Modeling Quantum Dots using Geometric Primitives

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Outline

1. Introduction
   - Explaining Quantum Dots
2. Method
   - Approximating the kinetic energy
   - Potential Energy Matrix
   - Combining The Two
3. Results
   - Results

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The Schödinger Equation

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

Where

$$\nabla^2 = \left(\frac{\partial^2}{\partial x} + \frac{\partial^2}{\partial y} + \frac{\partial^2}{\partial z}\right)$$

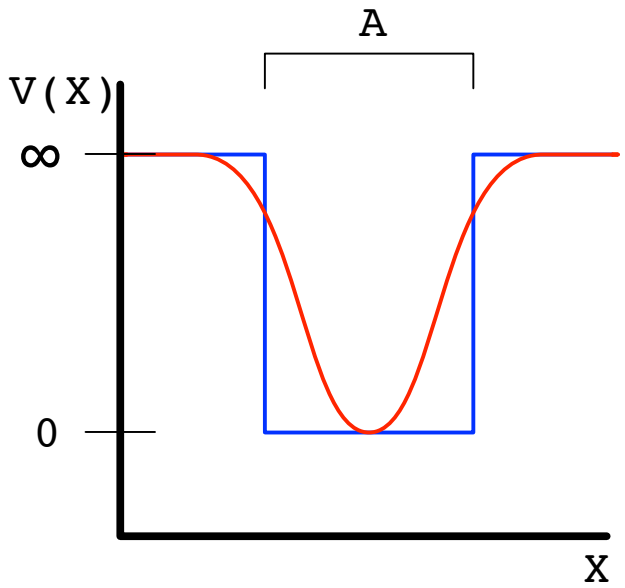
and

$\psi \rightarrow$ the wave equation for the particle

Understanding Potential Wells

Potential Wells

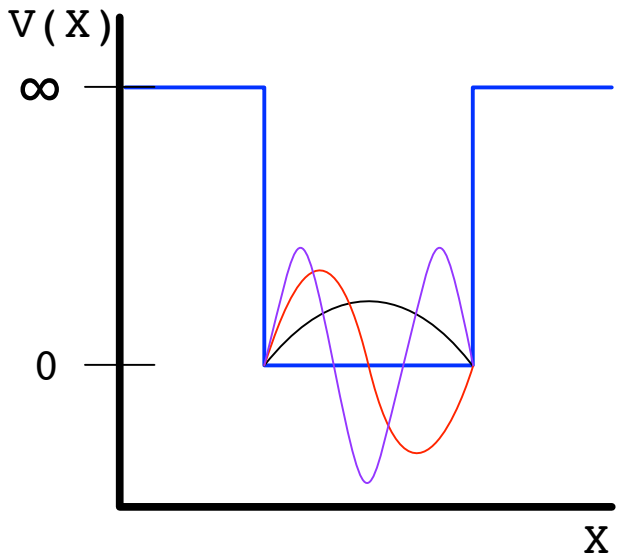
Free particles like to reside where the potential energy is low



Normally a function describing this function can be complex (the red line), so physicists approximate it using a trivial

Quantum Confinement

Infinitely deep well $\rightarrow$ quantum confinement



Quantum Dots as Artificial Atoms

Quantum Confinement in 3D -> Artificial atom

- Question: What atomic properties are we looking to exploit?
- Answer: Fluorescence.

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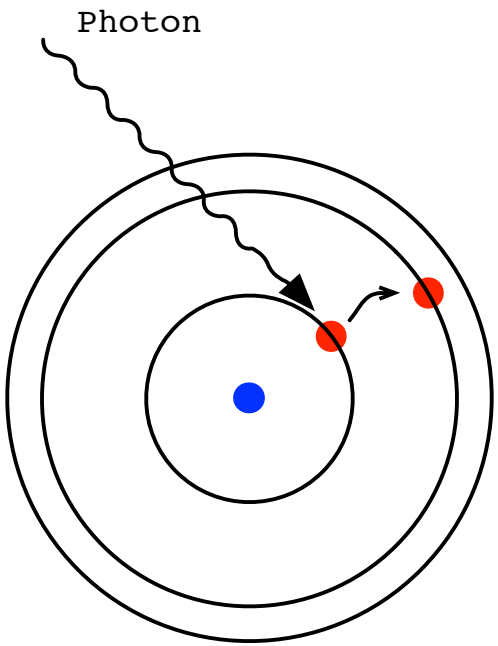
Fluorescence

