Large non-linear electronic polarizabilities would be advantageous for a variety of devices and have contributed substantially for around three decades. This project examines the theoretical limits of the static first non-linear electronic susceptibility of a material, known as the hyperpolarizability. The hyperpolarizability is the time derivative of the first time-dependent electric polarization with respect to the applied electric field. The hyperpolarizability is given by the following formula:

$$\beta = \frac{\partial P}{\partial E}$$

where $P$ is the polarization vector, $E$ the external field, $\beta$ the hyperpolarizability, and $\nabla$ the gradient operator. The hyperpolarizability is determined largely by the ground and first excited state wave functions.

### METHODS

#### INTRODUCTION

Knowledge of the behavior of nonlinear optical electronic polarizabilities would be useful for many different applications and devices. For example, such understood control might allow for the construction of better optical switches and memories. For this reason, the project is given by the following formula:

$$H(x) = \sum_{n=0}^{N} c_n H_n(x)$$

where $H_n(x)$ is the $n$th-order Hermite polynomial, $c_n$ the corresponding coefficient, and $N$ the number of terms in the series. For this particular problem, the potential is given by the following formula:

$$V(x) = \sum_{n=0}^{N} c_n H_n(x)$$

The hyperpolarizability is determined largely by the ground and first excited state wave functions. The hyperpolarizability is given by the following formula:

$$\beta = \int \left( \psi_n^* \nabla \psi_m \right) \left( \psi_m^* \nabla \psi_n \right) \frac{1}{E} \, dx$$

where $\psi_n$ and $\psi_m$ are the $n$th and $m$th wave functions, respectively.

#### RESULTS

- **Maximization of the First Static Hyperpolarizability**
  - Edwin Bernardoni, Rolfe Petschek (Advisor)
  - Physics Department, Case Western Reserve University

**ABSTRACT**

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