of Motion, while the other ellipses have their properties updated using free flight dynamics.

This section will first explore the free flight dynamics when ellipses are not colliding, then describe the algorithm used to determine the minimum distance of approach between two ellipses in contact, then it will detail the back tracing method of finding the time of collision of two ellipses and then goes on to describe the updated velocities of two ellipses when they collide.

2.2.1 Free-Flight Dynamics

All the molecules in the system are assumed to move freely between collisions. The center of mass of every ellipse moves in the $x-y$ plane with constant linear momentum and there is end-over-end rotation of the particles along the perpendicular of the axis of symmetry with a constant angular momentum.

If no collision is detected when advancing the system by a time step of length $\delta t$, then the angle and center of mass of every ellipse needs to be updated while linear and angular velocities remain unchanged. If $x_i$ and $y_i$ are the coordinates of the center of mass of an ellipse $i$, and $\theta_i$ is the angle of the major axis of an ellipse formed with the $x$-axis, then

\begin{align*}
x_i(t + \delta t) &= x_i(t) + u_i \delta t, \\
y_i(t + \delta t) &= y_i(t) + v_i \delta t, \\
\theta_i(t + \delta t) &= \theta_i(t) + \omega_i \delta t.
\end{align*}
2.2.2 Minimum Distance Between Ellipses

When dealing with the minimum distance allowed between the centers of two hard circles, the calculations are simple. The minimum distance allowed between the centers is simply twice the radius. However, these calculations becomes a lot harder when dealing with ellipses.

The maximum distance the centers of two ellipse in contact can have to each other is $2a$, while the minimum they can have is $2b$. However, these cases are the two extremes. The minimum distance is usually dependent on the relative orientations of the ellipses and the relative positions of their centers of mass. A detailed algorithm developed by Zheng and Palfy-Muhoray [8] describes in great detail the calculations necessary to detect overlap between ellipses.

To begin overlap detection, the algorithm chooses an ellipse and scans its neighbors to see if the $x$ or $y$ coordinates of the ellipses centers are within $2a$ units of each other. If either of the coordinates are further than $2a$ units from each other, then there could not possibly be an overlap, and the algorithm scans the next possibility. However, if both $x$ and $y$ coordinates are less than $2a$ units from each other, then the algorithm uses the function of the distance of closest approach to determine if the ellipses are overlapping.

![Figure 2.3: Two ellipses in contact. Forces act along the unit normal vectors $\hat{n}$ at the collision point.](image-url)
2.2.3 Back Tracing Method of Detecting Collisions

To advance the system through collision detection, a back tracing method is implemented. At time step $t$, all ellipses are advanced by a single time step of length $dt$. The choice of $dt$ depends on the number density. As the number density increases, $dt$ decreases. The overlap detection function described previously then scans all pairs of ellipse for an overlap. If an overlap between two ellipses is detected, the entire system is taken back to time step $t$ and advanced forward by a time step of length $\delta t = \frac{dt}{2}$. If an overlap is still detected, the entire system will be taken back to $t$ and this time advanced by a time step of length $\delta t = \frac{dt}{4}$. This procedure is continued until no overlap is detected or the overlap is less than an assigned tolerance. If this tolerance is reached, it is assumed that the ellipses are very close together and may be regarded as being in contact. The actual amount of time it takes to reach the next moment of collision is then given by $\delta t$.

Once the colliding ellipses are regarded as being in contact, the dynamics of the ellipses need to be updated. While the two colliding ellipses will have their dynamics updated as described in the next section, the ellipses that did not experience any collisions will be updated using free flight dynamics.

Note that this back tracing method does not detect the actual moment of collision, but rather the last known moment before the collision occurred. Therefore, the dynamics described in the following section are updated preemptively.

2.2.4 Collision Dynamics

Once the collision is detected, the velocities of the colliding ellipses must be updated. Suppose two ellipses labelled 1 and 2 are colliding and $i$ and $f$ represent the initial and final parameters of the ellipses. The linear and angular momentum and kinetic energy must be conserved in a system of elastic collisions. So if the momentum is exchanged along $\hat{n}$, the unit outward normal to ellipse 1 at the point of contact, and the impulse acting on the first ellipse is $\alpha \hat{n}$ as shown in Fig. 2.3, where $\alpha$ is the magnitude of the impulse, to be determined using conservation of energy, then the conservation of linear
momentum states that

\[ m_1(v_{1f} - v_{1i}) = \alpha \hat{n} \implies v_{1f} = v_{1i} + \frac{\alpha \hat{n}}{m_1}, \]

\[ m_2(v_{2f} - v_{2i}) = -\alpha \hat{n} \implies v_{2f} = v_{2i} - \frac{\alpha \hat{n}}{m_2}, \]

and conservation of angular momentum says that

\[ I_1(\omega_{1f} - \omega_{1i}) = \alpha \mathbf{p} \times \hat{n} \implies \omega_{1f} = \omega_{1i} + I_1^{-1}(\alpha \mathbf{p} \times \hat{n}), \]

\[ I_2(\omega_{2f} - \omega_{2i}) = -\alpha \mathbf{q} \times \hat{n} \implies \omega_{2f} = \omega_{2i} - I_2^{-1}(\alpha \mathbf{q} \times \hat{n}), \]

(2.8)

where \( \mathbf{p} \) and \( \mathbf{q} \) are the vectors from the center of ellipses 1 and 2 respectively to the contact point at the moment of collision [7]. Finally the conservation of kinetic energy requires that no energy is lost from the system, so the final energy must be the same as the initial energy. So

\[ E = \frac{1}{2}m_1v_{1i}^2 + \frac{1}{2}m_2v_{2i}^2 + \frac{1}{2}\omega_{1i}^2I_1 + \frac{1}{2}\omega_{2i}^2I_2, \]

\[ = \frac{1}{2}m_1v_{1f}^2 + \frac{1}{2}m_2v_{2f}^2 + \frac{1}{2}\omega_{1f}^2I_1 + \frac{1}{2}\omega_{2f}^2I_2, \]

