Modeling the Energy States of an Electron Trapped Between Two Sulphur Atoms.

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Introduction

In Quantum Mechanics, a common question is how a particle behaves in a potential well. Many systems can be modeled as such. Of interest here is an electron trapped in a single bond between two sulfur atoms.

Figure 1: Simple model of a single sulfur bond.

The potential well, itself, can be modeled in many ways. The simplest model is the infinite potential well where the potential in the well is zero and infinite everywhere else. Of greater interest here are the more complex models. The quantum harmonic oscillator (QHO) is a model where the potential well is shaped like that of a harmonic oscillator and is parabolic in shape. A similar model is a quantum aharmonic oscillator (QAHO). This is where the potential well is shaped as a function other than a parabola and should provide more accurate results.

The goal of this research is to compare experimental data for the difference in energy levels of the electron trapped in the single sulfur bond to a quantum harmonic oscillator and quantum aharmonic oscillator model in one dimension. Both of these models are further restricted by being placed into an infinite potential well for computational reasons. Because of these limitations, the best way to compare these three sets of values is to study the differences between the energy levels of the data sets. This allows the underlying trend of the data to show without large constants shifting the data.

Methods

The Fourth-Order Runga-Kutta Method (RK4) was used in conjunction with the secant method to find the energy eigenvalues of the Schrödinger equation. The RK4 method is needed to solve the second order Schrödinger equation with both speed and accuracy. The secant method was used to find the energy values by changing the initial energy value until the wave function fit into the potential well. The potential well, in this case, has a length of $2.05\text{x}10^{-10}$ m.

Original Schrödinger Equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\boldsymbol{x})\psi = E\psi$$

Potential Equation for the Quantum Harmonic Oscillator

$$V(x) = \frac{1}{2}kx^2$$

Potential Equation for the Quantum Aharmonic Oscillator

$$V(x) = \frac{ke^2}{x-1} + \frac{ke^2}{1+a-x}$$

Results

Figure 2: The fourth energy level's wave functions are shown below. The QHO wave function is slightly more pressed to the center then the QAHO which is closer to the square well.

