
Introduction to QDot Lab

James K Fodor
University of Florida
ECE Graduate Student

Introduction to QDot Lab

Description of the QDot Lab Simulator

- Simulate and visualize 3d Confined States in a Quantum Dot (powered by NEMO3D)
 - Five types of quantum dot geometry: (i) Box (ii) Cylinder (iii) Dome (iv) Ellipsoid and (v) Pyramid
 - Two types of quantum dot materials (i) GaAs (ii) InAs
 - Optical transitions can be computed and sorted into dark and light lines.

Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, R. Chris Bowen, and Paul von Allmen, Computer Modeling in Engineering and Science (CMES) Volume 3, No. 5 pp 601-642 (2002).

Introduction to QDot Lab

Description of the QDot Lab Examples

- Example 1: Eigenenergy and Wave Functions of Box Quantum Dots
- Example 2: Effect of the Shape of the Quantum Dot on Eigenenergy and Wave Functions
- Example 3: Effect of the Quantum Dot Material on Eigenenergy and Wave Functions

Quantum Dot Lab Problem 1

Problem 1: Box quantum dot

- a) *Simulate a box quantum dot with $L_x=12\text{nm}$, $L_y=11\text{nm}$, and $L_z=10\text{nm}$. Plot the eigenenergy as a function of the state number for the lowest 7 quantum states*
- b) *Plot the 3D wave function of the lowest 7 quantum states.*

1a) Eigenenergy vs. State

Settings and Parameters:

Number of States:

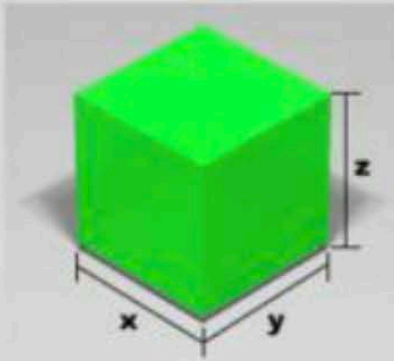
Device Structure | Light Source |

Geometry:

X dimensions:

Y dimensions:

Z dimensions:



Material:

Simulate >

1a) Eigenenergy vs. State

Results:

