Comparison of Molecular and Gravitational Three-Body Collisions

by

Aaron Larner
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Abstract

The present work aims to compare and contrast the topological structure of two-dimensional three body collisions using a molecular and a gravitational potential. The study presents the results of computationally determined trajectories in the form of topological representations of the configuration space. These representations describe the outcome of different trajectories based on specific initial conditions.

Introduction

The three-body problem is one of the most conceptually simple, yet practically elusive problems in physics. A general solution predicts positions of the three particles at all future moments of time, given any initial configuration. Many approaches have been taken to solve the problem, but questions still remain unanswered. A practical general solution is yet to be found. The fairly recent technique of computational orbit calculations has shed light on to why no useful analytical solution has been found: “the orbits are good examples of chaos in nature, and deterministic series expansions are utterly unsuitable for their description.” [1]

The presented approach aims to characterize the topology of the two dimensional three-body problem for a specific subset of initial conditions via computational integration of trajectories. The approach is taken from *The Topology of Three Body Scattering* by P. Hut [2]. The purpose of this investigation is to compare the topological structure of computationally determined orbits using the gravitational potential and the Lennard Jones 6-12 potential.

The study is divided into three phases. The first phase was completed as an informatics and modeling certificate. The goal was to reproduce Hut’s results (with the gravitational potential) at higher resolution. Using the Wesleyan University computer cluster simulations were run extremely quickly. Later phases of the project aim to expand upon Huts study by looking at a more molecular like potential, and
then comparing its topology to that of the gravitational potential. A general solution of the three-body problem requires a complete set of solutions to the differential equation:

$$m_i \ddot{r}_i = -\frac{\partial}{\partial r_i} U(r_1, r_2, r_3)$$ (1)

The potential chosen is of the form:

$$U(r_1, r_2, r_3) = \sum_{i\neq j} \frac{A}{|r_i - r_j|^{12}} - \frac{Gm_im_j}{|r_i - r_j|^N}$$ (2)

In equation 2, $|r_i - r_j|$ represents the distance between the two particles. $A$ is a constant that scales the repulsive element of the potential. $G$ is the gravitational constant. Units are scaled such that $G$ is one. $m_i$ and $m_j$ are the masses of the two particles. $N$ is another constant and affects the range over which the particles interact. The smaller $N$, the larger the distance over which interaction occurs.

This potential differs from the gravitational potential in two ways. First, a repulsive element prevents the particles from getting too close to one another. This repulsive element takes the form of $(A/r_i^{12})$ in equation 2. Second, the exponent in the numerator of the $Gm_im_j$ term is variable. For a typical gravitational potential $N = 1$. $N$ is increased from 1 to 6 in the second phase. For $N = 6$, the potential is the Lennard-Jones 6-12 potential, which is commonly used to model molecular behavior in computational simulations. Finally, vibration and rotation are added to the binary.

A variety of topological plots are produced varying the ratio of vibrational to rotational frequency.

For each phase data is obtained for two different initial velocities of particle three ($v_3$). In the high velocity $v_3$ is set to twice the critical velocity ($v_3 = 2v_c$). The
critical velocity \((v_c)\) is defined to be the velocity of particle three such that the total energy of the system is zero. In the low velocity case \(v_3\) is set to half the critical velocity \((v_3 = 0.5v_c)\). Varying the velocity of particle three allows for observations to be made at both positive and negative total energies.
Background

Historically, the three-body problem has been studied for the most part in the context of the gravitational potential. The original concern that prompted investigation into the problem was that the solar system might not be stable, and at some point in the future the earth would be pulled into the sun or expelled out of the solar system. These concerns were strongest in the eighteenth century when the belief was that the earth was only a few thousand years old. This is significantly less of a concern now that we believe the earth to be 4-5 billion years old, and to have been in a stable orbit for the entirety of that time. [1]

The three-body problem is an obvious extension of the two-body problem, which was solved by Newton in 1687. Since Newton, there have been many solutions to the problem for specific initial conditions, but none provide an adequate solution to the general problem. These specific solutions involve assuming a very special subset of initial conditions and have been worked out by many different physicists including Lagrange, Jacobi, Tisserand, Hill, and Delaunay [Valtonen]. Karl Sudman solved the problem in 1912 “by providing a convergent power series solution valid for all values of time.” Unfortunately Sudman’s solution converges extremely slowly (too slow for any practical use) and “gives no qualitative information about the behavior of the system…” [3]

Debatably the most important contributor in the effort to solve the three-body problem was Poincaré. His fame came about when he was awarded the Oscar prize. Oscar II, King of Sweden and Norway sponsored a competition in 1887 for which the challenge was to find a solution for the general three-body problem. “The solution
was to be in the form of a series expansion which describes the positions of the three bodies at all future moments of time following an arbitrary starting configuration” [2]. Even though Poincaré didn’t solve the presented problem, he was still awarded the prize for his contributions to the subject. Among these contributions were important strides towards understanding chaotic systems.

Shortly after Sudman’s solution was published, researchers began to use computers for numerical step-by-step integration. This was the approach that Hut as well as many other researchers took, and it has lead to a better understanding of the nature of the problem. Hut looks at a subset of gravitational three body interactions with certain defining features:

1. Two of the three particles are initially bound in a circular orbit;
2. The third particle starts at a position infinitely far away from the center of mass of the bound system in the $x$ dimension, and a varying distance away from the center of mass of the bound system in the $y$ dimension;
3. The masses of all particles are equal;
4. The third particle is given an initial velocity ($v_3$) in the $x$ direction towards the binary pair;

These specifications greatly limit the dimensionality of the problem. Since the goal is to be able to visualize the topology, limiting the configuration space to two (or possibly three) dimensions is highly desirable. This configuration space is particularly relevant to the present work because it has physical significance at both the stellar and molecular levels. At the stellar level the configuration space models a single star interacting with a binary pair. At the molecular level the configuration space models a
single atom interacting with a diatomic molecule. A schematic diagram of Hut’s setup is shown in figure 1.