(2.9)

solving for \( \alpha \) gives

\[ \alpha = \frac{2((\omega_{2i} \times \mathbf{q}) + v_{2i}) - ((\omega_{1i} \times \mathbf{p}) + v_{1i}) \cdot \hat{n}}{\frac{1}{m_1} + \frac{1}{m_2} + (\mathbf{p} \times \hat{n})I_1^{-1}(\mathbf{p} \times \hat{n}) + (\mathbf{q} \times \hat{n})I_2^{-1}(\mathbf{q} \times \hat{n})}. \]

(2.10)

Once all the parameters are updated, the system is advanced by another time step of length \( dt \) and the process is repeated.

### 2.3 Periodic Boundary Conditions

While studying a microscopic system of 900 particles may provide invaluable information, the study must also reflect well and be applicable on a macroscopic scale. Periodic boundary conditions help one study a small part of a larger system. Additionally, periodic boundary conditions conserve the energy as well as the density of the system. Otherwise, when an ellipse eventually moves outside the range of the visible simulation, the system will lose energy as ellipses continue to travel past the defined edges of the simulation box.

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An alternate system may have been created that had an ellipse that was moving at the edge of a simulation bounce back on an invisible “boundary wall,” thus keeping the ellipses within a defined workspace at all times. Instead, for the purposes of keeping any interaction of the ellipses solely between other ellipses, the original system, or visible simulation, has been replicated on all sides of the central simulation, thus creating an infinite invisible lattice around the visible simulation box. With this periodic boundary condition, any ellipse that moves through the original simulation box, also moves in the exact same manner in all the cells neighboring the original. This means that when an ellipse travels out of the visible simulation into the neighboring cell below, the replica of the ellipse, complete with identical linear and angular velocity and energy, enters the simulation box from above. So now, because there are no “walls” to bounce off of in the system, for any ellipse that travels through the “boundary” of the visible central simulation box, its images moves across their respective “boundaries” as well. This helps us keep the number of calculations done to a minimum, because when an ellipse travels out of the visible simulation box, attention may be turned to its image that is now entering the visible simulation from the opposite direction. A schematic illustration of the periodic boundary conditions is given in Fig. 2.4.
2.4 Cell Structures and Linked Lists

When looking for collisions between ellipses, it is a waste of time to consider the interactions between ellipses far away from one another. Since it is reasonable to assume that an ellipse will not interact or collide with every ellipse in the system, the computations may be minimized by only considering ellipses within a certain vicinity of the ellipse. To help with this minimization process, linked lists may be constructed where the system is split into cells and the interactions of an ellipse can be restricted to ellipses within that cell and its immediate neighboring cells.

If the central simulation containing $M \times N$ ellipses is divided into $K \times K$ cells, then, rather than compute $O((M \times N)^2)$ interactions, the linked list computes the interactions of ellipses in a cell only to the cell it belongs to and the 8 neighboring cells. So the number of computations is reduced to $O(9(\frac{M \times N}{K})^2)$.

A brief description of the pseudocode may be described as follows. Let $lcx$ and $lcy$ denote the number of cells of the simulation box in the $x$ and $y$ direction. So any cell that appears in the simulation box can be identified as $(1, 1), (1, 2), (1, 3)$ and so on. To simplify the algorithm, each cell $c$ is renumbered so it may be represented by a single number instead of a pair of numbers. For each ellipse $e_i, i = 1 \ldots M \times N$, we first sort it into a cell $c$ according to its center. We then set the $lsc\ell(i)$ to the head of the cell, and the head($c$) is reset to point to the index of the current ellipse $i$. This way, after sorting all ellipses to cells, head($c$) points to the highest indexed ellipse in the $c$-th cell or is empty if there are no ellipses in that cell, and linked list $lsc\ell(i)$ points to the next highest indexed ellipse in the same cell or is empty if the $i$-th ellipse is the smallest indexed ellipse in the cell [9]. This process is illustrated in Fig. 2.5. Using this linked list, the algorithm can then start with the head of a cell and, following the linked list, scan for and detect an overlap between ellipses.
Figure 2.5: The illustration of cell structures and linked list constructions.
Chapter 3

RESULTS

All results were processed on Intel Xeon E7-4820, 2.00GHz, 8 cores X 4 (32 cores total) computers with Intel Xeon E7-4820 and 64GB RAM. The results were generated on Matlab 2016b. Results took between three and forty hours to compute.

The results of this thesis can be divided into two further sections. The results shown in the first section are used to confirm the soundness of the system. This helps us confirm that the system is behaving as it should and there are no glaring faults in the algorithm. Once we are satisfied with the working of the algorithm, we come to the results in the second section. These results will study the behavior of the systems and analyze its physical properties.
3.1 Characterization of Thermodynamic Equilibrium

3.1.1 Ratio between Translational and Rotational Energy

The systems of this thesis assume that energy is entirely kinetic. The total energy of a system is the sum of its two components; rotational and translational energy. Translational energy in the $x$ and $y$ direction at a time $t$ is defined as

$$E_{x\text{-}trans} = \sum_{i=1}^{M \times N} \frac{m_i u_i^2}{2},$$

(3.1)

$$E_{y\text{-}trans} = \sum_{i=1}^{M \times N} \frac{m_i v_i^2}{2},$$

(3.2)

where $u_i$ and $v_i$ are the horizontal and vertical velocity components for the $i$-th particle. So the total translational energy is the sum of $E_{x\text{-}trans}$ and $E_{y\text{-}trans}$. The rotational energy, depending on the moment of inertia and angular velocity of the particle, is defined as

$$E_{rot} = \sum_{i=1}^{M \times N} \frac{I_i \omega_i^2}{2}.$$  

(3.3)