Fluorescence 1

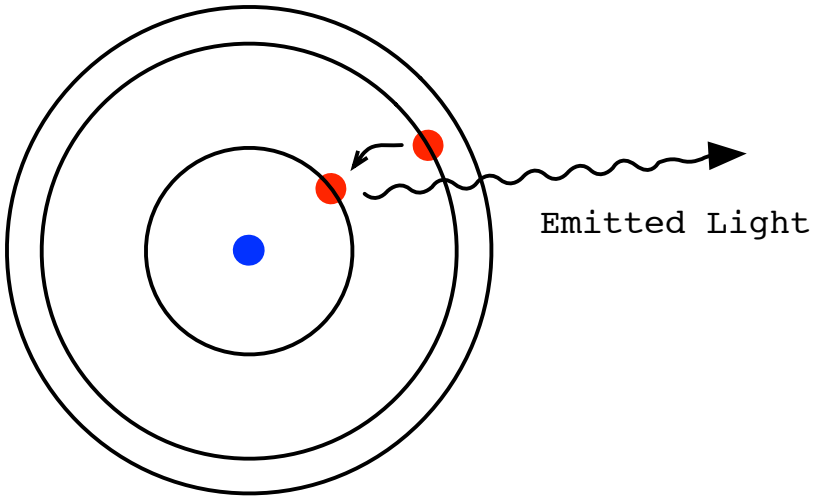
How fluorescence works



A photon ‘hits’ an electron into its excited state.

Fluorescence
Fluorescence 2

How fluorescence works



When the electron comes back ‘down’ form the excited state light is emitted [2].

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Remembering the Schrödinger equation

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

Let us first model the kinetic energy part

$$K = -\frac{\hbar^2}{2m}\nabla^2$$

where

$$\nabla^2 = \left(\frac{\partial^2}{\partial x} + \frac{\partial^2}{\partial y} + \frac{\partial^2}{\partial z}\right)$$

