

DIATOMIC

Ilana Berlin

September 25, 2025

1 Introduction

1.1 Purpose

Observe the shape of a wavefunction at different energy levels using the Diatomic software. Observe a practice example of degeneracy and the correspondence principle.

1.2 References

McQuarrie, D. A.; Simon, J. D. *Physical Chemistry: A Molecular Approach*; University Science Books: Sausalito, CA, 1997.

Reid, Brian P. *Diatomic: Classical, Quantum, and Statistical Mechanics of Diatomic Molecules*.

Wiser, D.; *Using DIATOMIC¹ to Understand Energy Contributions*; Lake Forest College: Lake Forest, IL, 2018; pp 1-4.

Reid B.P. *Diatomic* Ver. 2.1, Trinity Software: 1999.

1.3 Safety Information

There are no safety risks associated with this experiment.

2 Methods

Data was collected using version 2.1 of the Diatomic software.

3 Results/Data

3.1 Classical Learning

3.1.1 Average Energies at Different Temperatures

The average energy at room temperature (Table 1). was recorded from a graph of average energy at different temperatures.

Table 1: Average Energy of translational, vibrational, and rotational motion at room temperature, 273°K.

	Translation	Vibration	Rotation
Ave. Energy (kJ/mol)	4.39	12.79	2.712

3.2 Quantum Learning

3.2.1 Translational Energy Levels and Wave Functions

The spacing between each of the energy levels increases as the energy level increased. The ΔE between the energy levels is increasing. At the lowest energy level of 1, the energy is positive, therefore the lowest energy level was above zero. The number of half wavelengths in the function also increased as n increased (Fig. 1). There was one half wavelength for each n and there were $n-1$ nodes (Table 2).

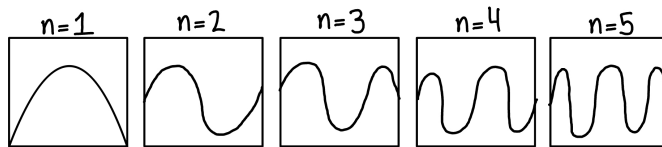


Figure 1: Sketch of shape of 1D wave function for $x = 1$ to $x = 5$.

Table 2: Half wavelengths and nodes visible in a graph of the a 1D wavefunction for $n = 1$ to $n = 5$.

n	1	2	3	4	5
Half Wavelengths	1	2	3	4	5
Nodes	0	1	2	3	4

The degenerate states (Table 3). were possible because x and y had equal length. Two state were degenerate if n_x and n_y could be flipped without affecting the energy.

Table 3: Energy in kJ/mol for a 2D wave from $n_{x/y} = 1$ to $n_{x/y} = 5$. Degeneracy is shown with the cell color.

$n_x \backslash n_y$	1	2	3	4	5
1	1.42E-19	3.55E-19	7.11E-19	1.21E-18	1.49E-18
2	3.55E-19	5.69E-19	9.24E-19	1.42E-18	2.06E-18
3	7.11E-19	9.24E-19	1.28E-18	1.78E-18	2.42E-18
4	1.21E-18	1.42E-18	1.78E-18	2.28E-18	2.91E-18
5	1.49E-18	2.06E-18	2.42E-18	2.91E-18	3.55E-18

For each 2D shape the total number of half wavelengths was the sum of n_x and n_y . The number of half wavelength in the x and y directions was not the same unless n_x equaled n_y .

3.2.2 Discrete Translational Energy Levels?

McQuarrie and Simon described the correspondence principle as the particle tending to behave classically in the limit of large n . As the number of energy levels increased up to 512, the gaps between the energy level disappeared. This follows the correspondence principle as in the face of a large number of levels, the energies stopped being discrete, a quantum condition, and became continuous as in classical physics.

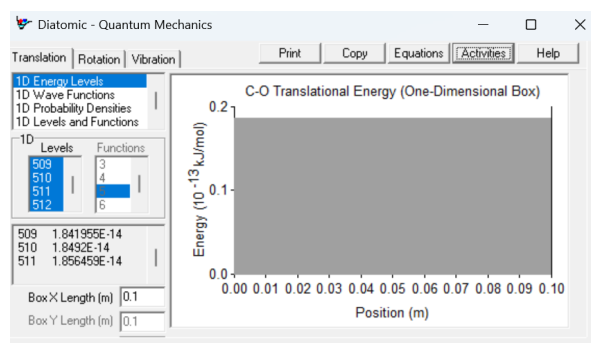


Figure 2: Graph of a 512 energy levels demonstrating the correspondence principle as energy appears to be continuous.

3.2.3 Rotational Energy Levels

As the rotational quantum number (J) increased the rotational energy levels increased exponentially. The degeneracy of the rotational energy levels in CO can be described by the equation:

$$y = 2x + 1 \quad (1)$$

3.2.4 Vibrational Energy Levels and Wave Functions

There was a difference of 34.33761 kJ/mol between the two lowest vibrational energies in F_2 . This corresponds to a frequency of $8.60554E+13$ Hz or a wavelength of 3483.717 nm. This belongs to the IR part of the electromagnetic spectrum. The number of half wavelengths of the vibrational wave functions increased as the vibrational quantum number (v) increased.