The total energy of the system, $E_{tot} = E_{trans} + E_{rot}$ is constant throughout the process. After the system reaches equilibrium, according to the equipartitioning theorem in classical statistical mechanics, energy is equally shared among all degrees of freedom [10]. In the 2D system, the ratio $\frac{E_{trans}}{E_{rot}}$ becomes steady around two because translational energy has two degrees of freedom, while rotational energy has one degree of freedom. In a 3D model, translational energy would have three degrees of freedom and rotational energy would have two, thus resulting in a ratio that stabilizes at the value $\frac{3}{2}$. Fig. 3.1 shows the ratio of $\frac{E_{trans}}{E_{rot}}$ stabilizing around 2 after achieving equilibrium for aspect ratio 2 at packing density $\eta = 0.7346$.

3.1.2 Distribution of Linear Speeds and Angular Velocities

To begin analyzing the distribution of the various properties of the ellipses, the data associated with each ellipse over $10^4$ time steps after equilibrium has been collected and
Figure 3.1: The ratio of $\frac{E_{\text{trans}}}{E_{\text{rot}}}$ settles around two for a system with 900 ellipses and aspect ratio 2 at packing density $\eta = 0.7346$.

analyzed. The resulting histograms are then fitted to the appropriate density functions, thus giving the parameters that best fit the function.

### 3.1.2.1 Distribution of Linear Speeds

In order to fit the linear speeds of the system, its two components in the $x$ and $y$ direction are combined as

$$V_i(t) = \sqrt{u_i(t)^2 + v_i(t)^2}. \quad (3.4)$$

James Clerk Maxwell and Ludwig Boltzmann [7] described the Maxwell-Boltzmann distribution in reference to the linear speed of particles in a system, where the particles could move freely without interacting with one another except for brief collisions during which the particles changed their energy and momentum [11][12]. The Maxwell-Boltzmann density function in 2D is given by

$$P(V) = \frac{V}{\sigma^2} e^{-\frac{V^2}{2\sigma^2}}, \quad (3.5)$$

where $\sigma = \sqrt{\frac{kT}{m}}$ is the standard deviation, where $\frac{3}{2}kT$ is the average energy per particle and $m$ is the mass of each particle [11].
Fig. 3.2 shows a Maxwell-Boltzmann fit of the linear speed probability distribution after the systems have reached the thermodynamic equilibrium. The parameters of the curve are presented in Table 3.1. The value of $\sigma$ increases with packing density because $kT/m$, increases with particle size.

![Distribution of Linear Velocity](image)

**TABLE 3.1:** Maxwell-Boltzmann fitting for linear speed distribution for a system of 900 ellipses with aspect ratio 2.
3.1.2.2 Distribution of Angular Velocities

Normalizing the histogram of the angular velocities of the system results in a bell shaped curve (see Fig. 3.3) that closely resembles the Gaussian density function given by

\[ P(\omega) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\omega^2}{2\sigma^2}} \]  

(3.6)

where \( \sigma = \sqrt{\frac{kT}{I}} \). Fitting the data to the Gaussian distribution results in the parameters presented in Table 3.2. The larger \( \sigma \) values for lower packing densities indicate higher variation among the angular velocities if there is more free volume for the particles to travel.

**Figure 3.3:** For aspect ratio 2, angular velocity follows the Gaussian distribution. The circles represent the data points while the lines are the fitted curves. The data from 100-1000 time steps is distributed into 50 bins and normalized to produce an estimation of the given Gaussian distribution.
<table>
<thead>
<tr>
<th>$\eta$</th>
<th>0.1451</th>
<th>0.2267</th>
<th>0.3265</th>
<th>0.4444</th>
<th>0.5804</th>
<th>0.7346</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma$ Value</td>
<td>2.136</td>
<td>1.738</td>
<td>1.459</td>
<td>1.258</td>
<td>1.114</td>
<td>1.002</td>
</tr>
<tr>
<td>$\sqrt{\frac{kT}{I}}$</td>
<td>2.138</td>
<td>1.723</td>
<td>1.448</td>
<td>1.252</td>
<td>1.107</td>
<td>0.995</td>
</tr>
</tbody>
</table>

**Table 3.2:** Gaussian fitting for angular velocity distribution for a system of 900 ellipses with aspect ratio 2.
3.2 Characterization of Phase Transition

In this section, we show the following results for a system of 900 ellipses for aspect ratios 2, 4 and 6: nematic orientational order, correlation functions, distribution of angles and collision frequency and system pressure.

Nematic Order Parameter
To characterize the average orientational order of the system, one defines the following symmetric traceless tensor,

$$Q_{\alpha,\beta} = \frac{1}{M \times N} \left\langle \sum_{i=1}^{M \times N} [2n_\alpha(i)n_\beta(i) - \delta_{\alpha\beta}] \right\rangle,$$

where $\alpha, \beta$ take $x, y$ and $n_\alpha(i)$ and $n_\beta(i)$ represent the $\alpha$ and $\beta$ Cartesian component of the unit vector specifying the direction of the $i$th ellipse with $x$ axis and $<>$ means time averaging [2]. If $\theta_i$ is the angle of the $i$th ellipse formed with a reference frame, then $Q$ may be written as follows:

$$Q = \frac{2}{M \times N} \left( \sum_{i=1}^{M \times N} (\cos^2 \theta_i - \frac{1}{2}) \sum_{i=1}^{M \times N} \cos \theta_i \sin \theta_i \right).$$

The absolute value of the eigenvalues $S$ of this matrix is usually referred to as the nematic order parameter which is a measure of degree of alignment of all particles. The eigenvectors are the average direction of particles and a direction perpendicular to it. A completely random or isotropic system will have a nematic order equal to zero, while a perfectly aligned system will have nematic order equal to 1.