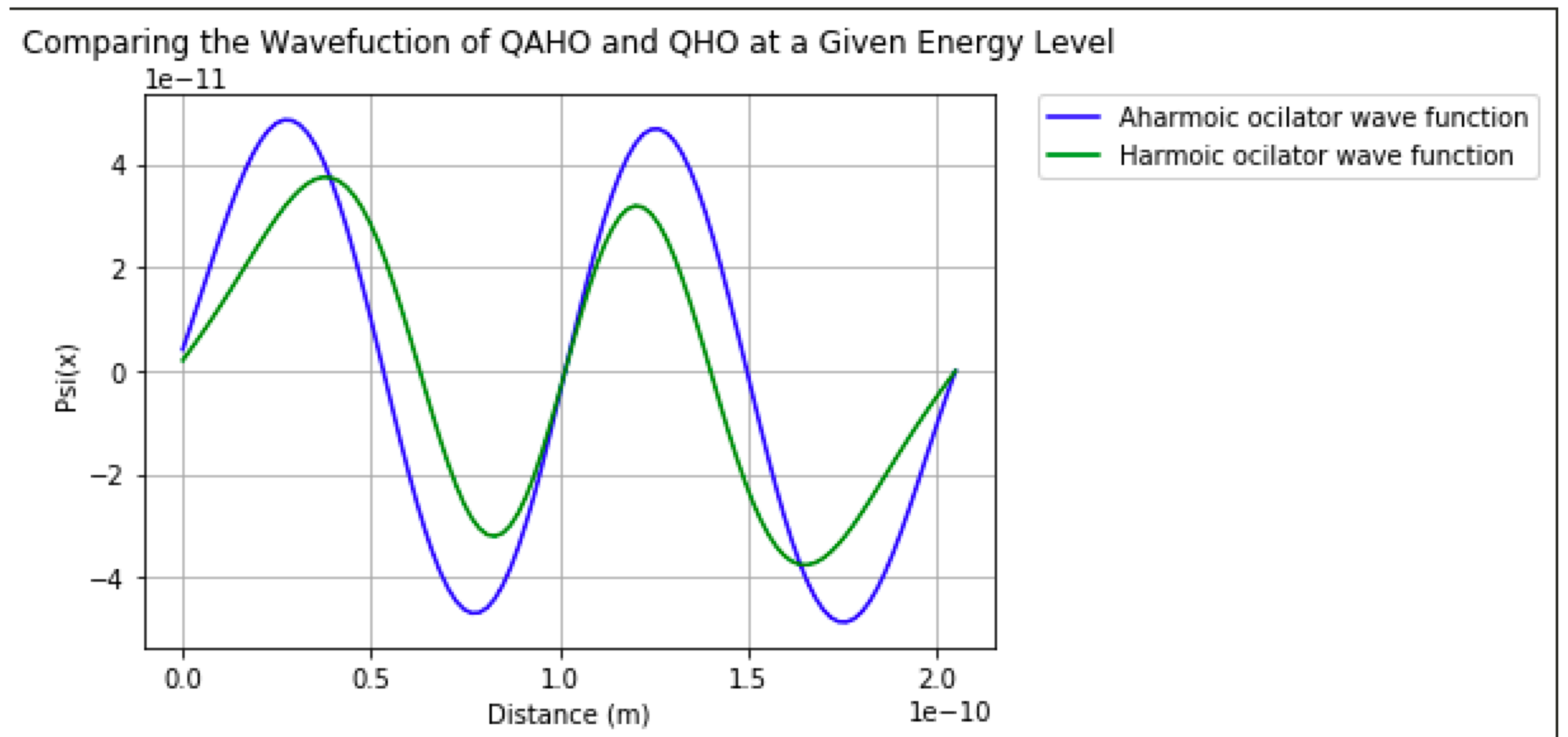


Figure 3: The energy eigenvalues of the two models are shown below over several energy levels. While the two models might both seem linear, the QAHO is closer to parabolic in nature. The QHO is in fact close to linear, which is in keeping with the theory of QHOs.