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

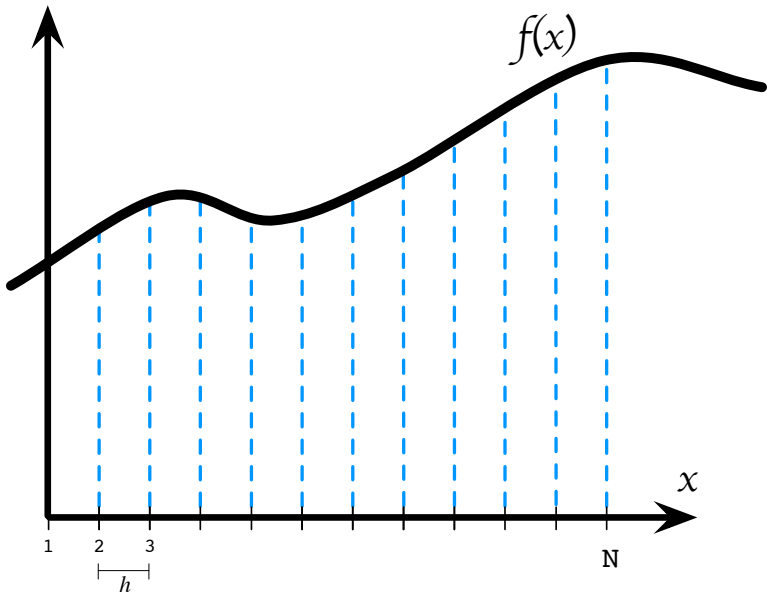
and

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

This gives us the following matrix for $f''(x)$

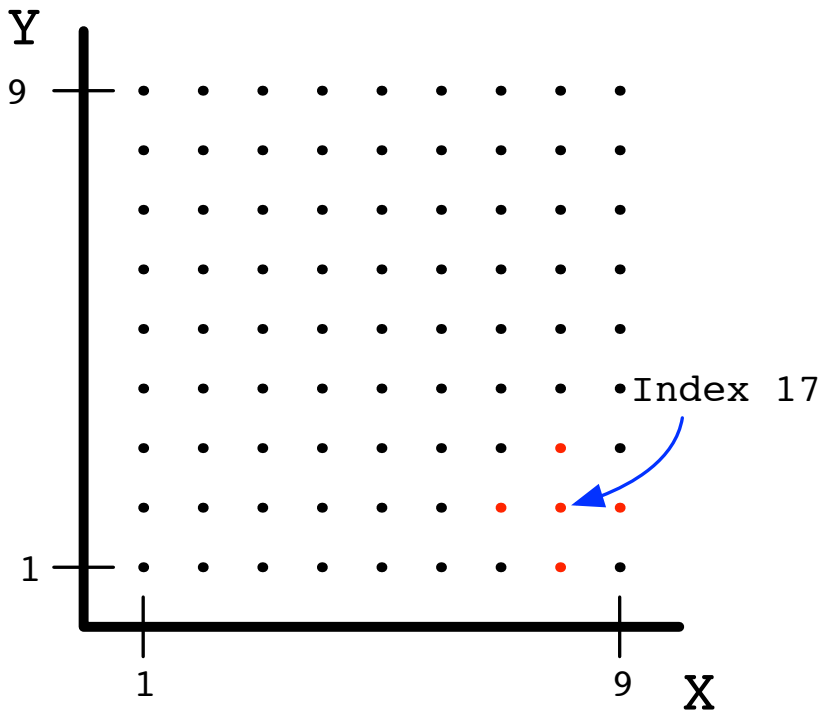
$$\begin{bmatrix} -2 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \cdots & 0 & 1 & -2 \end{bmatrix}$$

This works fine for a one dimensional function like this one



But what about higher dimensionality?

This is what we want!



Luckily, we can use the tensor product to achieve this.
For 2 dimensions

$$K = X \otimes I + I \otimes Y$$

For 3 dimensions

$$K = X \otimes I \otimes I + I \otimes Y \otimes I + I \otimes I \otimes Z$$

This process gives us the appropriate approximation of the kinetic energy matrix.