Figure 1.
Initial setup of each simulation. Particles 1 and 2 form a binary pair and particle 3 has a non-zero velocity towards the binary, coming from a large distance ($R$). $\phi$ is the angle between a line connecting the binary particles and the $x$-axis. $\rho$ is called the impact parameter and is defined to be the $y$ distance between the third particle and the center of mass of the binary pair. The binary pair is centered at the origin with binary members $r$ distance apart.

In order to characterize the topology, Hut limits the results of each interaction to one of four types: fly-by interaction, ionization event, dissociation event, and resonance interaction. The present work uses the same classification terminology except ionization events are re-labeled dissociation events. A more in-depth discussion of these types of collisions is presented in the next chapter.
Computational Techniques

The algorithm that is used for numerical integration is the Hermite Scheme. The Hermite Scheme gives future positions and velocities in time based on current values of position, velocity, acceleration, and jerk. Equations 3 and 4 describe the algorithm.

\[ r_{i+1} = r_i + \frac{1}{2} (v_i + v_{i+1})(dt) + \frac{1}{12} (a_i - a_{i+1})(dt)^2 \] (3)

\[ v_{i+1} = v_i + \frac{1}{2} (a_i + a_{i+1})(dt) + \frac{1}{12} (j_i - j_{i+1})(dt)^2 \] (4)

In equations 3 and 4, \( r \) is the position of a particle. \( v \) is the particles velocity and \( a \) is the particles acceleration. Finally, \( j \) is the particles “jerk” or “jolt.” Each variable is subscripted with a value that represents which time step it belongs to. \( i \) refers to the variables value at time \( t \) while \( i+1 \) refers to its value at time \( t+dt \). Since the investigation is of the two dimensional three-body problem, each equation is applied six times, once for each particle in each dimension. The Hermite Scheme is a fourth order integrator, so a reduction by one half in the time step yields results that are sixteen times more accurate. The code written is based on a Hermite Scheme integrator taken from [http://www.artcompsci.org][4] and adapted to fit the specific configuration space under investigation.

A few obstacles are encountered while using the Hermite scheme. First, equation 4 requires the jerk of each particle. This is simply the third derivative of position with respect to time. The potential (defined in equation 2) is differentiated with respect to the position \( r \) to obtain the force. Using the force, the acceleration is
calculated via Newton’s second law. Finally the acceleration is differentiated with respect to time to obtain the jerk.

\[
\vec{j} = \frac{NGm}{|r|^{N+2}} \left[ \vec{v} - \frac{\vec{r}(N + 2)(r_x v_x + r_y v_y)}{|r|^2} \right] - \frac{12A}{m|r|^{14}} \left[ \vec{v} - \frac{14\vec{r}(r_x v_x + r_y v_y)}{|r|^2} \right]
\]  

(5)

Furthermore, the future value of velocity is required in order to calculate the future value of position (notice \(v_{i+1}\) appears in the equation for \(r_{i+1}\)). Similarly, the future value of acceleration is required to calculate the future value of velocity. A Taylor series is used to obtain these values.

\[
r_{i+1} = (r_i) + (v_i)(dt) + \frac{1}{2}(a_i)(dt)^2 + \frac{1}{6}(j_i)(dt)^3
\]  

(6)

\[
v_{i+1} = (v_i) + (a_i)(dt) + \frac{1}{2}(j_i)(dt)^2
\]  

(7)

All values in the Taylor series equations above are in terms of current values (subscripted \(i\)), not future values. These Taylor series approximations are used to calculate the future value of the jerk \((j_{i+1})\) via equation 5. Finally, all calculated values \((v_{i+1}, a_{i+1} \text{ and } j_{i+1})\) are used to calculate more accurate future values for \(r\) and \(v\) using equations 3 and 4. \([4]\)

A variable time step algorithm is used to improve integration speed and accuracy. If the velocity of a particle is very small, by definition its position is changing slowly with respect to time. If this is the case, it is unnecessary to use a small time step, because computational time can be saved with very little loss of accuracy by using a larger one. Conversely, if the particles are moving quickly, smaller time steps are required in order to ensure accuracy. Furthermore, it is more difficult to integrate trajectories when the particles are very close to one another and
the time step should be reduced to maintain accuracy. The equation that is used to calculate the time step takes into accounts all of these factors.

$$dt = \varepsilon \min_{\{i,j\}} \left| \frac{r_i - r_j}{v_i - v_j} \right|$$  \hspace{1cm} (8)

The equation states that the time step $dt$ will be a scaling constant $\varepsilon$ multiplied by the minimum of the distance between two particles divided by their relative velocity, for all possible pairs of particles. Implementing this technique is very computationally inexpensive because it fits nicely into a loop that is already used in the implementation of the Hermite algorithm. The variable time step algorithm is taken from one of Hut’s previous publications [5]. Its advantages are most prevalent in complicated (usually low energy) trajectories where much of the collision time is spent in a semi-resonant state.

Unfortunately this technique does not work in all cases. With near zero relative velocities the time step shoots up and causes an unacceptably high energy error. Care is taken while implementing the algorithm to ensure that the time step value will never exceed a maximum value, even for very small relative velocities.

