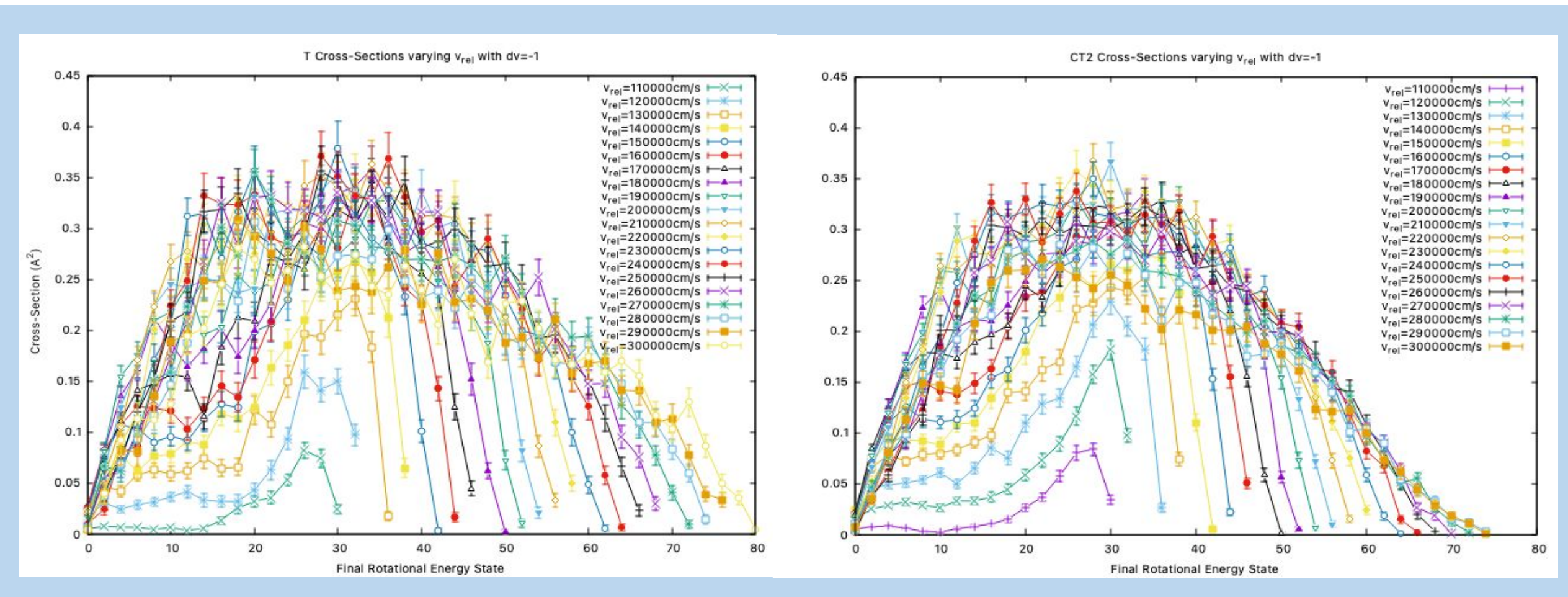


Introduction

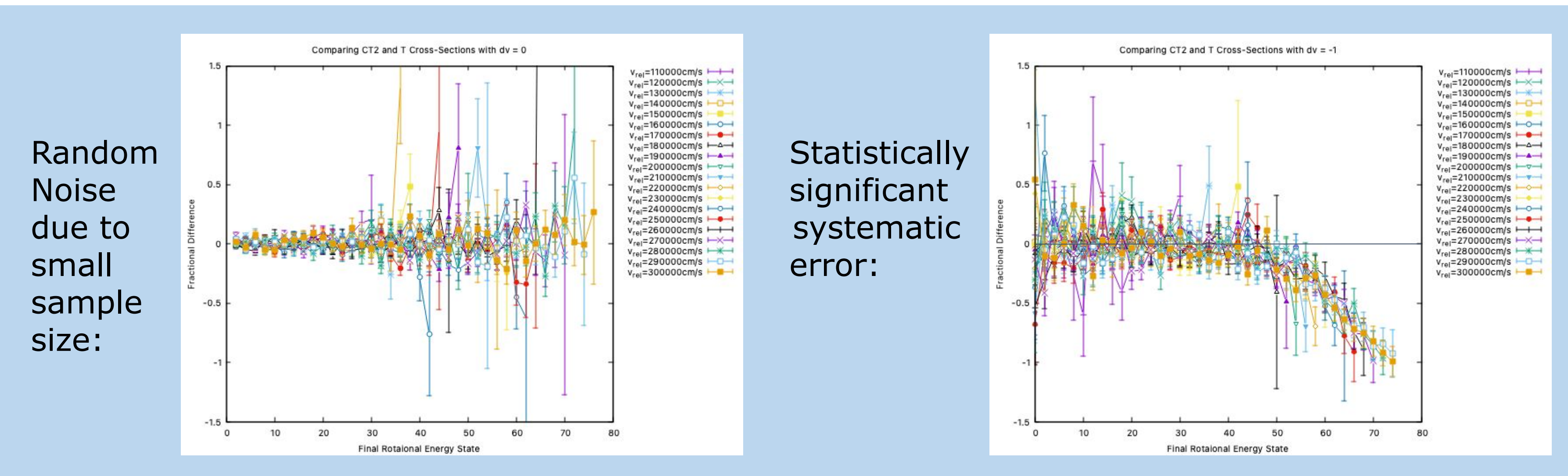
The Molecular Collisions Laboratory studies different kinds of few-body dynamics in atom-molecule collisions. The current experimental system involves Lithium dimer (Li_2) - Neon (Ne) non-reactive collisions, where we measure energy transfer rate coefficients and cross sections on a single excited-state potential surface. This summer we wanted to validate our quasi-classical trajectory programs by comparing the outputs of rotationally inelastic cross-sections when given the same input conditions. Here are two examples of the cross-section graphs we examine:



The graphs above were made using two different simulation programs our lab uses to compute collision cross sections. They depict the cross section for vibrationally inelastic collisions ($\Delta v = -1$) as a function of final rotational quantum number j_f . The first was calculated by the program **T**, which uses a computationally efficient algorithm, and the second is from the program **CT2**, which is slower but can be used for chemically reactive systems; both programs are important for the lab's work. Discrepancies had been noted between the output of these two programs in some situations, and my task was to determine the origin of the problem and to fix it.

Locating the Problem

First, we isolated variables such as the initial rotational and vibrational level, impact parameter, relative velocity and more. to look for systematic error by graphing fractional difference. Since each trajectory is ultimately a stochastic process, finding output differences is not trivial. Here, I was reminded of the importance of error bars and statistical significance. Graphs may look different but this could simply be due to random variance.



Ultimately, we found that variation was most apparent in cases of high relative velocities, which creates a high energy, as well as when $\Delta v < 0$.

Acknowledgements

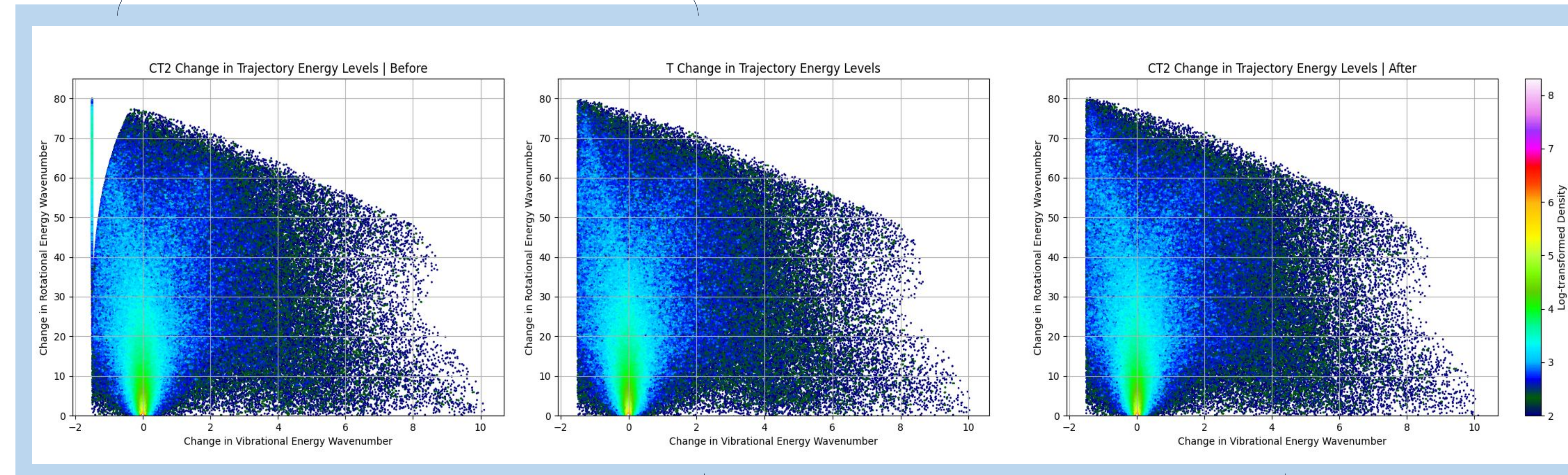
First, I would like to thank Dr. Stewart for being a great teacher and welcoming me into his lab. Next, I would like to thank my incredibly helpful lab members: Othmane for his continuous support and encouragement, Denuwan for taking time to guide me through the experimental lab, and Isaac, Jimmy and Mathis for their assistance and willingness to jump into a call. Last but not least, thanks to the QAC for granting me the opportunity and time to explore this fascinating sub-field of physics.