Result: Output Log

```
The number of OP*x is 304
The number of reorthogonalization steps is 304
The convergence criterion is 5e-07

Found eigval.
0 2.03374 -7.4678e-17
1 2.63894 5.5155e-17
2 2.63894 -1.84216e-16
3 3.24414 -1.82682e-16
4 3.24414 -1.8452e-17
5 3.63257 -8.66608e-17
6 3.63257 5.32426e-17

state 0 Eigval 1.940224e+00 Ritzval 1.940224e+00 residual 2.654283e-27 (Eigval-)
state 1 Eigval 2.368429e+00 Ritzval 2.368429e+00 residual 3.800141e-27 (Eigval-)
# of matrix-vector multiplies: 300
state 2 Eigval 2.445532e+00 Ritzval 2.445532e+00 residual 2.416809e-27 (Eigval-)
state 3 Eigval 2.545422e+00 Ritzval 2.545422e+00 residual 5.419051e-27 (Eigval-)
state 4 Eigval 2.873737e+00 Ritzval 2.873737e+00 residual 1.319393e-19 (Eigval-)
state 5 Eigval 2.973627e+00 Ritzval 2.973627e+00 residual 2.280881e-16 (Eigval-)
state 6 Eigval 3.050730e+00 Ritzval 3.050730e+00 residual 2.264389e-13 (Eigval-)

Memory usage: active: 8.56998 MB;max active: 12.3234 MB;freed: 6.59291 MB;total:
Memory usage: active: 8.52532 MB;max active: 12.3234 MB;freed: 6.63758 MB;total:

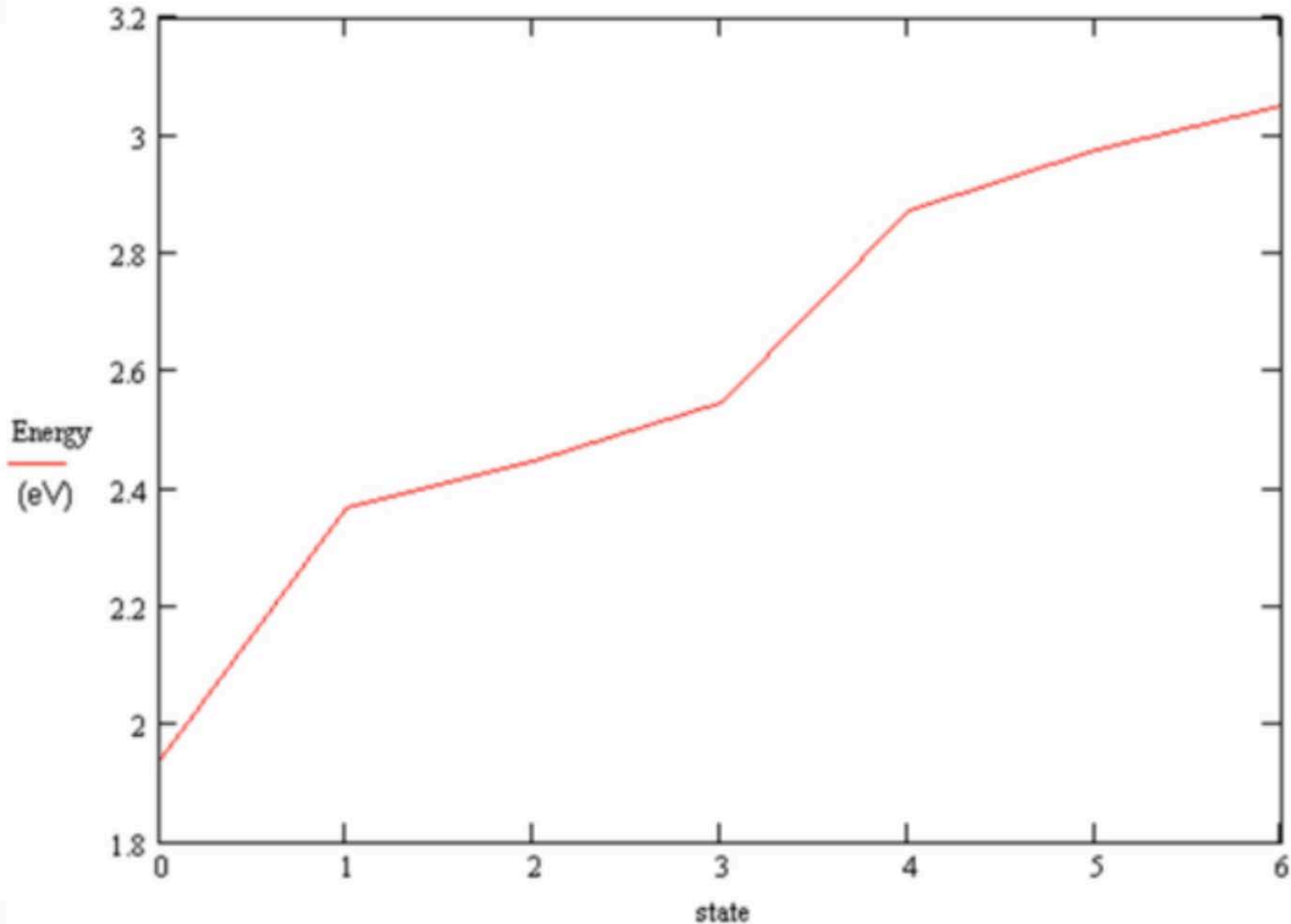
Exiting NEMO-3D
-----
Memory usage: active: 8.52532 MB;max active: 12.3234 MB;freed: 6.63758 MB;total:
Memory usage: active: 0 MB;max active: 0 MB;freed: 0 MB;total: 0 MB; End of fmd:
```

Find:

1 result Parameters

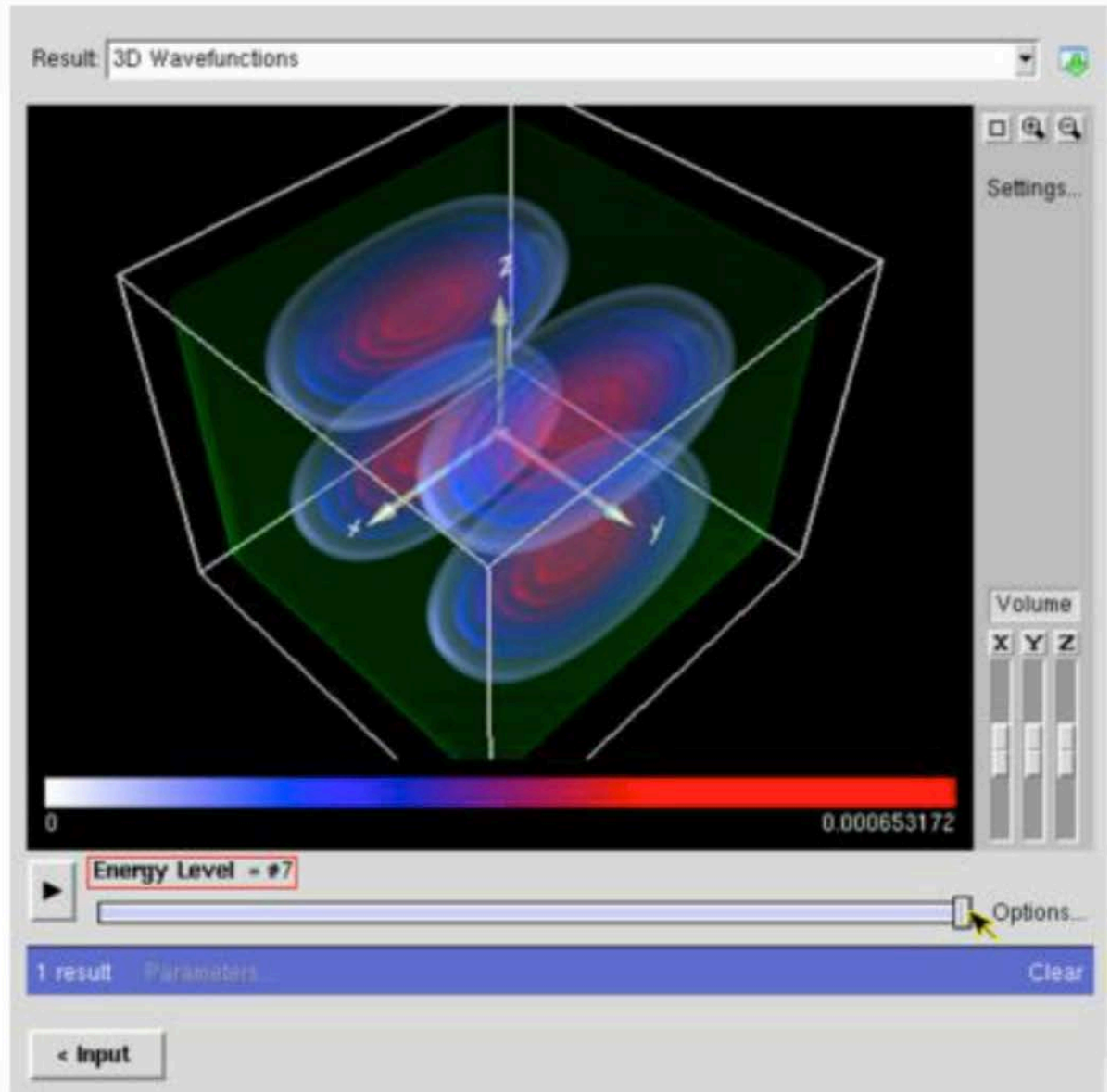
1a) Eigenenergy vs. State

Results:



1b) 3D Wave Function

Results:



Quantum Dot Lab Problem 2

Problem 2: Shape of the quantum dot

- a) *Simulate a box quantum dot, a cylinder dot, a sphere dot, and a pyramid dot, all with $L_x = L_y = L_z = 10\text{nm}$. Plot and compare the eigenenergy as a function of the state number for all quantum dots for the lowest 7 quantum states.*
- b) *Plot and compare the 3D wave function of the lowest quantum state for all quantum dots.*

2a) Eigenenergy vs. State

Settings and Parameters:

Number of States:

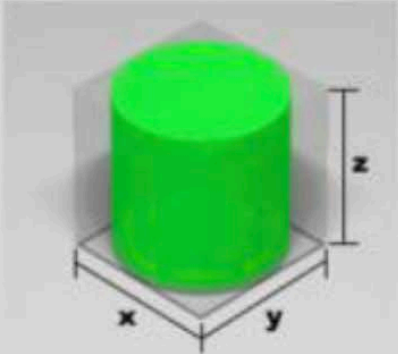
Device Structure | Light Source

Geometry:

X dimensions:

Y dimensions:

Z dimensions:



Material:

Simulate >

2a) Eigenenergy vs. State

Results:

Simulate

Result: Output Log

The convergence criterion is 5e-07

Found eigval.