The final, and probably most challenging computational hurdle is developing an algorithm to detect the result of each simulation. Developing this algorithm involves answering two related questions. First, “how do we know when the simulation is over?” Second, “what is the result when the simulation is complete?”

To answer the first question, “how do we know when the simulation is over?” the root of the mean square distance is calculated. The mean square distance is the average of the squares of the distances between all particles. Its root is given by $s$.  

10
\[ s(t) = \left[ \frac{1}{3} \sum_{i<j} |r_i(t) - r_j(t)| \right]^\frac{1}{2} \]  

(9)

The first thought is to only start checking for an end result once as much time has been spent after the first minimum in \( s \) is reached, as before it is reached. This makes sense because most high-energy collisions only have one minimum, so it is reasonable to assume that the minimum occurs half way through the interaction. This method does work for the high-energy simulations, however, it fails in the low-energy cases. This is because low-energy interactions are extremely variable, and particles become bound and then unbound many times over short periods. Therefore, if the algorithm begins checking while the particles are still interacting, the outcome is not accurate.

To deal with this issue, the algorithm is modified. Instead of starting to check for end conditions after an equal amount of time is spent after the first minimum as before it, the algorithm starts looking for an end condition after an equal amount of time is spent after the current minimum as before it. For example, say the system hits its first minimum at \( t = 10 \) and then hits another minimum at \( t = 15 \). Using the original algorithm, the program starts to look for an end condition at \( t = 20 \). Using the modified algorithm the program starts to look for an end condition at \( t = 30 \). This solves the problem of halting the simulation while the particles are still interacting because as the particles interact, \( s \) hits more and more minima. As the number of minima in \( s \) increases, the time required before the program starts to look for an end condition grows longer.
So what is an “end condition?” An end condition is the answer to the second question, “what is the result when the simulation is complete?” and involves looking at the energy of each of the three pairs of particles (\{1, 2\}, \{1, 3\}, \{2, 3\}). For each pair the algorithm asks: “are these particles bound?” (i.e. is their total energy with respect to one another negative). When this question evaluates to “true,” one might believe that the question is answered. However, the third particle cannot be ignored. Because of the nature of the problem, two particles can be bound at one instant and unbound the next if the third particle transfers energy to one or more of them. To deal with this issue, a modified total energy \(E_m\) is considered. This modified energy represents the total energy of the two particles with respect to one another if the particle not in the pair were to give all of its potential energy to the pair. The equation is shown below for an arbitrary pair of particles \{a, b\}:

\[
E_m = K_a + K_b + U_{ab} - U_{ac} - U_{bc}
\]  

\(K\) is the kinetic energy of the subscripted particle. \(U\) is the potential energy of the subscripted pair of particles. \(E_m\) provides an upper bound for the energy of the pair, so if this energy is negative then one can be confident that the pair is currently bound and will remain bound.

In order to characterize the topology, interactions are limited to one of four types. If the initial configuration is unchanged (i.e particles one and two are bound and particle three is unbound) the interaction is labeled a fly-by interaction. An interaction is labeled as a fly-by if \(E_m < 0\) for the pair \{1, 2\} and \(E_m > 0\) for all other possible pairs of particles. If \(\rho\) is very large and the potential declines with distance (as is the case for the gravitational and Lennard Jones 6-12 potential), then the third
particle may pass the binary pair without ever interacting at all. In fact, if $v_3 \neq 0$ there exists a value $\rho^+$ such that all trajectories where $\rho > \rho^+$ result in a fly-by interaction.

Similarly, there exists a value $\rho^-$ such that all trajectories where $\rho < \rho^-$ result in a fly-by interaction. The region between the largest possible value of $\rho^-$ and the smallest possible value of $\rho^+$ for a given configuration space is labeled the \textit{dynamic region}. While most fly-by interactions occur outside the dynamic region, a limited number occur within the dynamic region. A typical fly-by trajectory is shown in figure 2.

The second type of interaction occurs when the third particle collides into the binary system with enough energy to break the entire system apart, leaving all three

![Figure 2](image.png)

The above figure shows the trajectory for a \textit{fly-by interaction} in the $x$-$y$ plane. The initial binary particles (red and black) remain bound, while the third particle (green) flies past with minimal disruption.
Figure 3. The above figure shows the trajectory for a dissociation event in the x-y plane. All three particles are split apart due to the impact of particle 3 (green). This type of result is only possible if $v_c > 1$.

particles unbound. Hut calls this interaction an ionization event, but is labeled a dissociation event in the present work. Dissociation events only occur when the energy of the entire system is positive. Interactions are labeled as dissociation events if $E_m > 0$ for all possible pairs of particles.

A third type of interaction occurs when particle three becomes bound to one of the original binary particles during the collision. The other original binary particle becomes unbound. This is called an exchange event. There are two types of exchange events. Particle three can become bound to particle two, leaving particle one unbound. This is a type I exchange. Alternatively, particle three can become bound to particle one, leaving particle two unbound. This is a type II exchange. Interactions are labeled as type I exchange events if $E_m < 0$ for the pair $\{2, 3\}$ and $E_m > 0$ for all other possible pairs. Interactions are labeled as type II exchange events if $E_m < 0$ for the pair $\{1, 3\}$ and $E_m > 0$ for all other possible pairs.
Figure 4. Example of a type I exchange in the $x$–$y$ plane. Particle 3 switches places with one of the binary particles. In this case particle 2 (red) is replaced, and becomes unbound.

Figure 5. Example of a resonance interaction. All three particles (depicted in black, red, and green) remain bound for an extended period of time.