References:

- Figure 1: Review of the Universe, Harmonic Oscillator, Diatomic Potential. Available at: <http://universe-review.ca> (Accessed: July 25, 2024).
- Figure 2: Ling, S. J., Sanny, J., & Moebis, W. (n.d.). *The Quantum Harmonic Oscillator*. In *University Physics Volume 3*. Pressbooks. Retrieved from <https://pressbooks.online.ucf.edu/osuniversityphysics3/chapter/the-quantum-harmonic-oscillator/>

The Bug Revealed!

Here are graphs of our worst case: $v_{rel} = 300,000$ m/s, $v_i = 0$ and $j_i = 1$. As you can see, for CT2, there is a large area in the top left corner that fails to populate. This kind of behavior is abnormal from the density plot, you can see that there is an extremely sharp drop off to zero as well as a highly populated area of a change in rotational energy level equal to -1.5.



Calculating Vibrational Turning Points

Figure 1: Simple Harmonic Oscillator Vibrational Energy levels

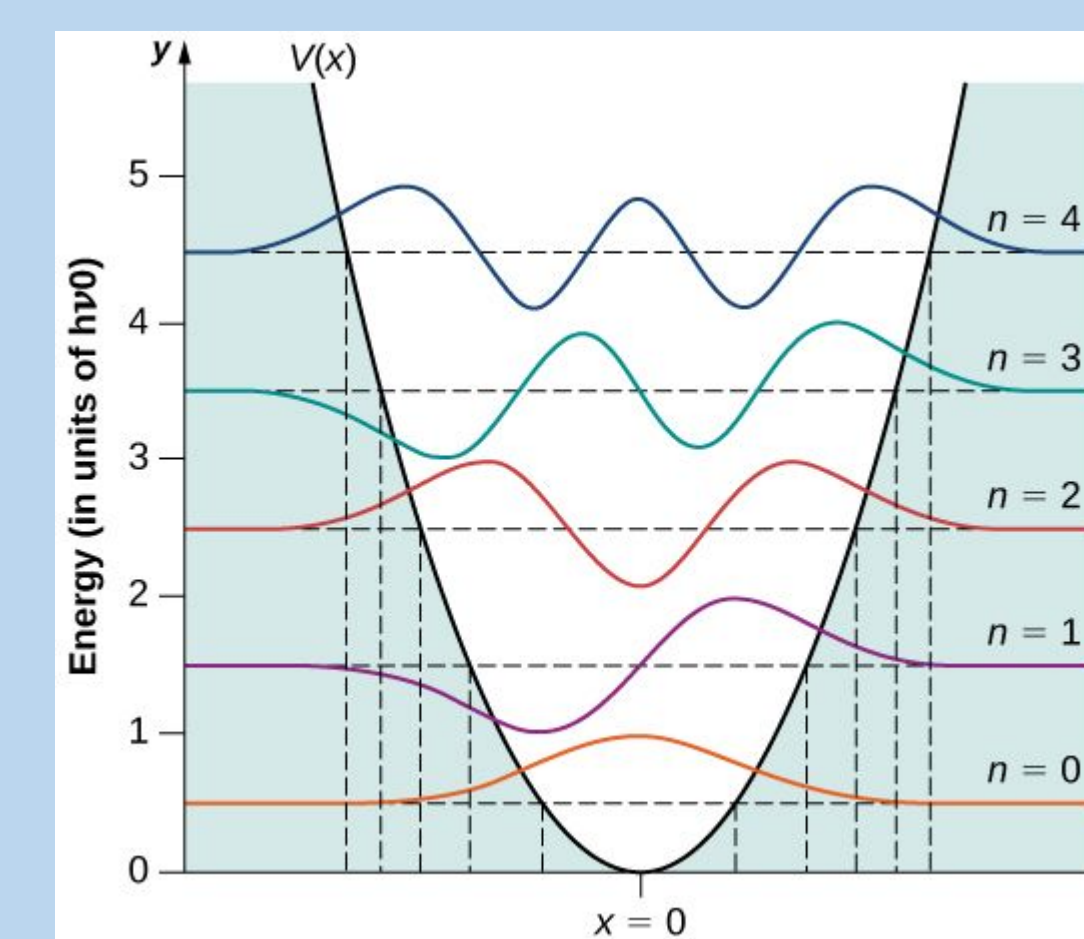