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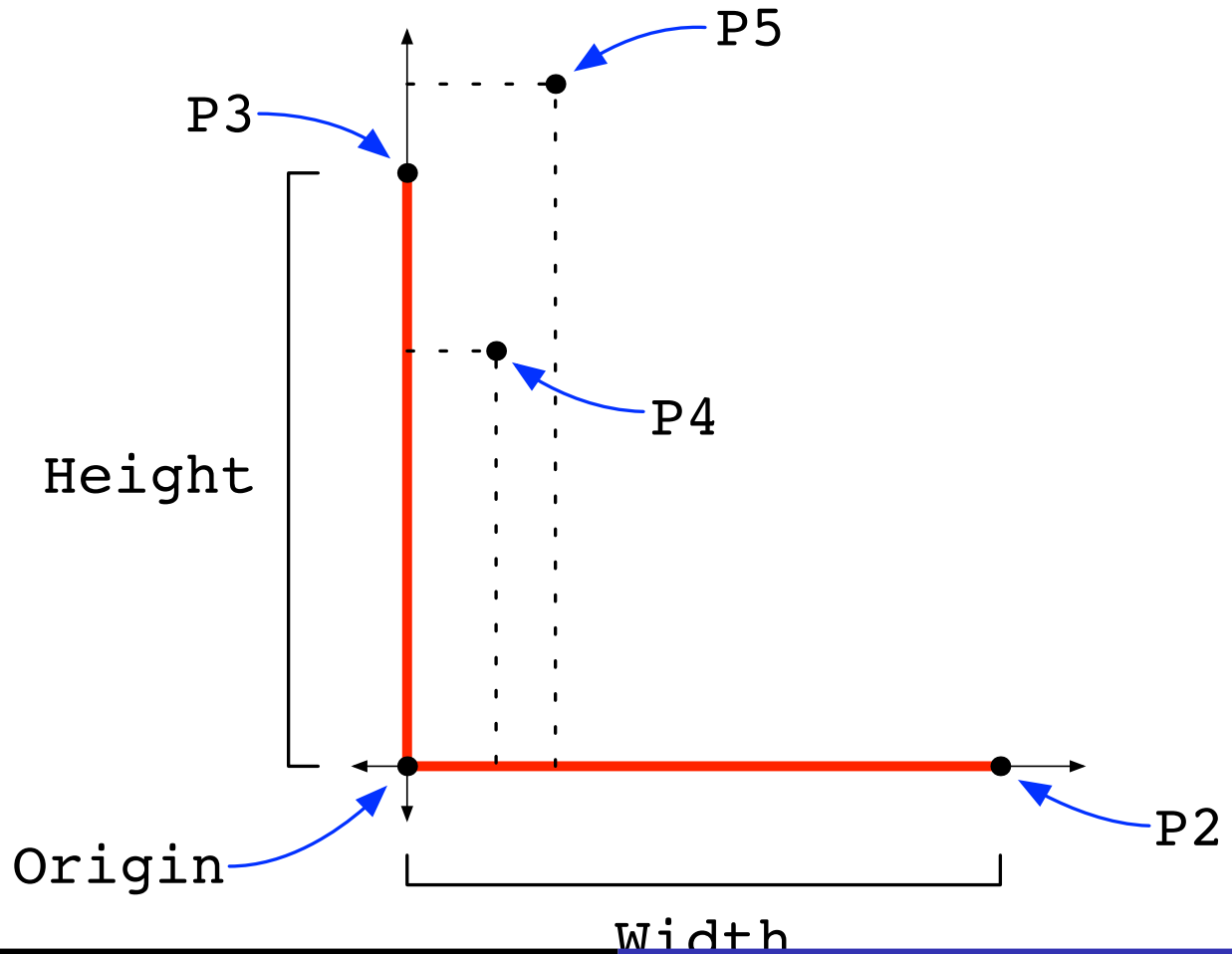
Now we can create our potential energy matrix.

- Have a set of defined primitives
- Iterate through the set of sample points
- For each point determine if it is inside any of the primitves
- Place results along the diagonal of a matrix.

Set of primitives

- Sphere
- Rectangular Prism
- Cylinder

Determining if a point is inside a prism



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Now that we have both matrices we can add them together and solve for the eigenvalues.

$$E\psi = K\psi + V\psi$$

The eigenvalues of E codify the spectral information of the quantum dot.