Finally, all three particles can remain bound. The probability that all three particles are permanently bound is zero, however, in some interactions they are bound for an extended period of time. After a certain amount of time spent in resonance, the simulations are too computationally expensive to find the “true” result, and are simply labeled resonance interactions. Resonance interactions can only occur when
Very few cases are encountered in which integration cannot be completed due to this issue in the present work, so this category of results is less important.

To determine when a resonance interaction occurs, a slightly different method is used. For each minimum in $s$ that is encountered during a given simulation, a counter is incremented. If this counter exceeds a preset value (typically 300) then the simulation is halted and the result is recorded as a resonance interaction. The idea behind this solution is that in quasi-resonant states the particles are continually colliding with one another and incrementing the counter frequently. Therefore the counter provides a good indication of how long the system has been resonating. The number of minima in $s$ is important for data analysis and will be referred to in future sections. It should be noted that Hut uses this same method to determine resonance interactions, however he ends interactions after only 2 minima in $s$ as opposed to 300.

Two other results are coded into the algorithm to prevent practical problems. The first aims to prevent the simulation from running on forever if none of the conditions are ever met. This is done by halting the integration if the number of time steps ever exceeds a maximum value (100,000,000). The second result aims to highlight poor simulations by halting integration if the total energy error exceeds a threshold value (0.1%). The total percent energy error was calculated for each time step, so this check is not difficult to implement.
The first task is to reproduce Hut’s work described in *The Topology of Three-Body Scattering*. The initial setup for the simulations is pictured in figure 1 and exactly mimics Hut’s initial conditions except for a differing value of R. Data is calculated at six different velocities ($16v_c$, $8v_c$, $4v_c$, $2v_c$, $v_c$, and $0.5v_c$). All subsequent molecular studies are done at $2v_c$ and $0.5v_c$. Only those velocities are shown for the gravitational collisions below. In the color figures black points represent type I exchanges, red points represent type II exchanges, green points represent dissociation interactions, blue points represent resonance interactions, and yellow points are simulations that failed to meet the energy conservation requirement. White space represents fly-by interactions. Hut’s original data are also included for comparison purposes. The new figures are done at significantly higher resolution and have a stricter energy error requirement. Hut requires trajectories to conserve energy to within 1% of the initial energy of the system, ten times higher than the requirement used for this work. Hut’s figures distinguish between different types of outcomes by symbols as opposed to colors. For the reader’s reference:

- “*” represents a dissociation event (equivalent to green points)
- “1” represents a type I exchange (equivalent to black points)
- “–” represents a type II exchange (equivalent to red points)
- “@” represents a resonance interaction (equivalent to blue points)

It should be noted that the rotational phases do not line up perfectly. This is because a different starting distance (R) is used. In the present work, particle three is backed up to a distance $1000r$ away from the binary. Hut uses a trick in order to allow particle
Figure 6.
A comparison of data for gravitational scattering in the high velocity case ($v_3 = 2v_c$). Current results are shown at top. Hut's results are shown at bottom. Black and red points represent exchanges and green points represent dissociation interactions. White points represent fly-by interactions. Finally, yellow points represent trajectories that failed to conserve energy.
Figure 7. A comparison of data for gravitational scattering in the low velocity case ($v_\beta = 0.5 v_c$). Current results are shown at top. Hut’s results are shown at bottom. Black and red points represent exchanges. White points represent fly-by interactions. Finally, yellow points represent trajectories that failed to conserve energy.
three to start closer to the binary \((40r)\) while still maintaining a velocity and \(y\) position that mimic a particle that started an infinite \(x\)-distance away from the center of mass of the binary pair. To achieve this goal, Hut approximates the trajectory of particle three in the limit where the binary pair acts as a single mass. This transforms the situation into a two-body problem, which is analytically solved. Using this estimate Hut is able to make a good prediction of where particle three will be after falling from an infinite distance towards the binary pair. The use of this technique was unnecessary in the present work because more computational power allows for integration from very large distances fairly quickly. The differing approaches cause a phase shift in the high velocity case of about \(\pi\) radians. The data line up fairly well in the low velocity case by chance.

The advantage of the higher resolution images is highlighted in the high velocity case. Because of the higher resolution, small features in the topology can be seen that are lost in the lower resolution figures. For example, there is a small region of dissociation interactions within the large exchange regions in figure 6 (top) that is apparent in the higher resolution data. Similar features are visible in the higher resolution data for other values of \(v_3\) (not shown) as well.

The lower threshold requirement for energy conservation however, seems to have little effect on the overall structure of the topology. This is a reassuring fact. If the topology changes dramatically after a decrease in the error requirement threshold for energy conservation, the validity of all the points is questionable. After all, if a 10 fold reduction in the energy error requirement caused dramatic changes, what is to say that another 10 fold reduction won’t further change the topology? The static
nature of the topology when the error threshold is reduced provides confidence that the data are reliable.

Unfortunately the lower energy conservation threshold leaves many points undetermined in the low energy simulations. In an attempt to describe the structure of these undetermined points, Individual trajectories are compared within the solid yellow regions. These regions represent areas where numerical integration is extremely difficult. The common attribute amongst these trajectories is nearly head on collisions between one or more particles. These trajectories are difficult to integrate because at close distances, the position and velocity of the particles change quickly. The variable time step algorithm partly solves this problem, but in head on collisions, $dt$ must be reduced so much that either round-off error causes undetermined points, or the variable time step algorithm simply fails to reduce the time step enough to ensure energy conservation. Fortunately, the gravitational potential is unique in this regard. Adding a repulsive term to the potential prevents many of the energy conservation issues.