Correlation Functions
Radial distribution function or pair correlation function shows how the number density of a system varies as a function of distance from a reference particle. For completeness, $g(r)$ is defined as follows:

$$g_0(r) = \frac{1}{\eta(M \times N)} \left\langle \sum_{i=1}^{M \times N} \sum_{j \neq i} \delta(r^2 - r_{ij}^2) \right\rangle.$$
where $<>$ means averaging over all ellipses having center to center distance of $r$ from each other. A general algorithm determines the number of ellipses that are within an $r$ and $r + \delta r$ distance from a reference particle [4]. Weak positional ordering, indicative of a liquid phase, shows minor oscillations that eventually settle into a constant. For strong positional ordering, indicative of the solid crystalline phase, the radial distribution function oscillates with large amplitude, demonstrating the long range order of the molecules. See top left of figures 3.7, 3.12 and 3.17.

The angular spatial correlation function measures the average relative angle around an ellipse at a certain distance $r$ from its center. The function is defined as

$$g_2(r) = \langle \cos(2[\theta(r) - \theta(0)]) \rangle.$$  \hfill (3.10)

The average is over all ellipses having a distance $r$ between their centers [4]. If $g_2(r)$ is close to 1, it means the particles at distance $r$ are parallel to the reference particle. If $g_2(r)$ is close to zero, it corresponds to weak correlation and means that the angles between particles at a distance $r$ to the reference particle are uniformly distributed in the interval $(0, \pi/2)$. See top right of figures 3.7, 3.12 and 3.17.

In the solid phase, if $g_0$ initially oscillates with strong peaks indicating strong short range spatial order but eventually settles around one, this indicates a lack of long range order. The angular spatial correlation function $g_2$ does not play a role in determining a solid phase.
In the nematic phase, \( g_0 \) does not oscillate but rather increases to and settles at one, indicating the weak spatial order of the system. The angular spatial correlation function \( g_2 \) settles above zero for the nematic phase.

In the isotropic phase, \( g_0 \) shows no significant oscillation and increases to one, much like the nematic phase, however, unlike the nematic phase, the angular spatial correlation function \( g_2 \) oscillates and settles at zero, indicating short range orientational order but not long range order.

Angular spatial correlations of the fourth and sixth order are defined as

\[
\begin{align*}
g_4(r) &= \langle \cos(4[\theta(r) - \theta(0)]) \rangle, \quad (3.11) \\
g_6(r) &= \langle \cos(6[\theta(r) - \theta(0)]) \rangle. \quad (3.12)
\end{align*}
\]

These order parameters will dominate over \( g_2(r) \) if the system shows a local fourfold or sixfold orientational order other than twofold orientational order. In our simulation, we do not find fourfold or sixfold local structure. See bottom left and bottom right of figures 3.7, 3.12 and 3.17.

**Collision Frequency and System Pressure**

The average number of collisions in a system per unit time provides an insight into the behavior of the system at high density. The study of the dependence of collision frequency \( \Gamma \) on \( \eta \) in the elliptical system described in this study displays strongly nonlinear behavior with a drastic increase in \( \Gamma \) when \( \eta \) exceeds a certain value that changes with the aspect ratio. See figures 3.8, 3.13 and 3.18

In molecular dynamics of hard molecules, the virial expansion can be written in a form involving an average over collisions such that \([9]\)

\[
<W> = \frac{1}{2T} \sum_{\text{colls}} r_{ij} \cdot \alpha \hat{n}
\]

(3.13)

where \( i \) and \( j \) represent a colliding pair and \( r_{ij} \) is the vector joining the centers of the ellipses at the moment of collision. The sum is over all collisions occurring in time period \( T \). This expression may be written in terms of collision frequency and the average of \( r_{ij} \cdot \alpha \hat{n} \) per collision. In our simulation, we assume that the average of the quantities \( r_{ij} \cdot \alpha \hat{n} \) are essentially the same for all packing densities, but may vary for different aspect
ratios. Thus the system pressure is simply a constant multiplying the collision frequency. If there is a nonsmooth change or a kink presents in the collision frequency curve, that is the packing density where the first order phase transition would be expected to occur. If the curve is smooth near the transition, then the phase transitions are expected to be continuous or at least second order.

**Distribution of Angles**

Creating a histogram by distributing the angles of the system with aspect ratio 2 into 40 bins results in a bell shaped curve. Figures 3.9, 3.14 and 3.19 indicate that as the density increases, the distribution of angles becomes more concentrated around zero, resulting in narrower and higher curves than those of smaller density. This is due to the increase in packing fraction, which limits the rotational movement of the ellipses.
3.2.1 Aspect Ratio = 2

From the radial distribution function and angular correlation functions, we observe an isotropic phase and a solid phase but no nematic phase, see Fig. 3.7. The transition from isotropic to nematic is first order as can be seen from the fact that the collision frequency of the system exhibits a kink around the density $\eta = 0.7510$ as density increases, see Fig. 3.6. Fig. 3.8 shows that the nematic order parameter $S$ starts to depart from zero after packing density $\eta = 0.6864$ and increases to one at the dense packing limit.

Figure 3.5: Snapshots of a system of 900 ellipses with $AR = 2$. Left: $\eta = 0.4444$ shows isotropic phase. Middle: $\eta = 0.7510$ shows plastic solid phase which is characterized by strong positional ordering and weak orientational ordering. Right: $\eta = 0.8271$ shows a solid phase.
Figure 3.6: Nematic Order Parameter for $AR = 2$.

