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3D Imaging of a Binary Colloidal Fluid

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Abstract:
In order to understand the nature of colloidal fluids, we wanted to visualize a 3D representation of their thermodynamic distribution. Colloidal fluids are fluids that consist of two parts: colloidal particles and a dispersing medium. Some examples include toothpaste, mayonnaise, plaster, and muddy water. We could also think about colloidal fluids simply as a mixture of two or more parts. In this poster, we used the hard-sphere system to represent the structure of colloidal fluids in a 3D graph using Mathematica (MMA). In the hard-sphere system, we used two different sizes of impenetrable spheres that could not overlap to represent particles in a binary colloidal fluid. We focused on how their interactions caused probable arrangements. We located big and small particles in the hard-sphere system by finding their pressure distribution, where the pressure distribution was found by calculating the forces created by the particle collisions. The results of our 3D graph representation of the particle distribution of a binary colloidal fluid showed that the particles’ interactions with each other caused ray and sheet-like structures. Understanding this particle distribution and structure of a colloidal fluid can help us in several applications. For example, we could apply this knowledge when dealing with separation processes of binary mixtures, which are similar to colloidal fluids. In addition, understanding the thermodynamic distribution of colloidal fluids could help in understanding buoyancy seen in colloidal mixtures, which has been seen to break Archimede’s principle.

Introduction:
We wanted to visualize a 3D snapshot of the particle arrangement in colloidal fluids and determine if the particles get locked into any sort of arrangement with a thermodynamically favorable distribution. To find the highly probable locations of big and small particles in colloidal fluids we calculated a radial distribution function (RDF) of the hard-sphere system. We used the same method as Shinomoto [2] when he calculated the pair distribution function. His method uses forces and net forces to describe the interaction between two particles. Others found that they could use this method with more iterations to describe the interaction between hard-sphere particles [3]. With the use of FORTRAN, we were able to create a RDF with numerous iterations until the function converges to be self-consistent. With this data we located the big and small particles and created a 3D image of their placements in MMA. For the particular case we chose to present in this poster we used a ratio of big particles to small particles of 4 to 1, a volume filling fraction of 26.18%, with 60% (x=0.6) of the particle volume being filled with big particles. Below, Figure 1, is a graph of the RDF for x=0.6, demonstrating long-range structure with periodic peaks, and a normal case of x=0.2, which does not have long-range structure.

Methods:
Our goal was to find a 3D representation of the distribution of particles in hard-sphere fluids in thermodynamic equilibrium. We worked through a series of steps in order to generate this:
- Created a series of RDFs that show the probability of the placement of a second particle being located at a distance from a first particle for four different cases: big particle to small particle, big particle to big particle, small particle to big particle, and small particle to small particle. Using the data shown in Figure 1, we placed the second particle at a location of high probability where there was a peak in the graph.
- Generated a table and 3D representation of the probability of a big third particle being located in a 60x60x60 area based on the RDFs of the first two big particles, shown below. Using the data in Figure 2, we placed the third particle at a location of high probability.

This could be a property of the structure of colloidal fluids. On the other hand, this could also be a result of our choice of placement of particles. In order to look further into this, we posed a normal case, with 20% (x=0.2) of the particle volume being filled with small particles. When we made a 3D representation of this data in MMA, like that in Figure 3, this structure of rays and sheets was nonexistent, and instead, the big particles were concentrated at the origin. Because of this, we would conclude that this structure is due to the periodic peaks as seen in Figure 1, and that this structure was not seen for the x=0.2 case because there were not periodic peaks in Figure 1. Also, we can notice that the small particles seem to form spherical sheets around the big particles. See Figure 4. However, we did not focus on this because it seems that the big particles are the ones that determine the arrangement.

Results:
In Figure 3 below, we can notice that the big particles seem to form sheets made of rays expanding out from the origin. We saw this for the majority of cases when dealing with long-range structures.

Conclusion:
With what we have seen, it seems colloidal mixtures only form these favorable ray and sheet-like arrangements when the particle volume of the small particles is high.

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References:

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