Two prominent features stand out in the topological maps (figures 6 and 7). In the high velocity case dissociation interactions are possible and fairly prevalent. In the low velocity case granular regions (mostly yellow but with red, black and white points present as well) are highly prevalent. These granular regions are believed to be chaotic. Dissociation interactions are missing in the low velocity case because particle three is not given enough energy to break the system apart.
Varying the Exponent $N$ – Low Velocity

Obtaining data for this phase is considerably easier than the last because reasonable initial conditions are obvious and very little code modification is necessary. While varying the exponent $N$ in equation 2, binary particles are set to be initially stationary. Particles neither vibrate nor rotate initially. Furthermore, the repulsive part of the potential prevents a lot of issues that are caused by the strictly gravitational potential because there are no extremely close “head-on” encounters (little to no angular momentum) after the repulsive term is introduced. The potential used conveniently establishes a minimum distance that the particles can reach before they repel each other. Simulations are done for high and low energy cases ($v_3=2v_c$ and $v_3=0.5v_c$ respectively), and for $N$ values of 1, 2, 4, and 6. The low velocity results are shown in figures 8 through 11. In the figures, black and red points both represent exchange reactions (black points represent type I exchanges, red points represent type II exchanges). Green points represent dissociation events. Blue points depict resonance reactions. Finally, yellow points show trajectories that fail to satisfy the energy error requirement. Yellow points are discussed in further detail below.

In the low energy case there are several notable observations. First, the cross section for exchanges increases as $N$ decreases. This is to be expected; for higher values of $N$ the magnitude of the potential approaches zero more quickly as $r$ is increased. This means that for higher values of $\rho$, particle 3 is less likely to interact with the binary when $N$ is high.
Figure 8 shows the topology for $N = 6$ at $v_3 = 0.5v_c$. Black points represent type I exchanges. Red points represent type II exchanges. Blue points represent resonance interactions. Yellow points represent trajectories that failed to conserve energy.

Figure 9 shows the topology for $N = 4$ at $v_3 = 0.5v_c$. Black points represent type I exchanges. Red points represent type II exchanges. Blue points represent resonance interactions. Yellow points represent trajectories that failed to conserve energy.
Figure 10 shows the topology for $N = 2$ at $v_3 = 0.5v_c$. Black points represent type I exchanges. Red points represent type II exchanges. Blue points represent resonance interactions. Yellow points represent trajectories that failed to conserve energy.

Figure 11 shows the topology for $N = 1$ at $v_3 = 0.5v_c$. Black points represent type I exchanges. Red points represent type II exchanges. Blue points represent resonance interactions. Yellow points represent trajectories that failed to conserve energy.
Another interesting set of features that is investigated is the fly-by regions that are buried within the dynamic region. As $N$ decreases from 6 to 1, these regions grow, and somewhere between $N = 4$ and $N = 2$, these regions “break through” the boundary and become connected with the area where “typical” fly-by interactions are found.

“Typical” fly-by interactions are found at large values of $\rho$ in which particle 3 has little to no effect on the original binary pair. The trajectories that make up these atypical fly-by regions have an interesting property. They always have exactly two minima in the mean square distance (equation 9) for $N = 4$ and $N = 6$, and have exactly one minimum in the mean square distance for $N = 2$ and $N = 1$. As soon as these islands “break though” the boundary between the “typical” fly-by regions and the dynamic region they assume the properties of the region to which they are connected (i.e. only one minimum). However, while they are still contained within

![Figure 12](image_url)

This figure gives an example of two typical trajectories found within the fly-by regions buried within the interactive region. The trajectories are plotted in the x-y plane. Green represents particle three’s path. Similarly black and red represent one and two’s trajectories respectively. For $N = 4$ and 6 typical trajectories exhibit a double bounce feature (two minima). For $N = 1$ and 2 the regions break through the interactive region boundary and typical trajectories only exhibit one minimum. Arrows denote movement direction.
the dynamic region they always have exactly two minima.

Further investigation into this phenomenon shows that in a typical trajectory, particle 3 is pulled towards and then bounces off of one of the binary particles. It is then pulled in by the second binary particle and bounces off of this particle as well. As \( N \) is decreased, this characteristic trajectory becomes less pronounced, until it resembles a typical fly-by interaction with only one minimum. Typical trajectories in these regions for \( N = 6 \) and \( N = 1 \) are shown in figure 12. It should be noted that trajectories in the regions under investigation are unusual because the average number of minima for fly-by interactions in the dynamic region ranges between 24 and 41 depending on \( N \).

Similar generalizations can be made about the solid regions of red and black. For example, all clearly visible regions of red and black have exactly one minimum. There is also some structure that is less discernible in the above figures, but which represents small regions with two minima. The regions with two minima are most prevalent at low \( N \), and are non-existent for \( N = 6 \).

Finally, it appears that resonance interactions are more highly concentrated at high \( \rho \). For \( N = 1 \) and \( N = 6 \) the resonant trajectories (depicted by blue points) are clustered around the boundary of the dynamic region and the fly-by region. This observation prompts a closer look at how the number of minima varies as a function of \( \rho \). Data are divided into 10 equally spaced bins, and the average number of minima in each bin is calculated. To prevent skewed data, only points for which the number of minima is greater than two are considered. Specifically, the pure exchange/fly-by
regions are ignored and the remaining granular regions are considered. Histograms of this data show peaks that vary depending on the value of $N$. When $N$ is 4 or 6, the histogram peaks at the edge of the interaction zone ($\rho = \pm 2.65$ and $\rho = \pm 2.15$ respectively). For $N=2$ the data peaks at $\rho = \pm 1.2$. For $N=1$ there is a set of major peaks at the edge of the interaction zone ($\rho = \pm 3.7$), and a set of minor peaks at $\rho = \pm 2.0$. The composite histogram is shown in figure 13.