Figure 3.7: Correlation Functions for $AR = 2$. Top left: $g_0(r)$, top right: $g_2(r)$, bottom left: $g_4(r)$, bottom right: $g_6(r)$. The radius $r$ of the anuli is plotted on the horizontal axis.
**Figure 3.8:** Collision frequency for $AR = 2$ follow highly nonlinear paths.

**Figure 3.9:** For $AR = 2$, angles of the system follow Gaussian distribution.
3.2.2 Aspect Ratio = 4

From the radial distribution function and spatial correlation functions, see Fig. 3.12, we observe an isotropic, nematic and solid phase. From the collision frequency of the system, see Fig. 3.13, we see that there is a first-order isotropic-nematic phase transition around $\eta = 0.6173$ and a first-order nematic-solid phase transition around the density $\eta = 0.7346$. The nematic order parameter $S$, see Fig. 3.11, is once again highly nonlinear and becomes nonzero at a density much lower than that observed for aspect ratio 2.

Figure 3.10: Snapshot of a system of 900 ellipse with $AR = 4$: On the left $\eta = 0.4444$ shows isotropic phase, while in the middle $\eta = 0.6173$ shows nematic phase, and on the right $\eta = 0.8185$ shows solid phase.
Figure 3.11: Nematic Order Parameter for $AR = 4$.

Figure 3.12: Correlation Functions for $AR = 4$. Top left: $g_0(r)$, top right: $g_2(r)$, bottom left: $g_4(r)$, bottom right: $g_6(r)$. The radius $r$ of the anuli is plotted on the horizontal axis.
Figure 3.13: Collision frequency for $AR = 4$ follow highly nonlinear paths.

Figure 3.14: $AR = 4$: Angles follow the Gaussian distribution.
3.2.3 Aspect Ratio = 6

As we did with systems of aspect ratio 4, we observe an isotropic, nematic and solid phase, see Fig. 3.17. From the collision frequencies of the systems, see Fig. 3.18, the continuous curve with no kinks suggests a continuous second order phase transition between isotropic-nematic and a first order nematic-solid phase around $\eta = 0.7600$. The nematic order parameter, see Fig. 3.16 is once again highly nonlinear and becomes nonzero at a density much lower than that observed for both aspect ratios 2 and 4.

**Figure 3.15:** Snapshot of a system of 900 ellipse with $AR = 6$: On the left $\eta = 0.2267$ shows isotropic phase while in the middle $\eta = 0.5804$ shows nematic phase and on the right $\eta = 0.8013$ shows solid phase.
Figure 3.16: Nematic Order Parameter for $AR = 6$.

Figure 3.17: Correlation Functions for $AR = 6$. Top left: $g_0(r)$, top right: $g_2(r)$, bottom left: $g_4(r)$, bottom right: $g_6(r)$. The radius $r$ of the annuli is plotted on the horizontal axis.
Figure 3.18: Collision frequency for $AR = 6$ follow highly nonlinear paths.

Figure 3.19: $AR = 6$: Angles follows the Gaussian distribution.
Chapter 4

CONCLUSION

To summarize, we study the phase transition of a system of 900 ellipses with aspect ratio 2, 4 and 6, via molecular dynamics. The ellipses interact with each other exclusively through elastic collisions in an NVEP system. Free-flight dynamics and collision dynamics are used to advance the system and a back tracking method is implemented to detect the moment of collision. This algorithm is also aided by our use of periodic boundary conditions that help us view the system as a microscopic part of a whole while not compromising the integrity of the outcome, and the use of linked lists makes the algorithm time efficient. This comprehensive algorithm lets us collect data after the system has reached equilibrium and thus allows us to study the energy, linear speeds and angular velocities of the ellipses.

The dynamic properties of the system of ellipses with aspect ratio 2 let us confirm that the system is effective and accurate. We observe that the ratio of translation over rotational energy settled around 2, which is compliant with the equipartition theorem of classical statistical mechanics. We also observed that linear speeds of ellipses in the system follow Maxwell-Boltzmann distribution while the angular velocities of the ellipses follow Gaussian distribution.

The focus of this paper is to show the phase transitions from an isotropic phase to nematic phase to solid phase for different aspect ratios. Through the results on nematic order parameters, correlation functions and system pressures, we show that the system with aspect ratio 2 does not have any nematic phase but rather transitions directly from an isotropic phase to a plastic solid to a solid phase. From the system pressure, we conclude that the phase transition from isotropic to solid is first order. Systems with aspect ratio 4
and 6, in addition to isotropic and solid phase, also show nematic phase. In particular, for the systems with aspect ratio 4, we observe first order isotropic-nematic phase transition followed by a first order nematic-solid phase transition. For aspect ratio 6, the systems appear to exhibit continuous second order isotropic-nematic transition followed by first order nematic-solid phase transition. However, to conclusively accept this observation, more densities must be studied. All results are in accordance with works by Vieillard-Barron [1] and Cuesta and Frenkel [2], who use Monte-Carlo simulation to achieve their results, as well as Foulaadvand and Yarifard [4], who used molecular dynamics.