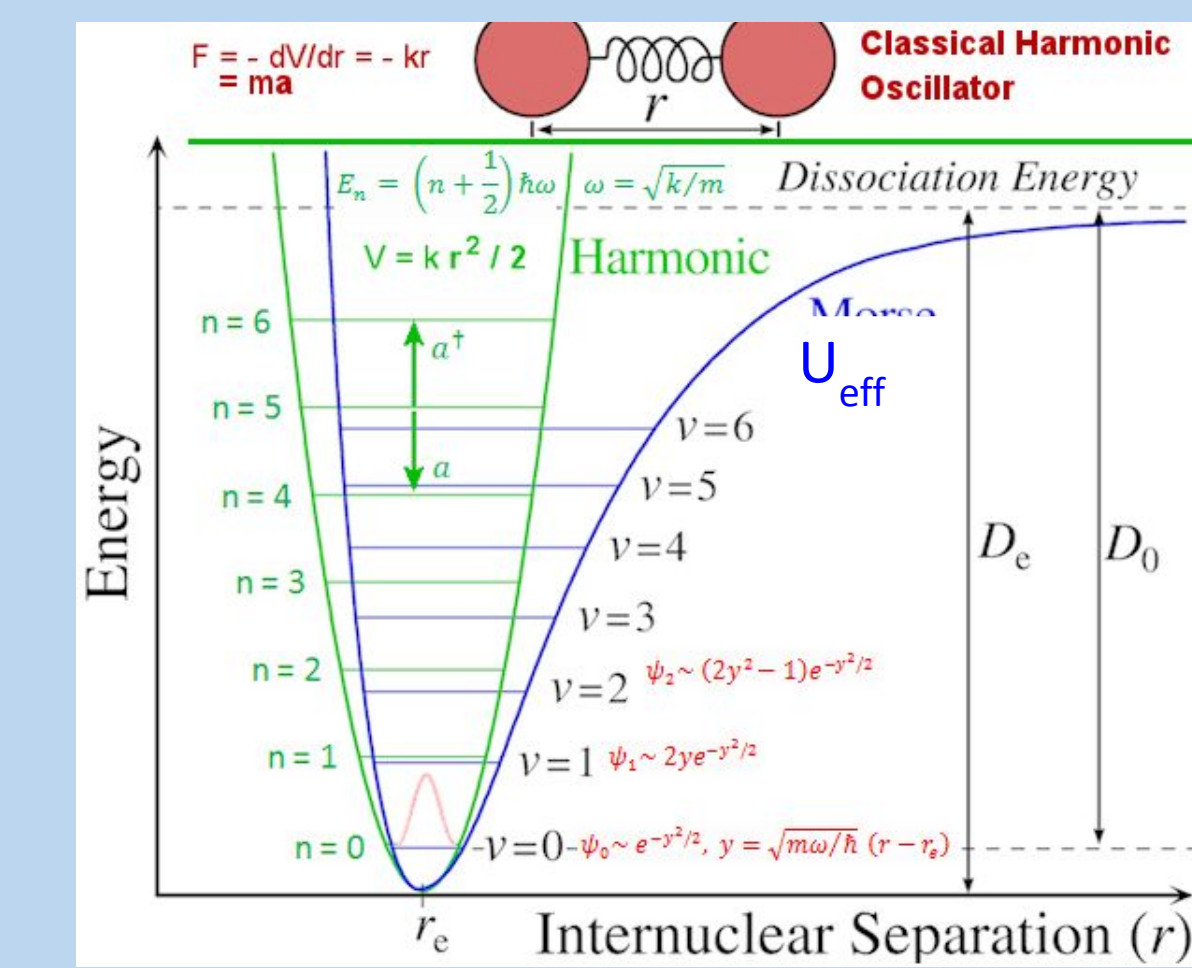


Figure 2: Effective Potential Vibrational Energy levels



Finally, we found cases where the vibrational action was equal to 0 which is physically impossible. We soon figured that this was the result of incorrectly finding the vibrational turning points. We employ the simple harmonic oscillator as the vibrational potential energy function between the two lithium atoms. However, the effective potential (U_{eff}) also accounts for rotational energy of the atom. I have implemented a binary search to first find the radius of the effective minimum and then the two turning points are also found through binary searches for a final internal energy using a radius angle given by the search. Given more time, I would like to lower the complexity of this calculation by doing both searches simultaneously. Furthermore, we could utilize the previously used Newton-Raphson method, which was more efficient but was implemented incorrectly.

Final Contour Maps