![Histogram](image)

**Figure 13.**

This histogram shows the average number of minima, binned from the lower to upper interactive boundary for different values of $N$. To avoid skewing the results from fly-by and exchange regions (number of minima always less than three), only points where the number of minima was greater than two were considered.

It is necessary to briefly discuss the points that fail to converge (depicted in yellow in figures 8-11). Individual trajectories for points in yellow regions, specifically those passing through the islands of red and black, are observed. These points represent exchanges in which energy conservation fails before end conditions
are tested. With a larger computational investment it is likely that these points would be computationally determined. However, investigating other aspects of the problem take precedence over computationally determining the result for these few points.

Related to the yellow regions are the granular regions that make up much of the dynamic region. These trajectories in the granular regions are computationally expensive to calculate much like the trajectories that fail to meet energy conservation requirements. These regions are observed in the strictly gravitational case as well, and are believed to represent chaotic trajectories. This claim is supported by the fact that they have many times more minima in $s$ than the solid regions. Trajectories with many minima in $s$ are observed to resonate for an extended period of time before the result of the trajectory is resolved. Small changes in initial conditions at the start of these trajectories are more likely to cause differing outcomes because of the time spent in resonance.
Varying the Exponent $N$ – High Velocity

There is considerably less going on in the high-energy case. Because of
the nature of high energy collisions, dissociation events are possible and fairly
prevalent. Table 1 shows the percent values for each type of result over the range $\rho = -1.43$ to $+1.43$. A notable difference between the high and low energy cases is that the
height of the dynamic region varies in the low energy case but is essentially constant
in the high energy case.

<table>
<thead>
<tr>
<th>$N$</th>
<th>Exchange (Type 1)</th>
<th>Exchange (Type 2)</th>
<th>Dissociation</th>
<th>Fly-by</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>21.36 %</td>
<td>21.36 %</td>
<td>33.37 %</td>
<td>23.91 %</td>
</tr>
<tr>
<td>2</td>
<td>20.29 %</td>
<td>20.29 %</td>
<td>36.23 %</td>
<td>23.19 %</td>
</tr>
<tr>
<td>4</td>
<td>17.94 %</td>
<td>17.94 %</td>
<td>38.93 %</td>
<td>25.19 %</td>
</tr>
<tr>
<td>6</td>
<td>16.61 %</td>
<td>16.61 %</td>
<td>38.74 %</td>
<td>28.00 %</td>
</tr>
</tbody>
</table>

Table 1. Shows proportions of each type of interaction within the dynamic region.

A notable difference between the high and low energy cases is that while the
number of minima for a given interaction in the low energy case can vary from 1 to
over 300, the number of minima in any given interaction for the high energy case is
strictly 1. It doesn’t matter whether the reaction is an exchange, dissociation, or fly-by.

Although the number of minima doesn’t give any new information about the
different topological regions in the high energy case ($v_3 = 2v_c$), distinctions can be
made. For each value of $N$ there are the two types of exchanges (type I and type II).
However, there are also two sub-categories within each type of exchange. They
Figure 14 shows the topology for $N = 6$ at $v_3 = 2v_c$. Black points represent type I exchanges. Red points represent type II exchanges. Blue points represent resonance interactions. Yellow points represent trajectories that failed to conserve energy.

Figure 15 shows the topology for $N = 4$ at $v_3 = 2v_c$. Black points represent type I exchanges. Red points represent type II exchanges. Blue points represent resonance interactions. Yellow points represent trajectories that failed to conserve energy.
Figure 16 shows the topology for $N = 2$ at $v_3 = 2v_c$. Black points represent type I exchanges. Red points represent type II exchanges. Blue points represent resonance interactions. Yellow points represent trajectories that failed to conserve energy.

Figure 17 shows the topology for $N = 1$ at $v_3 = 2v_c$. Black points represent type I exchanges. Red points represent type II exchanges. Blue points represent resonance interactions. Yellow points represent trajectories that failed to conserve energy.
This figure gives an example of two different sub categories of type two exchanges. The trajectories for particle 1 (black), particle 2 (red) and particle 3 (green) are pictured in both cases. The image on the left depicts a typical trajectory for the region A in figure 17. Particle three is immediately captured by particle two. The image on the right depicts a typical trajectory for region B. Particle three bounces off of particle one and is subsequently captured by particle two. Arrows denote the direction of motion. Dots denote starting positions.

manifest themselves in the two differing types of exchange regions. There is an elongated diagonal strip in the center of each figure (labeled region A in figure 17), and two more distorted regions at either side of the elongated region (labeled region B in figure 17). These differing regions represent two distinctly different types of collisions.

The distinguishing factor between region A and region B is with which binary pair the third particle initially interacts. For example, in all type II exchanges the end result is that particle three is bound with particle two, and particle one is unbound. However, in the region B particle three has its closest approach with particle one, bounces off, and finally becomes bound with particle two. Alternatively, in region A
particle three interacts with particle two from the start and they become bound immediately. Example trajectories are shown in figure 18.
Vibrating Rotating Binary

In the vibrating rotating case the ratio of vibrational to rotational frequency was varied from 5 to 290. Data collection over such a large range is necessary because the topology is dramatically affected by this ratio. $N$ is fixed at 6 for this phase so that the amount of data is manageable, and to mimic a molecular potential. The topology is somewhat symmetrical when there is no rotation in the binary pair. It then becomes asymmetric as rotational energy is added to the binary. Finally, as the limit of rotational velocity is reached, the topology becomes nearly symmetrical about the $\phi$ axis. In addition to an investigation of this phenomenon, notes on how the number of minima in the mean square distance is affected by the addition of rotational energy to the initial configuration are included. Finally, a discussion on how the percentage of exchanges varies as a function of rotational energy is presented. All presented figures are for the low velocity case ($v_3 = 0.5v_c$).