APPENDICES

A Output

function Output_1_A

clear all;

global M N a b a1 b1 a2 b2

M = 30; % number of particles along horizontal direction
N = 30; % number of particles along vertical direction

AR = 2; % aspect ratio

a = 1; % half size of the grid along the horizontal direction
b = a * sqrt(3) / 2 / AR; % half size of the grid along the vertical direction

ratio = 4. / 10; % artificially create different densities

a1 = ratio * a; % major axis of all ellipses
b1 = a1 / AR; % minor axis of all ellipses

a2 = a1; % for ellipse routine, do not do anything
b2 = b1;

eta = pi * a1 * b1 / (4 * a * b); % eta is the packing density

main_dynamics
function main_dynamics
% global parameters
global M N a b a1 b1 a2 b2
global first second rshiftxx rshiftyy px py qx qy
global time angle center_x center_y vel_x vel_y omega

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%% INITIALIZATION HERE %%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

for i = 1 : M
    for j = 1 : N
        index = (j - 1) * M + i; % index of the ellipse
        if(mod(j,2) == 1)
            center_x(index,1) = (i - 1) * 2 * a + a; % x-coordinates of the center of the ellipse
        else
            center_x(index,1) = (i - 1) * 2 * a;
        end
        center_y(index,1) = (j - 1) * 2 * b + b; % y-coordinates of the center of the ellipse
        angle(index,1) = 0; % angle of the major axis
        vel_x(index) = 2*rand - 1; % horizontal velocity
        vel_y(index) = 2*rand - 1; % vertical velocity
        omega(index) = 2*rand - 1; % angular velocity
        mass(index) = pi * a1 * b1; % mass of the ellipse
        ine(index) = mass(index) * (a1^2 + b1^2) / 4; % moment of inertia of the ellipse
    end
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%% DYNAMICS STARTS HERE %%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

dt_global = 0.001; % global time step
k = 1;
time(k) = 0; % save time during dynamics
time_now = 0; % keep track of current time
flag = 0; % if flag=0 no overlapping, if flag=1 overlapping
while(flag == 0 && time_now < 100) % time evolution
    dt = dt_global;
    flag = 1;
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

while(flag == 1)
    for i = 1 : M * N
        % free flight for all particles
        angle(i,k + 1) = angle(i,k) + omega(i) * dt;
        center_x(i,k + 1) = center_x(i,k) + vel_x(i) * dt;
        center_y(i,k + 1) = center_y(i,k) + vel_y(i) * dt;
        % implement periodic boundary conditions
        if(center_x(i,k + 1) > 2 * a + M)
            center_x(i,k + 1) = center_x(i,k + 1) - 2 * a + M;
        elseif(center_x(i,k + 1) < 0)
            center_x(i,k + 1) = center_x(i,k + 1) + 2 * a + M;
        end
    end
end
if(center_y(i,k + 1) > 2 * b * N)
    center_y(i,k + 1) = center_y(i,k + 1) - 2 * b * N;
elseif(center_y(i,k + 1) < 0)
    center_y(i,k + 1) = center_y(i,k + 1) + 2 * b * N;
end

[flag,dt] = checking_overlap(center_x(:,k + 1),center_y(:,k + 1),angle(:,k + 1),
dt);
end

% end of checking for overlap
k = k + 1;
time(k) = time(k - 1) + dt;
% collision dynamics
if(dt < dt_global)
    theta1 = angle(first,k);
    theta2 = angle(second,k);
    theta3 = atan2(center_y(second,k) - center_y(first,k) + rshiftyy,center_x(second,
k) - center_x(first,k) + rshiftxx);
    xc1 = center_x(first,k);
    yc1 = center_y(first,k);
    [min_dist,px,py,qx,gy] = ellipse2(a1,b1,a2,b2,theta1,theta2,theta3,xc1,yc1);
    A11 = (sin(theta1) / b1)^2 + (cos(theta1) / a1)^2;
    A12 = cos(theta1) * sin(theta1) * ((1 / a1^2) - (1 / b1^2));
    A21 = cos(theta1) * sin(theta1) * ((1 / a1^2) - (1 / b1^2));
    A22 = (cos(theta1) / b1)^2 + (sin(theta1) / a1)^2;
    Nx = (A11 * px + A12 * py) / sqrt((A11 * px + A12 * py)^2 + (A21 * px + A22 * py)^2);
    Ny = (A21 * px + A22 * py) / sqrt((A11 * px + A12 * py)^2 + (A21 * px + A22 * py)^2);
    alpha = (2 * Nx * ( - omega(second) * qy + omega(first) * py + vel_x(second) -
    vel_x(first))) / (1 / mass(first) + 1 / mass(second) ... + 1. / ine(first) * (px * Ny - py * Nx)^2 + 1. / ine(second) * (qx * Ny - qy *
    Nx)^2);
    % updating velocities of colliding ellipses
    vel_x(first) = vel_x(first) + 1 / mass(first) * alpha * Nx;
    vel_y(first) = vel_y(first) + 1 / mass(first) * alpha * Ny;
    omega(first) = omega(first) + 1 / ine(first) * alpha * (px * Ny - py * Nx);
    vel_x(second) = vel_x(second) - 1 / mass(second) * alpha * Nx;
    vel_y(second) = vel_y(second) - 1 / mass(second) * alpha * Ny;
    omega(second) = omega(second) - 1 / ine(second) * alpha * (qx * Ny - qy * Nx);
end

end
C Checking Overlap of all Ellipses in the System

function [flag, dt] = checking_overlap(centerx, centery, anglei, dt)

global first second rshiftxx rshiftyy px py qx qy M N a b a1 b1 a2 b2
flag = 0; % if flag=0 no overlapping, if flag=1 overlapping

tol = 1.e-14;

% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% % % CELL STRUCTURE AND LINKED LIST CONSTRUCTION % %
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

lcx = floor(M / 4); % number of cells in the x-direction
lcy = floor(N / 4); % number of cells in the y-direction

for c = 1 : lcx * lcy
    head(c) = 0;
end

% check for overlapping
for mc_x = 1 : lcx
    for mc_y = 1 : lcy
        c = lcx * (mc_y - 1) + mc_x; % index of the cell
        % scan neighborhood cells of c including itself
        for mc1_x = mc_x - 1 : mc_x + 1 % left and right
            % impose periodic boundary condition by shifting coordinates
            % horizontally
            if mc1_x <= 0
                rshiftx = - 2 * a * M;
            elseif mc1_x >= lcx + 1
                rshiftx = 2 * a * M;
            else
                rshiftx = 0; % else keep (centerx, centery), no shift
            end
        % impose periodic boundary condition by shifting coordinates
        % vertically
        if mc1_y <= 0
            rshifty = - 2 * b * N;
        elseif mc1_y >= lcy + 1
            rshifty = 2 * b * N;
        else
            rshifty = 0; % else keep (centerx, centery), no shift
        end
        % Calculate the scalar cell index of the neighbor cell
        if(mod(mc1_x + lcx, lcx) ~= 0)
ccx = mod((mc1_x + lcx),lcx);
else
    ccx = lcx;
end
if(mod(mc1_y + lcy,lcy) ~= 0)
    ccy = mod((mc1_y + lcy),lcy);
else
    ccy = lcy;
end
c1 = (ccy - 1) * lcx + ccx;
i = head(c); % Scan atom i in cell c
while (i ~= 0)
    j = head(c1); % Scan atom j in cell c1
    while (j ~= 0)
        if (i < j) % Avoid double counting of pair (i, j)
            dist_x = centerx(i) - (centerx(j) + rshiftx); % Image-corrected relative pair position
            dist_y = centery(i) - (centery(j) + rshifty);
            dist_center = sqrt(dist_x^2 + dist_y^2);
            if (dist_center < 2 * a) % Compute distance of closest approach between (i, j)
                theta1 = anglei(i);
                theta2 = anglei(j);
                theta3 = atan2(centery(j) - centery(i) + rshifty, centerx(j) - centerx(i) + rshiftx);
                [min_dist, px, qx, py, qy] = ellipse2(a1, b1, a2, b2, theta1, theta2, theta3, xc1, yc1);
                if(dist_center < min_dist - tol) % overlapping
                    flag = 1;
                    first = i; % first is the index of first ellipse in the collision pair
                    second = j; % second is the index of second ellipse in the collision pair
                    rshiftxx = rshiftx;
                    rshiftyy = rshifty;
                    break
                end
            end
        end
    end
end
end
if(flag == 1) break; end
i = lscl(i);
end
if(flag == 1) break; end
end
if(flag == 1) break; end
end
if(flag == 1) break; end

end

if(flag == 1)
    dt = dt / 2;
    break;
end
end
Minimum Distance Allowed Between Two Ellipses

\% a1, b1, a2, b2 are length of semi-axes of two ellipses
\% theta1 and theta2 are the angles of major axes of two ellipses formed
\% with respect to x-axis
\% theta3 is the angle of center line formed wrt x-axis
\% xc1, yc1, are coordinates for first ellipse
\% dist is the distance between centers at collision
\% xt, yt are coordinates of the contact points
\function [dist, px, py, qx, qy] = ellipse2(a1, b1, a2, b2, theta1, theta2, theta3, xc1, yc1)
\% assign variables cosine and sines of three angles
\cs1 = cos(theta1); sn1 = sin(theta1);
\cs2 = cos(theta2); sn2 = sin(theta2);
\cs3 = cos(theta3); sn3 = sin(theta3);
\k1d = cos(theta1 - theta3); \% inner product of k1 and d
\k2d = cos(theta2 - theta3); \% inner product of k2 and d
\k1k2 = cos(theta2 - theta1); \% inner product of k1 and k2
\% eccentricity of ellipses
\e1 = 1. - b1^2 / a1^2;
\e2 = 1. - b2^2 / a2^2;
\% component of A'
\eta = a1 / b1 - 1.;
\a1 = b1^2 / b2^2 * (1. + 0.5 * (1. + k1k2) * (eta * (2. + eta) - e2 * (1. + eta * k1k2)^2));
\a2 = b1^2 / b2^2 * 0.5 * sqrt(1. - k1k2^2) * (eta * (2. + eta) + e2 * (1. - eta^2 * k1k2^2));
\a22 = b1^2 / b2^2 * (1. + 0.5 * (1. - k1k2) * (eta * (2. + eta) - e2 * (1. - eta * k1k2)^2));
\% eigenvalues of A'
\lambda1 = 0.5 * (a11 + a22) + 0.5 * sqrt((a11 - a22)^2 + 4. * a12^2);
\lambda2 = 0.5 * (a11 + a22) - 0.5 * sqrt((a11 - a22)^2 + 4. * a12^2);
\% major and minor axes of transformed ellipse
\b2p = 1. / sqrt(lambda1);
\a2p = 1. / sqrt(lambda2);
\deltap = a2p^2 / b2p^2 - 1.;
\if abs(k1k2) == 1;
\if a11 > a22
\kpmp = 1. / sqrt(1. - e1 * k1d^2) * b1 / a1 * k1d;
\kpmps = 1. / sqrt(1. - e1 * k1d^2) * sin(theta3 - theta1);
\else
\kpmp = 1. / sqrt(1. - e1 * k1d^2) * b1 / a1 * k1d;
\kpmps = 1. / sqrt(1. - e1 * k1d^2) * sin(theta3 - theta1);
\end
\kpmp = (a12 / sqrt(1. + k1k2) * (b1 / a1 * k1d + k2d + (b1 / a1 - 1.) * k1d + k1k2) + (lambda1 - a11) / sqrt(1. - k1k2) * (b1 / a1 * k1d - k2d - (b1 / a1 - 1.) * k1d + k1k2)) / sqrt(2 + (a12^2 + (lambda1 - a11)^2) * (1. - e1 * k1d^2));
\kpmps = (- (lambda1 - a11) / sqrt(1. + k1k2) * (b1 / a1 * k1d + k2d + (b1 / a1 - 1.) * k1d + k1k2) / sqrt(2 + (a12^2 + (lambda1 - a11)^2) * (1. - e1 * k1d^2));
\end
\if kpmp == 0.0 || deltap == 0.0
\Rc = a2p + 1.;
\end