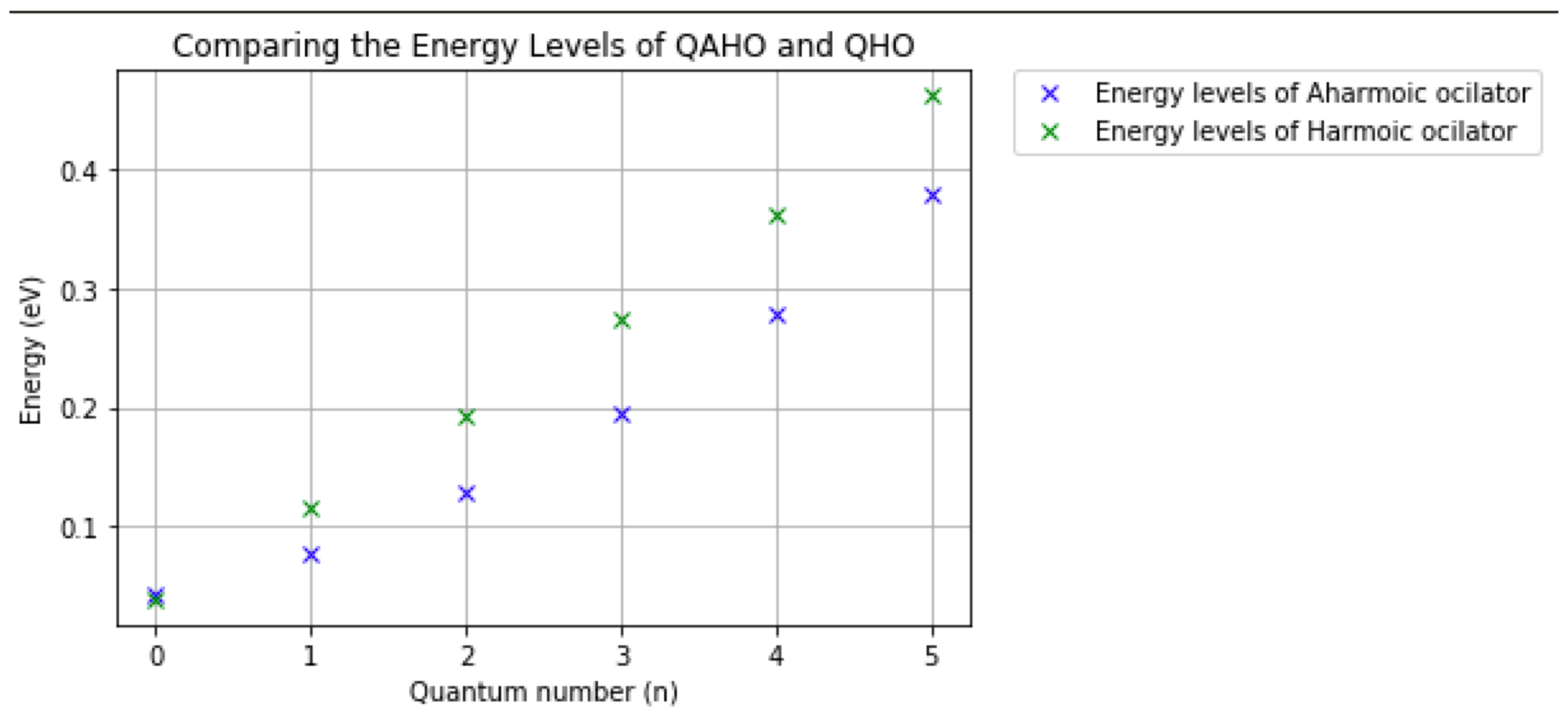
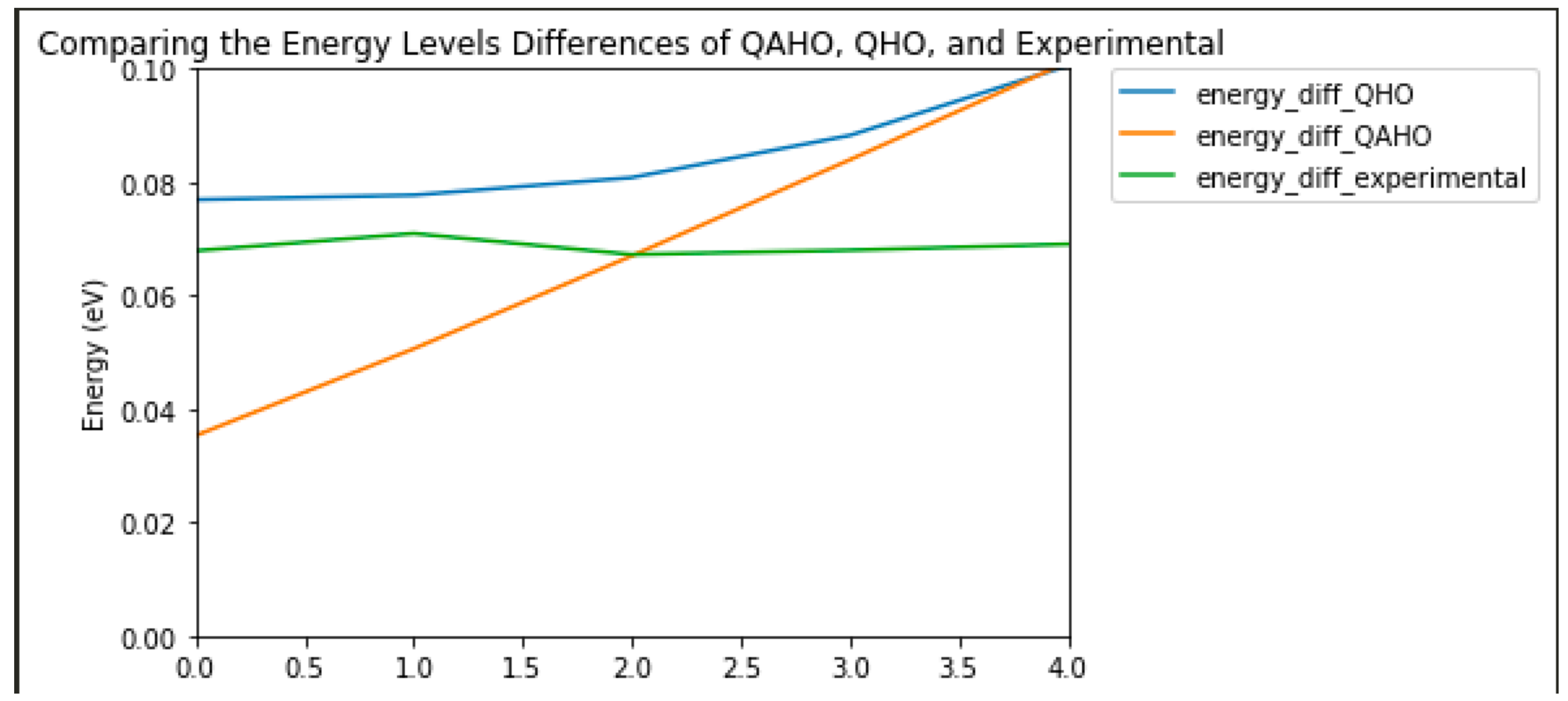


Figure 4: The differences in the energy levels of the two models and the experimental data are compared below. Of note, the comparatively simple QHO model seems to be a better model as it captures the difference in energy levels better than the more complicated QAHO model.



Conclusion and Future Work

The model that most closely resembles the experimental data is the simpler QHO model. This seems to imply that the more complicated QAHO model is not capturing a nuance that is captured by the QHO.

While each seems to be a reasonable model of the trapped electron, it would be helpful to try modeling this system in more then one demission to see how things behave in a model closer to reality. Further, refining how the wells are structured numerically in the models could be helpful. Currently the model has to skirt the problem of infinite potential for the QAHO.

References

- Mark Newman, *Computational Physics.* University of Michigan, 2013.
- Kenneth S. Krane, *Modern Physics, 3rd Edition.* John Wiley & Sons, 2012.