At very low rotational energy (figure 19), the topology within the dynamic region is not symmetric, but the overall shape of the dynamic region is symmetric across the $\phi$ axis. As rotational energy is added to the binary system, the topology becomes asymmetric. Finally, as the limit of rotational energy is reached (past this point the binary is not bound) the topology becomes completely symmetric about the $\phi$ axis. Even the structure inside the dynamic region is symmetric. To understand the progression as rotational energy is added to binary system, the rotational adiabaticity of the system is considered. An adiabatic collision is one in which energy transfer is inefficient. In the adiabatic limit the duration of the collision is long compared to the
Figure 19. Shown above is a topology plot for a vibration to rotation frequency ratio of 290 to 1. This corresponds to a binary tangential velocity of 0.01 and a displacement in $r$ of +0.02. All units are scaled such that the gravitational constant is one.

Figure 20. Shown above is a topology plot for a vibration-rotation frequency ratio of 29 to 1. This corresponds to a binary tangential velocity of 0.1 and a displacement in $r$ of +0.02. All units are scaled such that the gravitational constant is one.
Figure 21. Shown above is a topology plot for a vibration-rotation frequency ratio of 14 to 1. This corresponds to a binary tangential velocity of 0.2 and a displacement in $r$ of +0.02. All units are scaled such that the gravitational constant is one.

Figure 22. Shown above is a topology plot for a vibration-rotation frequency ratio of 8 to 1. This corresponds to a binary tangential velocity of 0.3340 and a displacement in $r$ of +0.02. All units are scaled such that the gravitational constant is one.
Figure 23. Shown above is a topology plot for a vibration-rotation frequency ratio of 6 to 1. This corresponds to a binary tangential velocity of 0.43 and a displacement in $r$ of +0.02. All units are scaled such that the gravitational constant is one.

Figure 24. Shown above is a topology plot for a vibration-rotation frequency ratio of 5 to 1. This corresponds to a binary tangential velocity of 0.473 and a displacement in $r$ of +0.02. All units are scaled such that the gravitational constant is one.
period of rotation. The adiabaticity parameter ($\xi$) describes how close the collision is to this limit and is defined to be:

$$\xi = \frac{t_c}{t_r}$$

where $t_c$ is the collision time and $t_r$ is the rotational period. If $\xi > 1$ then the collision is entering the adiabatic regime. [6]

The idea is that when $t_r$ is very large the topology appears semi-symmetric because the rotational contribution to the relative speed between particle three and the binary particle that it interacts with is small. Therefore, the difference between a collision in which the binary particle is moving towards particle three ($\rho < 0$) and a collision in which the binary particle is moving away from particle three ($\rho > 0$) is small. As the rotational velocity increases, this distinction becomes more and more significant, and the topology is distorted. This causes the asymmetry seen in figures 20 and 21. Finally, as the rotational period becomes so small that collisions become adiabatic, horizontal symmetry is established.

Calculating the collision time is non-trivial. There is no standard way to do this. However, there are two intuitive approaches. For each simulation, the time between the first and last minima in $s$ is recorded. This value is the resonance time. The resonance time provides a measure of the collision time. Unfortunately, for collisions in which there is only one minimum, this value is zero. Furthermore, the resonance time only accounts for time after the first minimum and before the last. This is equivalent to assuming that the collision starts at the first minimum and ends at the last, when it in fact starts before the fist minimum and ends after the last. For
these reasons, the resonance time provides a lower limit for $t_c$. Another technique for determining the collision time involves looking at the potential energy of the system as a function of time. This function peaks as the collision occurs. The peak has a width that relates to the collision time. Using the full-width half-max of this peak is a reasonable way to determine the collision time. The disadvantage of this approach is that it requires analysis of thousands individual trajectories, one by one. Figure 25 shows an example plot of the potential energy as a function of time for an interaction with multiple minima in $s$.

![Figure 25](image.png)

The above plot shows an example of the potential energy as a function of time for an interaction with multiple minima in $s$. The collision time is set to be the full width at half maximum.

Both methods are used in conjunction. A limited number of individual trajectories are examined and the value for the collision time obtained using both
methods is compared. Taking the difference of the two values, a correction constant (3.75 scaled time units) is calculated for the resonance time. The resonance time values are then corrected by adding this constant. This gives a more accurate value for the collision time, without requiring analysis of an unreasonable number of individual trajectories. As the rotational energy is increased, the adiabaticity parameter increases as well. The data are shown in figure 26. Although $\xi$ never exceeds 0.7 (suggesting that the collisions are not adiabatic), none of the figures are completely symmetrical. Figure 24, which has the highest rotational velocity, is symmetrical about the line $\rho = 0.21$, not the line $\rho = 0.0$. It is expected that as the rotational velocity is further increased, $\xi$ exceeds 1. Furthermore, because the collision time is ill defined, using a different method (or different correction constant) would yield different numerical results. However, it is clear that as rotational energy is added to the binary system, the adiabaticity increases, and the topology becomes more symmetrical.
Shown above is the adiabaticity parameter as a function of rotational velocity. The rotational velocity refers to the tangential velocity that the binary particles are given initially.