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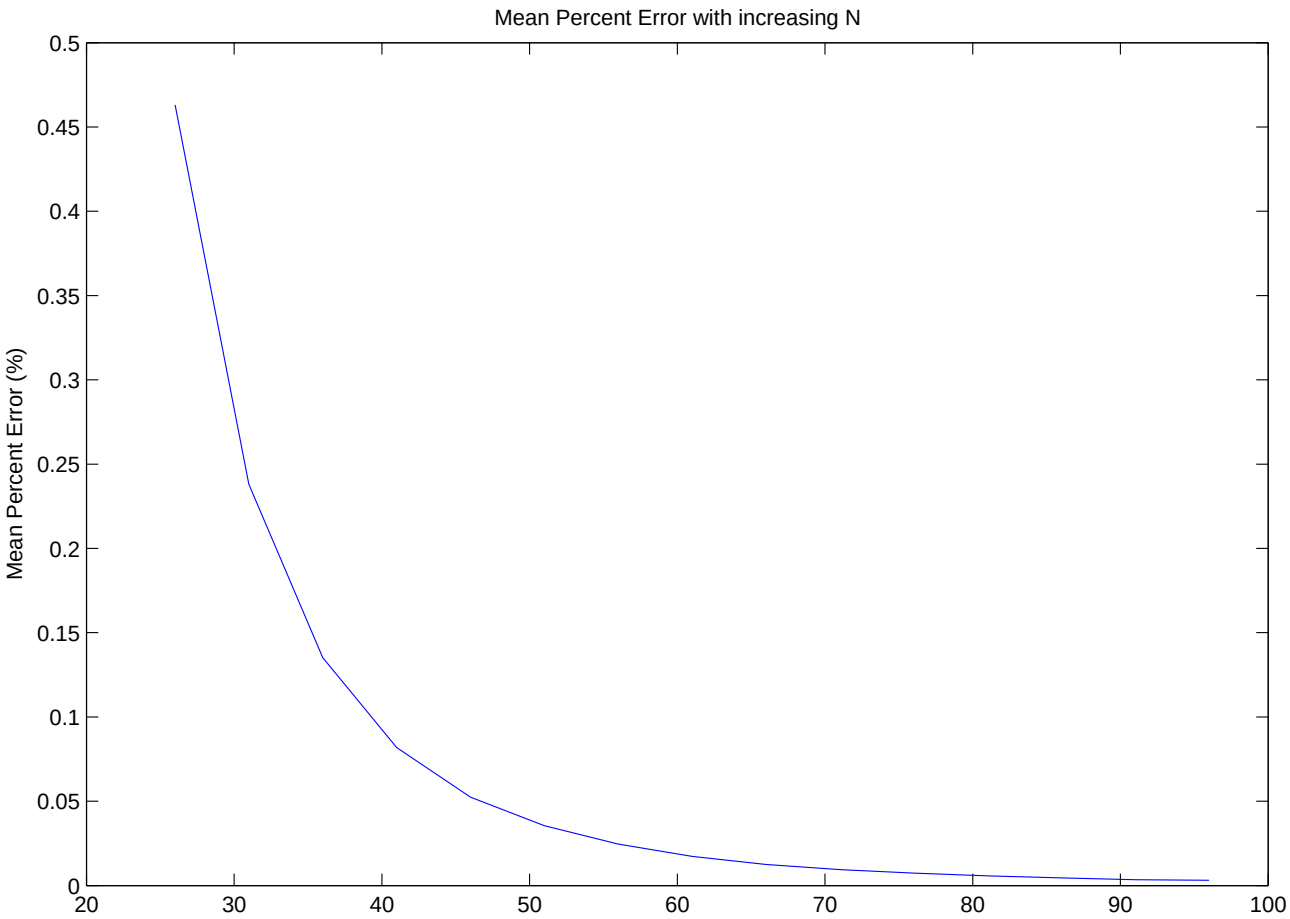
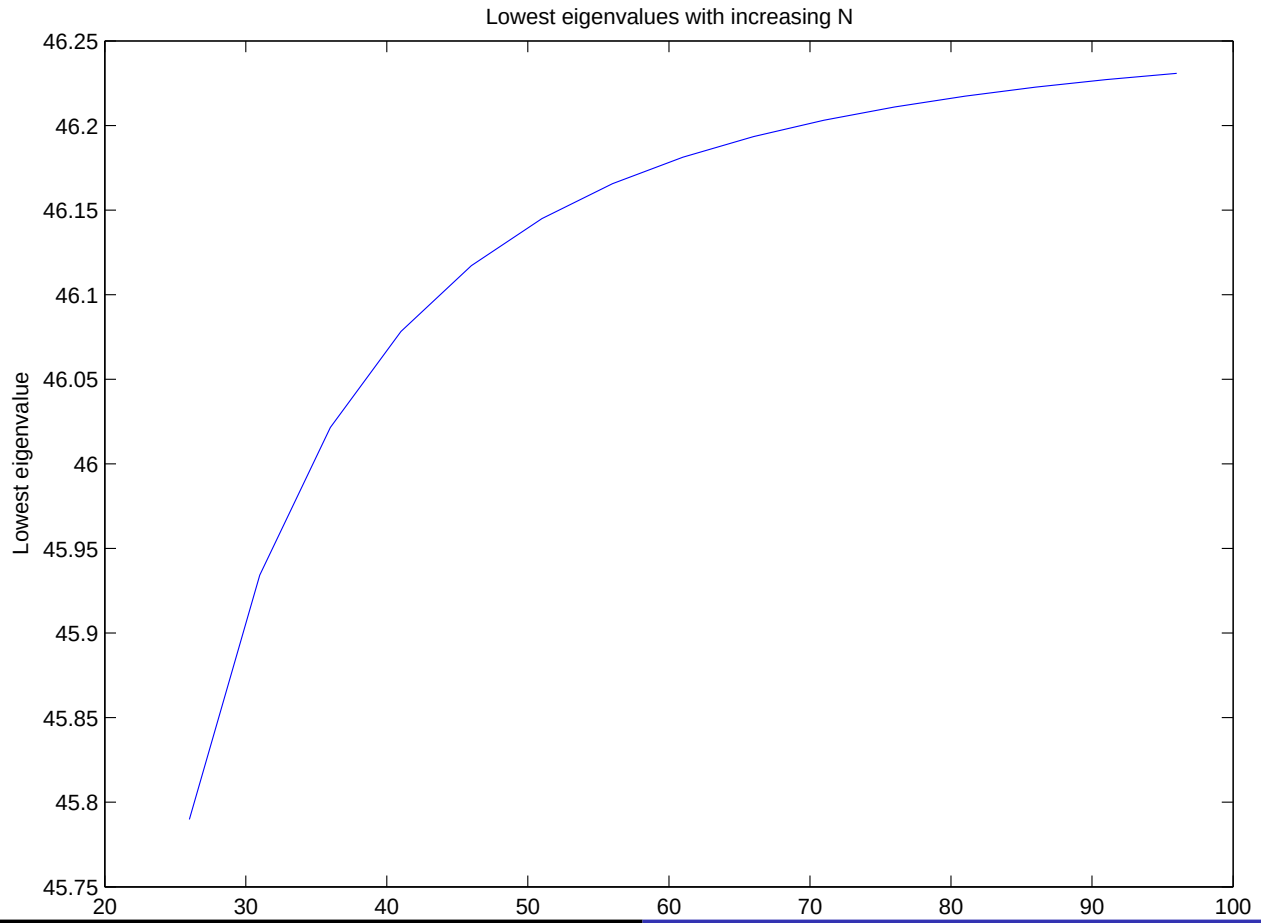
Having an implementation, we can now compare its results to an analytical solution (of a very simple case).
Two comparisons can be made

- First ten eigenvalues should be $3, 6, 6, 6, 9, 9, 9, 11, 11, 11$
- For a cube of .8 the length of the sample cube, the lowest eigenvalue should be 46.2638

Percent error of the first ten eigenvalues (increasing the sample rate)



Value of first eigenvalue with cube of .8 the length of the sample cube.



Conclusion

- By using primitives we can abstract away from the sample-point level.
- Using the approximation methods based on the Taylor series provides a simple yet effective approximation of the energy levels.
- Finding computers that had sufficient memory resources proved to be a problem.
- Outlook
  - Run more tests, including the variation of the potential field (changing the surrounding electric field)
  - Use this to create an evolutionary algorithm to find optimal shapes for desired spectral properties.

Questions

[1] P. Harrison, *Quantum Wells, Wires, and Dots*. Wiley-Interscience, John Wiley and Sons Inc, 2005.

[2] S. Gasiorowicz, *Quantum Physics*. John Wiley and Sons Inc, 1996.