5-2014

Computational Modeling of Doped Helium Clusters

Ryan Carlsen
Utah State University

Phys 4900 Report

Ryan Carlsen

Computational Modeling of Doped Helium Clusters

Prior to starting my coursework for this class, I had little experience in this area. I had done some related coursework in physical chemistry and computer science, but I had little direct experience. Thus, over the course of the year I learned very many things that are important to the research, but I did not reach a stage at which a lot of output occurred. Thus, in general this is a report of the things that I learned that will enable me to be effective in generating research output in the future, as I plan to continue participating int his research project.

My first effort in the project was to become more familiar with the program Mathematica, which is used in the research in order to solve differential equations so that they can from there be translated into computer code. These differential equations deal with the underlying quantum mechanics of the system, and the solutions thereof allow the equations to be solved by numerical computing methods. Some of my work (primarily copied from a Mathematica notebook) on the simplified system of two particles confined to a ring is shown below.

In this notebook we have some of the solutions for the two-particle on a ring quantum mechanical system. We compare the values obtained from a matrix solution method of the differential equation with values obtained by direct solution using Mathieu functions.

Given that the Hamiltonian for this system is as follows:

$$\hat{H} = -\frac{\hbar^2}{mass\, r^2}\frac{\partial^2}{\partial \alpha^2} + V_0 \cos\alpha$$

and that our basis functions have the form:

$$\psi = e^{i m \varphi}$$

We obtain the values for our function by constructing an n x n matrix where n is an odd number. Then to obtain the values to populate our matrix, we evaluate the following integral:

$$\int \psi_i^{'} \hat{H} \psi_k \, d\tau$$

for all values of i and k between 1 and n. The results of this integral are then used to populate the matrix, with the integral giving the following results:

$$i = k \;:\; \int \psi_i' \hat{H} \psi_k \, d\tau = m^2 \frac{\hbar^2}{mass\, r^2}$$

$$i = k \pm 1 \;:\; \int \psi_i' \hat{H} \psi_k \, d\tau = \frac{V_0}{2}$$

$$i = k \pm 2,3 \ldots \infty \;:\; \int \psi_i' \hat{H} \psi_k \, d\tau = 0$$

Following some variable substitutions to simplify the problem, the matrix was constructed, allowing *i* and *k* to run from -12 to 12. After numerical quantities were included so that the elements of the matrix had value, the eigenvalues and eigenvectors of the matrix were obtained. The eigenvalues estimate the energy of the different states of the system, while the eigenvectors can be used in obtaining the coefficients for linear combinations of the basis set functions that will most nearly represent the solution, which is a Mathieu function.

Upon plotting the appropriate linear combinations of the basis function and comparing them with the Mathieu function they were approximating, there was no visible difference between the Mathieu function and the linear combination. Therefore, it is determined that this method was successful.

My next focus involved learning the basics of FORTRAN, as the computer programs used to analyze these clusters are written primarily in FORTRAN because of the need for the speed with which calculations can be performed in this computing language. Here my experience with basic computer coding in C++ was an advantage, as it allowed me to recognize the elements of the language more simply, so that I could focus primarily on learning the syntax rather starting from the basics of how to write computer programs. I made some progress in this over the course of the semester, and wrote part of a FORTRAN program to generate and solve matrices that provided solutions to a simplified model of the quantum mechanical system.

Another major focus of the semester was gaining a better understanding of the literature in the field. I spent quite a bit of time reading articles concerning superfluidity, especially microscopic superfluidity. This effort was inspired in part by my application for the Goldwater scholarship, which was closely related to my research during the first semester and the first part of the second semester. This aided me both in my understanding of the field in general and in my ability to effectively express myself in a scientific manner.

Another important skill that I learned was how to use a UNIX command line. This is the method by which the FORTRAN programs are run, so it is essential to the project. I particularly

became familiar with the command line during the second semester, when I ran a FORTRAN program a large number of times while varying the potential used by the program. I started by doing some simple work with this in the first part of the second semester. The FORTRAN method I was using was a basis set method, which in general is accurate but also computationally intensive. The computing power required for the calculations was reduced by utilizing a reduced dimensional model of the quantum system, which is shown in the image to the side.

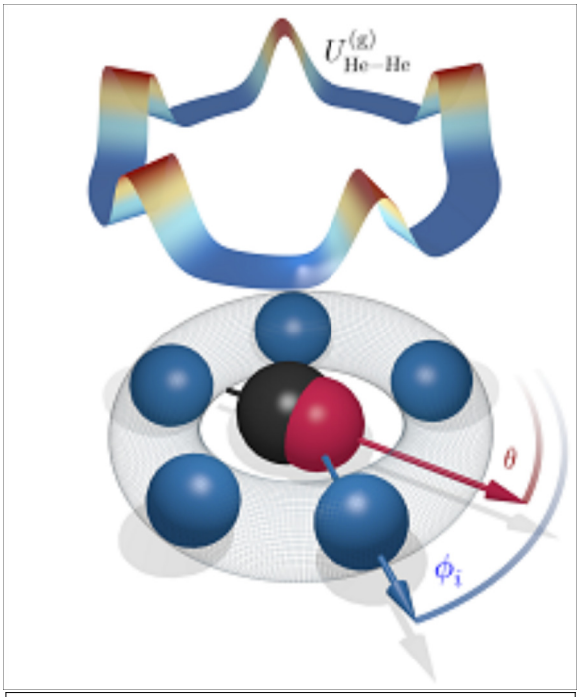

Fig. 1 – Reduced Dimensionality Model of a doped ^{4}He cluster. The ^{4}He atoms are confined to a ring. The molecule is fixed at the center but can freely rotate in the plane of the ring. The ribbon above the ring illustrates the He-He interaction.

The basis set method constructs a mathematical configuration space in which the wave function is allowed to develop. The larger the basis set is, the more fully the wave function can develop; however, the size of the wave function is limited by the computational resources available. Each atom needs its own configuration space, which is why the reduced dimensionality models are necessary in order to keep the problems computationally tractable. Each atom added to the system increases the computing time factorially, so basis set methods are only feasible for small systems. To help determine their accuracy they can be compared with the results of Monte Carlo simulations of the systems. These provide numerically accurate results but fewer physical details can be extracted.

My final project was based on running several of these basis set simulations for small cluster of helium-4 atoms doped with a single HCN molecule, calculating the energies of the ground and excited states. The potentials were altered for the different calculations, as well as the number of surrounding helium atoms. From the ground and excited state energies the effective rotational constant can be calculated, and by comparing the effective rotational constants as the number of helium atoms surrounding the HCN molecule is varied the point at which superfluid behavior begins can be determined. The goal was to determine if the potentials affected the point of superfluidity onset. Unfortunately one of the codes had some problems and so the project was not completed, although a decent amount of data was gathered.