Looking at the number of minima for the figures 19-21, similar conclusions are reached as those described in chapter where $N$ is varied. All solid colored regions have either one or two minima in $s$. Solid regions that represent exchanges (depicted in red and black) have exactly one minimum and solid regions that represent fly-by interactions (depicted in white) that are within the dynamic region have exactly two minima. As is true for all the data, the two regions of fly-by interactions above and below the dynamic region all have one minimum.

However, in the high rotational energy cases (figures 22-24) these rules don’t necessarily hold true. As the rotational energy is increased, the solid exchange regions begin to contain trajectories for which the number of minima is greater than one. This

Figure 27.
This figure shows and overlay of minima information on top of figure 24. The same vibration-rotation frequency ratio of 5 to 1 is used. This corresponds to a binary tangential velocity of 0.473 and a displacement in $r$ of +0.02. All units are scaled such that the gravitational constant is one. Pink points represent trajectories with one minimum. Orange points represent trajectories with two minima. The figure highlights solid regions that have more than two minima, a feature that is not prevalent in other topologies. Phenomenon is shown in figure 27. The number of minima associated with each point is overlaid on figure 24 (pink represents points with 1 minimum, orange represents points with two minima) to produce figure 27. Figure 24 starts with a binary pair in a 5:1 vibration to rotation frequency. Notice that there are solid exchange regions (depicted in red and black) that are visible even with the overlay; obscuring all points with two or less minima in $s$. This suggests that these regions have more than two minima in $s$. For no other initial conditions have solid regions with more than two minima been observed. Furthermore, some solid regions switch from one minimum to two abruptly. This feature is also missing in the lower rotational energy figures.

In his paper *Effect of Reagent Rotation on Elementary Bimolecular Exchange Reactions*, Sathyamurthy claims that “For most of the direct reactions, there is an initial decline in $\sigma(J)$ followed by an increase and possibly a leveling off.” [7] The presented results are compared to Sathyamurthy’s results but appear to differ. An initial small decline is observed, followed by a slight rise, and then an additional decline in the percentage of exchanges as a function of rotational energy. Figure 28 illustrates this point.
Figure 28. Shown above is the percentage of exchange reactions as a function of initial rotational velocity.
Summary

Comparisons between results that use the gravitational potential and results that use the Lennard Jones 6-12 potential are not easy to make. Because there are so many free parameters in the problem, it is difficult to find values for each parameter that make the system behave (at least initially) like its molecular or gravitational counterpart. Parameters like vibrational energy, rotational energy, and even the magnitude of the repulsive force in the Lennard Jones potential are all variable quantities and require one to make specific decisions about their value. These decisions were by no means empirical or objective. A completely objective study would require one to vary all of these parameters and it would be nearly impossible to take in all of the information.

Practical restrictions limited some of these choices. For example in order to define a critical velocity ($v_c$) the energy of the binary pair cannot be positive. In the vibrating rotating case, it is actually possible to have a binary with positive energy because the effective potential peaks above zero. Therefore, in order for the critical velocity to be defined, the rotational energy of the binary was limited. This is why data was not taken for vibration to rotation ratios of less than 5 to 1. It would have been nice to take data for 2:1, or 1:1 ratios because they would more closely resemble the gravitational case but with the parameters that are chosen, this is impossible.

Nonetheless, general comparisons can be made between the two cases. In both the gravitational and molecular cases, granular regions appear in the low velocity cases. In both cases these granular regions consist of type I exchanges, type II exchanges, and fly-by interactions. In both cases these regions represent initial
parameters that lead to highly tangled trajectories with many minima in $s$. It is likely that these regions are chaotic.

There are similarities between the high velocity, non-vibrating, non-rotating case where the Lennard Jones potential is used (figure 17) and the high velocity gravitational case (figure 6) as well. In both cases dissociation interactions are prevalent in the dynamic region. Furthermore, in both cases there are two differing regions for each type of exchange (notice two distinctly different black shapes in each figure).

Obviously there are many differences as well. The most notable is that in the low velocity, high rotational energy Lennard Jones cases, some solid regions have more than two minima in $s$. This is observed in neither the gravitational case nor lower rotational energy molecular cases.

Comparisons of the topological structure for the gravitational and molecular potentials are limited to these observations. Further similarities may exist, but possibly require more similar initial configurations to be observed. For example, in the low velocity gravitational case the topology is asymmetrical about the $\phi$ axis (figure 7). This same observation is made in the low velocity, medium rotational energy, vibrating rotating molecular case (figures 20 and 21). However, as the rotational velocity of the binary is increase in the later case, the topology becomes more any more symmetrical about the $\phi$ axis. Increasing the velocity of binary members in the gravitational case may expose similar behavior.
Given more time there are many specific areas of interest that can be explored further. Four areas are particularly interesting to me. First, I would like to study the granular regions that appear in all low velocity figures in more depth. I suspect that these regions are chaotic, and would like to obtain data with a lower energy error threshold to see how the points in these regions are affected by an increase in precision. Second, a more in-depth examination of how the average number of minima in the mean square distance varies as a function of $\rho$ would be enlightening. Figure 13 highlights many interesting features as $N$ is varied and it would be interesting to see the differences when rotational period and vibrational period are varied as well. Third, an investigation into the adiabaticity of the gravitational case might shed some light on how symmetry in the figures is established. It would be interesting to see if symmetry would be re-established in the low velocity gravitational case if the rotational velocity of the binary were increased. Finally, an investigation into elliptical orbits in the gravitational case would not only provide insight into the gravitational problem, but also allow for closer comparisons between the molecular and gravitational cases.
Bibliography