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% coefficients of quartic for q
\[
t = 1. / kpm^2 - 1.;
A = - 1. / b2p^2 * (1. + t);
B = - 2. / b2p * (1. + t + deltap);
C = - t - (1. + deltap)^2 + 1. / b2p^2 * (1. + t + deltap + t);
D = 2. / b2p * (1. + t) * (1. + deltap);
E = (1. + t + deltap) * (1. + deltap);
\]
% solution for quartic
\[
\alpha = \frac{-3.}{8.} * \left( \frac{B}{A} \right)^2 + \frac{C}{A};
\beta = \left( \frac{B}{A} \right)^3 / 8. - \left( \frac{B}{A} \right) * \left( \frac{C}{A} \right) / 2. + D / A;
\gamma = \frac{-3.}{256.} * \left( \frac{B}{A} \right)^4 + \frac{C}{A} * \left( \frac{B}{A} \right)^2 / 16. - \left( \frac{B}{A} \right) * \left( \frac{D}{A} \right) / 4. + \frac{E}{A};
\]
if beta == 0
\[
qq = - \frac{B}{4.} / A * \sqrt{\left( \frac{\alpha}{2.} - \sqrt{\alpha^2 - 4 * \gamma} \right) / 2.};
\]
else
\[
P = \frac{-\alpha^2}{12.} - \gamma;
Q = \frac{-\alpha^3}{108.} + \gamma * \alpha / 3. - \frac{\beta^2}{8.} / \frac{B}{A};
U = \text{mycbrt}(\frac{-0.5 * Q + \sqrt{Q^2 / 4 + P^3 / 27}}{8.});
if abs(U) == 0.0
\]
\[
y = \frac{-5.}{6} * \alpha + U - P / 3. / U;
\]
else
\[
y = \frac{-5.}{6} * \alpha - \text{mycbrt}(\gamma);
\]
end
\[
qq = \frac{-B}{4.} / A * \left( \frac{\alpha}{2.} + \sqrt{\alpha + 2. * y + 2. * \beta / \sqrt{\alpha + 2. * y}} \right);
\]
end
% substitute for R'
\[
Rc = \frac{\sqrt{\left( \frac{qq^2 - 1.}{deltap} \right) + \left( \frac{1. + b2p * (1 + deltap)}{qq} \right)^2 + \left( \frac{1. - \left( \frac{qq^2 - 1.}{deltap} \right)}{1. + b2p / \frac{qq}{qq}} \right)^2}}{\frac{1. + b2p / \frac{qq}{qq}}{qq}^2};
\]
% this is the solution for the closest approach
\[
dist = \text{real}(Rc * b1 / \sqrt{1. - e1 * k1d^2});
\]
% the following block is to find the coordinates of the contact point
if deltap == 0 || kpmp == 0.0 % case of two circles
\[
x_t = \text{real}(xc1 + b1 / \sqrt{1. - e1 * k1d^2} * \cos(\theta3));
y_t = \text{real}(yc1 + b1 / \sqrt{1. - e1 * k1d^2} * \sin(\theta3));
\]
else
\[
sps = \sqrt{(qq * qq - 1.0) / deltap};
cps = \sqrt{(1.0 - (qq * qq - 1.0) / deltap)};
\]
% now make sure that the sign of psi is same as of phi
\[
sps = sps * \text{sign}(kpmp);
cps = cps * \text{sign}(kpmp);
if abs(k1k2) == 1
\]
if a11 > a22
\[
x_t = \text{real}(xc1 + a1 * cps * cs1 - b1 * sps * sn1);
y_t = \text{real}(yc1 + a1 * cps * sn1 + b1 * sps * cs1);
\]
else
\[
x_t = \text{real}(xc1 - b1 * cps * sn1 + sps * a1 * cs1);
y_t = \text{real}(yc1 + b1 * cps * cs1 + sps * a1 * sn1);
\]
end
else
\[
 rp = \sqrt{1. + k1k2};
\]
\[ \text{rm} = \sqrt{1. - k1k2}; \]
\[ \text{ami} = \frac{1.}{\sqrt{2. \times (a_{12} \times a_{12} + (\lambda_{1} - a_{11})^2)}} \times a_{12}; \]
\[ \text{bmi} = \frac{1.}{\sqrt{2. \times (a_{12} \times a_{12} + (\lambda_{1} - a_{11})^2)}} \times (\lambda_{1} - a_{11}); \]
\[ \text{ama} = \text{cps} \times \left( \frac{\text{ami}}{\text{rp} + \text{bmi}} + \frac{\text{sps}}{\text{rm} - \text{bmi}} \right) + \text{sps} \times \left( \frac{\text{ami}}{\text{rm} - \text{bmi}} + \frac{\text{sps}}{\text{rp}} \right); \]
\[ \text{bma} = \text{cps} \times \left( \frac{\text{ami}}{\text{rp} - \text{bmi}} - \frac{\text{sps}}{\text{rm} + \text{bmi}} \right) - \text{sps} \times \left( \frac{\text{ami}}{\text{rm} + \text{bmi}} - \frac{\text{sps}}{\text{rp}} \right); \]
\[ \text{xt} = \text{real}(\text{xcl} + \text{ama} \times a_{1} \times \text{cs1} + \text{bma} \times (a_{1} - b_{1}) \times k_{1k2} \times \text{cs1} + \text{bma} \times b_{1} \times \text{cs2}); \]
\[ \text{yt} = \text{real}(\text{ycl} + \text{ama} \times a_{1} \times \text{sn1} + \text{bma} \times (a_{1} - b_{1}) \times k_{1k2} \times \text{sn1} + \text{bma} \times b_{1} \times \text{sn2}); \]