The Formation of Particle Lumps in N-Body Systems

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In several fields of physics it is often of great interest to study systems of interacting particles. Consequently, there exist equations describing the states of these systems. One of these equations is the Virial Theorem which relates the kinetic energy and the potential energy of such systems. Particle systems are, however, most often studied with the purpose of determining how particles with a specific way of interacting with each other behave. On the contrary, this study compares systems where the potential energy of a bond between particles is proportional to r^n, where n is the independent variable in this study and r is the distance between particles. The potential and kinetic energy of the system are studied and compared to the Virial Theorem and their ratio is related to the formation of particle lumps. Namely, the Virial Theorem predicts that the most favorable condition for particle lump formation is when $n = -2$. By comparing the predictions of the Virial Theorem and numerical simulations of particles, this study has shown that predictions of the Virial Theorem match well with the simulations, where a significantly greater number of particle lumps and clusters form for $n = -2$, compared to other values of n.

I Introduction

Systems of interacting particles have been studied by physicists for centuries. Such systems are commonly called N-body systems and play an important role in the study of many fields of physics ranging from thermodynamics to astronomy [1]. Most commonly, such systems are studied to describe real world systems [2] rather than a general system of interacting particles. This study investigates some of the properties of more general N-body systems of particles with non zero radius, where interactions between two particles are determined by the relation

$$V = cr^n. \tag{1}$$

Here, V is the potential energy of the interaction, r is the distance between the particles, and c and n are constants. More specifically the kinetic and potential energy of the system are studied and related to certain qualitative properties of the system such as the formation of large lumps of particles.

A The Virial Theorem

The Virial Theorem [3], describes the relationship between the potential energy and the kinetic energy in systems of particles where the integral of the force between two particles, i.e. the potential energy, can be written as Equation 1. The Virial Theorem then states that

$$2\langle K\rangle_\tau = n\langle V\rangle_\tau, \tag{2}$$

where $\langle K\rangle$ is the kinetic energy and $\langle V\rangle$ is the potential energy, both averaged over time. Combining this relationship with Equation 1 and using the fact that the total energy of the system E is conserved gives the equation

$$\frac{4E}{N(N-1)} = c(n+2)\langle r^n\rangle_{N,\tau}, \tag{3}$$

where $\langle r^n\rangle_{N,\tau}$ is the average value of r^n between two particles averaged over both time and all pairs of particles. Note that $\frac{N(N-1)}{2}$ is the amount of pairs of particles.

Since $\langle r^n\rangle$ always is a positive number, the equation can never be satisfied if $\frac{E}{c(n+2)}$ is negative. These cases will not be discussed in great detail in this paper but it should be noted that one possible outcome of these situations is that the potential energy of the system could go towards infinity.

It is also important to note that these equations are derived for and apply to systems where particles do not have a radius, meaning that in the systems studied in this paper these equations will not be perfectly accurate. Placing the particles in a box also contributes to further deviations from these equations. It will be shown empirically however that these deviations are relatively small except for one important consequence: that the potential energy cannot go toward infinity.

B Lump Formation

In this section the relationship between the Virial theorem and the formation of "lumps" or very dense clusters of particles will be discussed. Equation 3 gives a relationship between the total energy of the system and the quantity $\langle r^n\rangle$. To find a condition for whether or not the particles form lumps, the approximation

$$\langle r\rangle^n \approx \langle r^n\rangle \tag{4}$$

needs to be used. Using Jensen's Inequality [4] it can be shown that in reality

$$\langle r\rangle^n \geq \langle r^n\rangle \tag{5}$$

for all $n \leq 0$ which are the values of n this paper will mainly focus on.

Approximation 4 and Equation 3 give the equation

$$\langle r\rangle = \left(\frac{4E}{cN(N-1)(n+2)}\right)^{\frac{1}{n}}. \tag{6}$$

This distance will furthermore be called the characteristic distance of the system and be denoted r_c. If r_c is smaller than r_p the Virial theorem predicts that lumps should start to form.

When $n = -2$, this expression is undefined for every value of E. The Virial Theorem in this case gives $\langle V\rangle = -\langle K\rangle$. If $E \neq 0$ this will only be satisfied in the limit where $\langle K\rangle$ and $\langle V\rangle$ go to positive and negative infinity. Therefore the Virial theorem predicts that in this case particles will get very close to each other and lumps will almost always form.

II Specifications

To be able to analyze the various systems with different values of n, computer simulations coded in C++ will be used for numerical analysis[1].

To accurately simulate these systems, there Furthermore the particles have a radius r_p, meaning that no two particles can be closer than $2r_p$ to each other. This means that particles can collide and exchange energy through this mean. Furthermore, all particles are confined in a cubical box with side length L. All particles have an initial velocity v_0 where the force and the velocity is calculated for each frame to determine the new position of each particle. The total number of frames and time step between each frame is given by I and dt respectively. The only parameter that is varied between simulations, i.e. the independent variable, is the exponent n. All other parameters are defined as $N = 200, r_p = 0.1, L =$

$10, v = 2, c = \frac{1}{n}, dt = 10^{-5}$, and $I = 10^7$. The same units for length and time are used for all parameters.

Using these simulations, the predictions by the Virial theorem will be tested, i.e. that most lumps form for $n = -2$.

III Results

In this section the results from the simulations will be shown[1].

The distribution of distances between particles for cases $n = -1, -2, -3$ is shown in Figure 1.

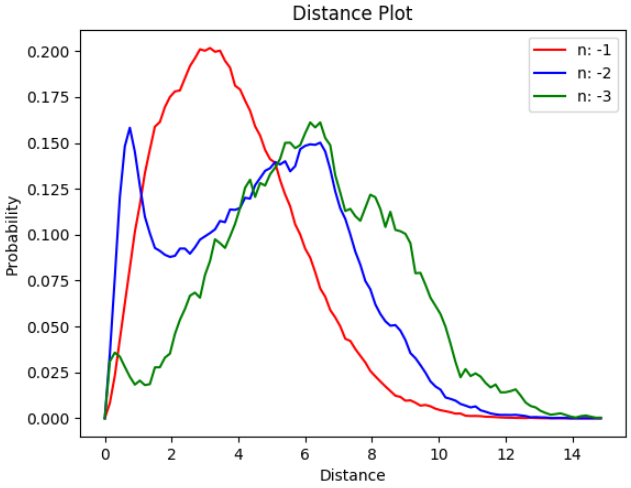

Figure 1: Radial distribution for different values of n.

Table 1 shows the energy per particle, characteristic radius, and actual average distance for each of these plots.

Table 1: Important characteristics for the simulated systems

n	E/N	r_c	$\langle r \rangle$
-1	-16.4	3.03	3.84
-2	-0.82	0	4.71
-3	0.33	3.69	6.25

The developement of the potential and kinetic energy over time is shown for $n = -2$ in Figure 2. The total energy is included as a control, as it should remain constant.

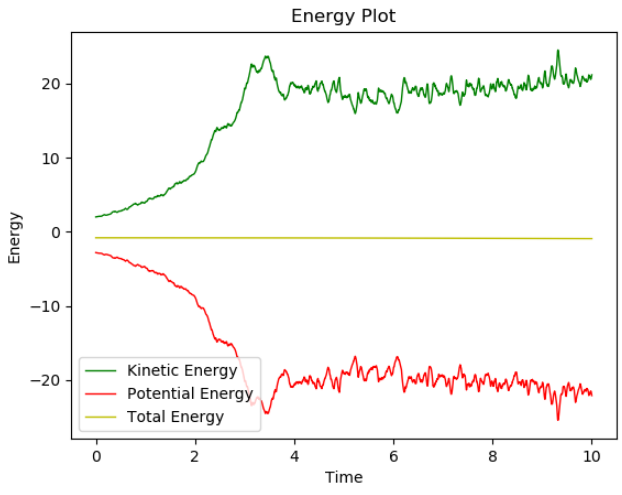

Figure 2: Potential and kinetic energy per particle for $n = -2$.

[1] Videos showing the full simulation, as well as all the code can be found in this Github repository

IV Discussion

When analyzing Figure 1, there is a clear difference for different values of n. For $n = -2, -3$, there are two distinct peaks in the distribution. The peak closest to 0 shows that many particles are close to each other, which by definition is a lump of particles. The second peak corresponds to a "normal distribution" of the particles in the box. While the "normal distribution" peak exists for all values of n, the lump peak is only visible for $n = -2, -3$ and is significantly larger for $n = -2$. This means that lump formation is much more likely for $n = -2$ compared to other values of n, confirming the theoretical prediction by the Virial Theorem.

Table 1 shows expected results according to Inequality 5 when comparing r_c and $\langle r \rangle$. It should, however, be noted that these values would most likely be closer to each other if the particles had zero radius. Since there is a minimal radius for the particles they will be forced to be further away from each other and thus the average distance between particles will increase. It should also be mentioned that due to simulation inaccuracies the total energy of the system decreases slightly for $n = -3$, rendering this value for r_c less meaningful.

When viewing the development of the kinetic and potential energy over time for $n = -2$ in Figure 2, it becomes apparent that the Virial Theorem also makes accurate predictions here. The kinetic energy increases at first as particles attract and approach each other. Many particles will then form lumps at $t \approx 3.7$, after which the kinetic and potential energy stabilizes. In theory, the kinetic and potential energy should go towards positive and negative infinity respectively, but this is not possible in our simulation due to the non-zero radius of the particles. It is therefore impossible for the prediction of the Virial Theorem to be accurate here. However, the relationship between the kinetic and potential energy almost perfectly matches Equation 2, which states that for $n = -2$, the absolute value of the kinetic and potential energy should be equal. Once again, the Virial Theorem proves to match the numerical results.

V Summary and Conclusion

This study has investigated the Virial Theorem and how its predictions compare to numerical simulation of an N-body system. These two have a high correspondence according to the results of this study, despite the fact that the Virial Theorem requires particles with zero radius while the simulation was constructed with particles with non-zero radius. Furthermore, this analysis has confirmed, theoretically, numerically, and visually, that particles in a N-body system are more likely to cluster and form lumps when $n = -2$.

VI References

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