0	2.03374	-7.4678e-17
1	2.63894	5.5155e-17
2	2.63894	-1.84216e-16
3	3.24414	-1.82682e-16
4	3.24414	-1.8452e-17
5	3.63257	-8.66608e-17
6	3.63257	5.32426e-17

state 0	Eigval	2.033738e+00	Ritzval	2.033738e+00	residual	2.136617e-27	(Eigval-I
state 1	Eigval	2.638937e+00	Ritzval	2.638937e+00	residual	2.666933e-27	(Eigval-I
state 2	Eigval	2.638937e+00	Ritzval	2.638937e+00	residual	2.742975e-27	(Eigval-I
state 3	Eigval	3.244135e+00	Ritzval	3.244135e+00	residual	1.415110e-20	(Eigval-I
state 4	Eigval	3.244135e+00	Ritzval	3.244135e+00	residual	9.149689e-26	(Eigval-I
state 5	Eigval	3.632568e+00	Ritzval	3.632568e+00	residual	2.607226e-14	(Eigval-I
state 6	Eigval	3.632568e+00	Ritzval	3.632568e+00	residual	8.171155e-20	(Eigval-I

Memory usage: active: 8.56998 MB; max active: 12.3234 MB; freed: 6.59291 MB; total:
Memory usage: active: 8.52532 MB; max active: 12.3234 MB; freed: 6.63758 MB; total:

Find:

Select All

4 results Parameters... Clear

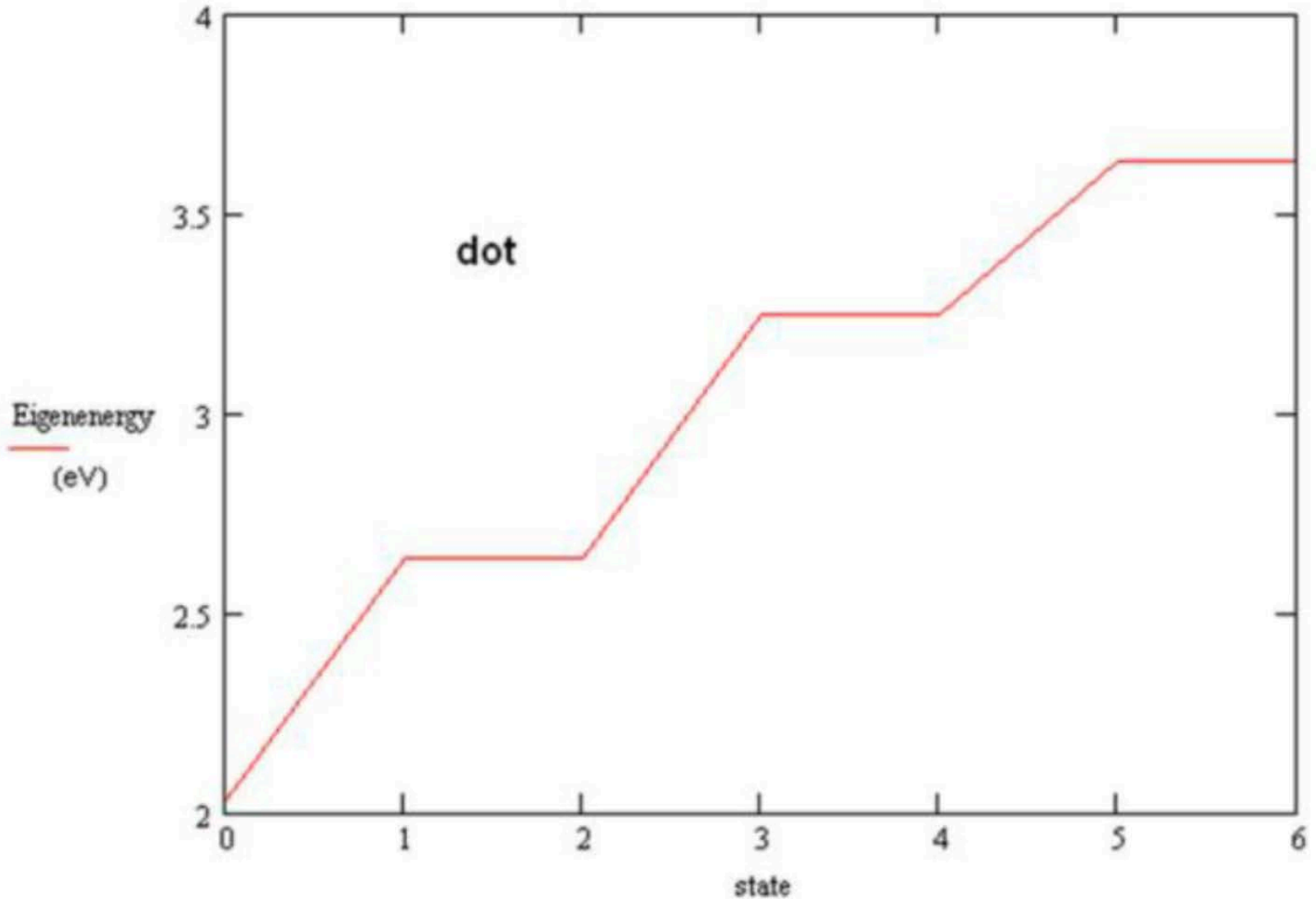
All **Simulation = #1**

Geometry = Box

< Input

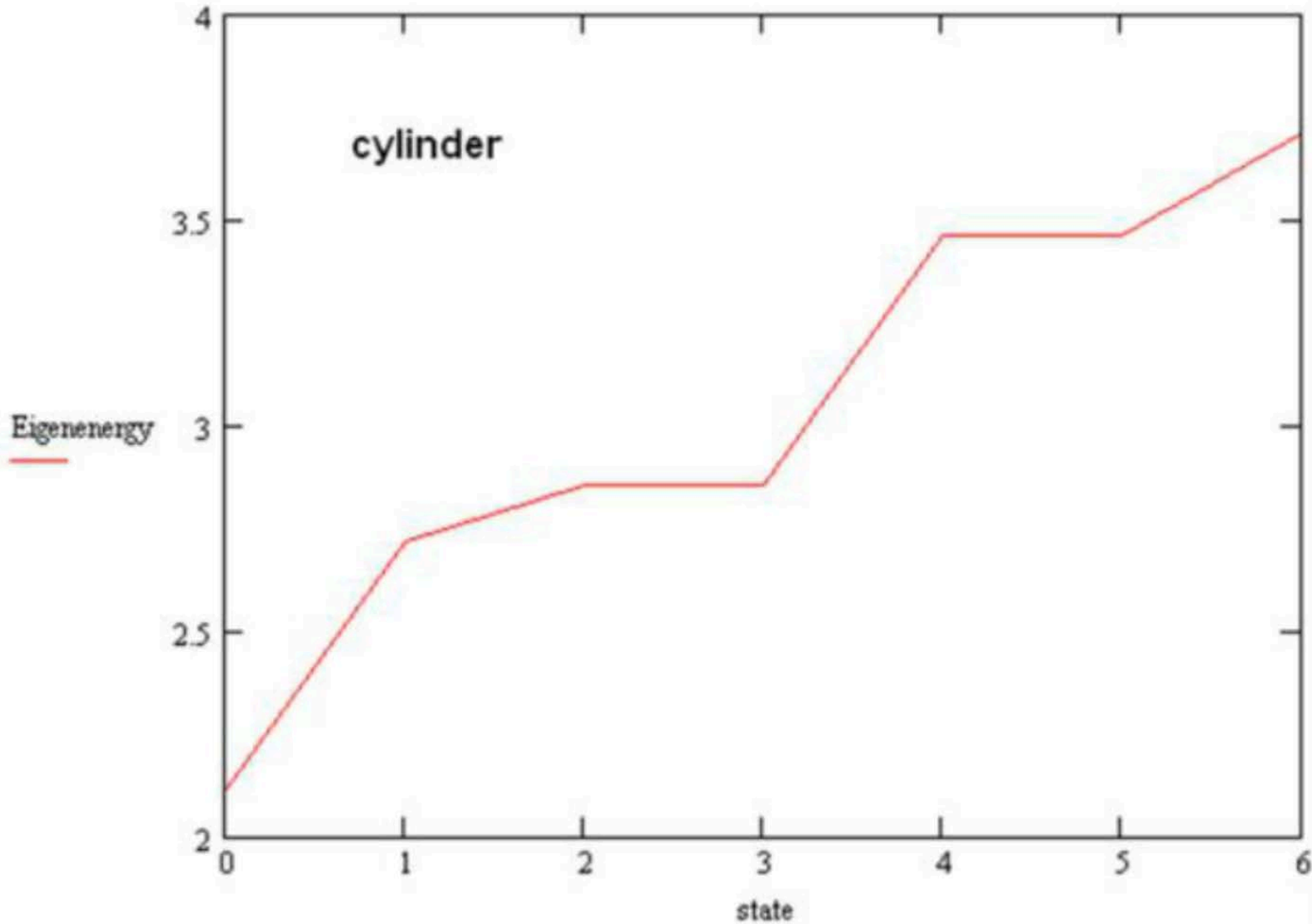
2a) Eigenenergy vs. State

Results:



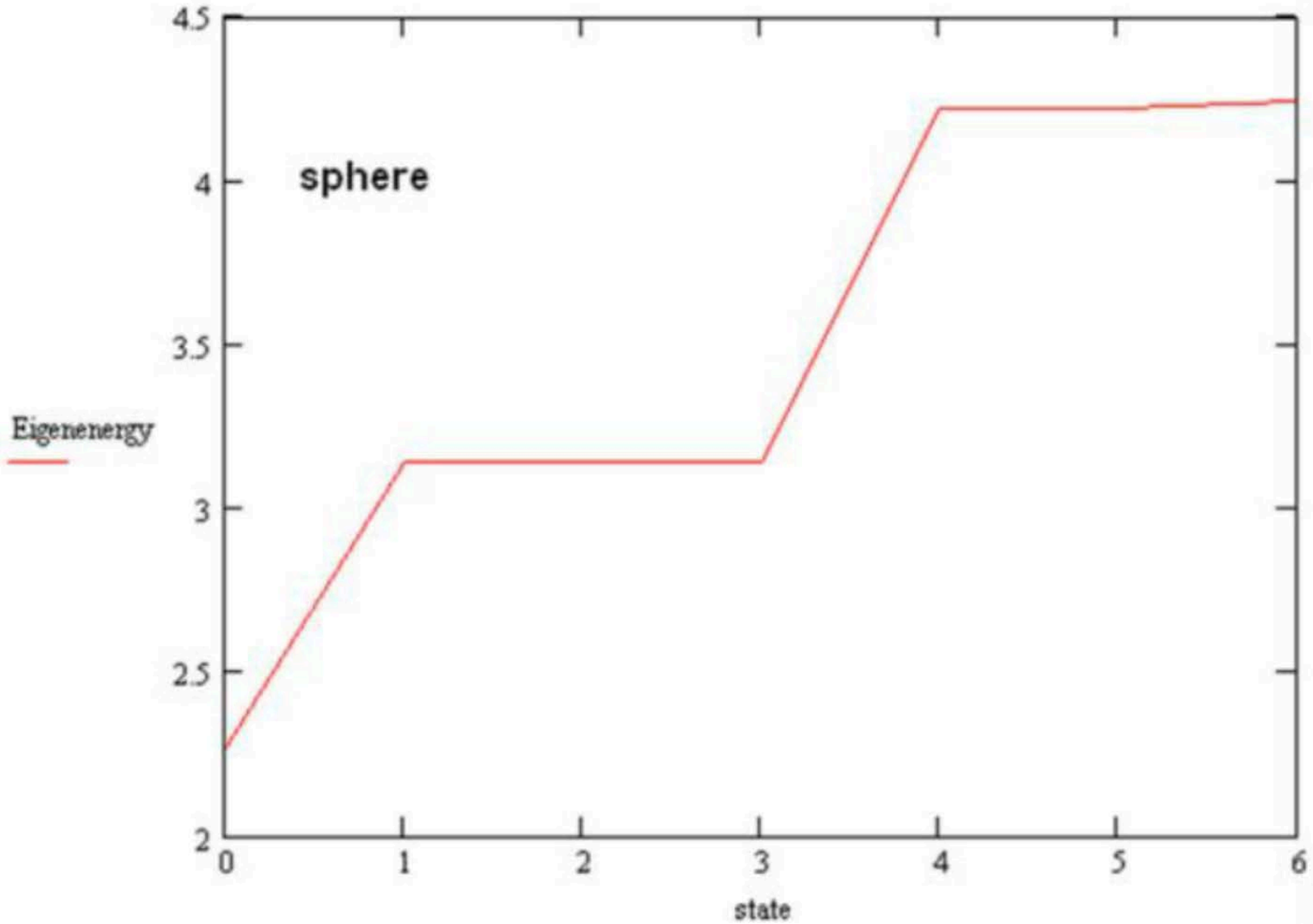
2a) Eigenenergy vs. State

Results:



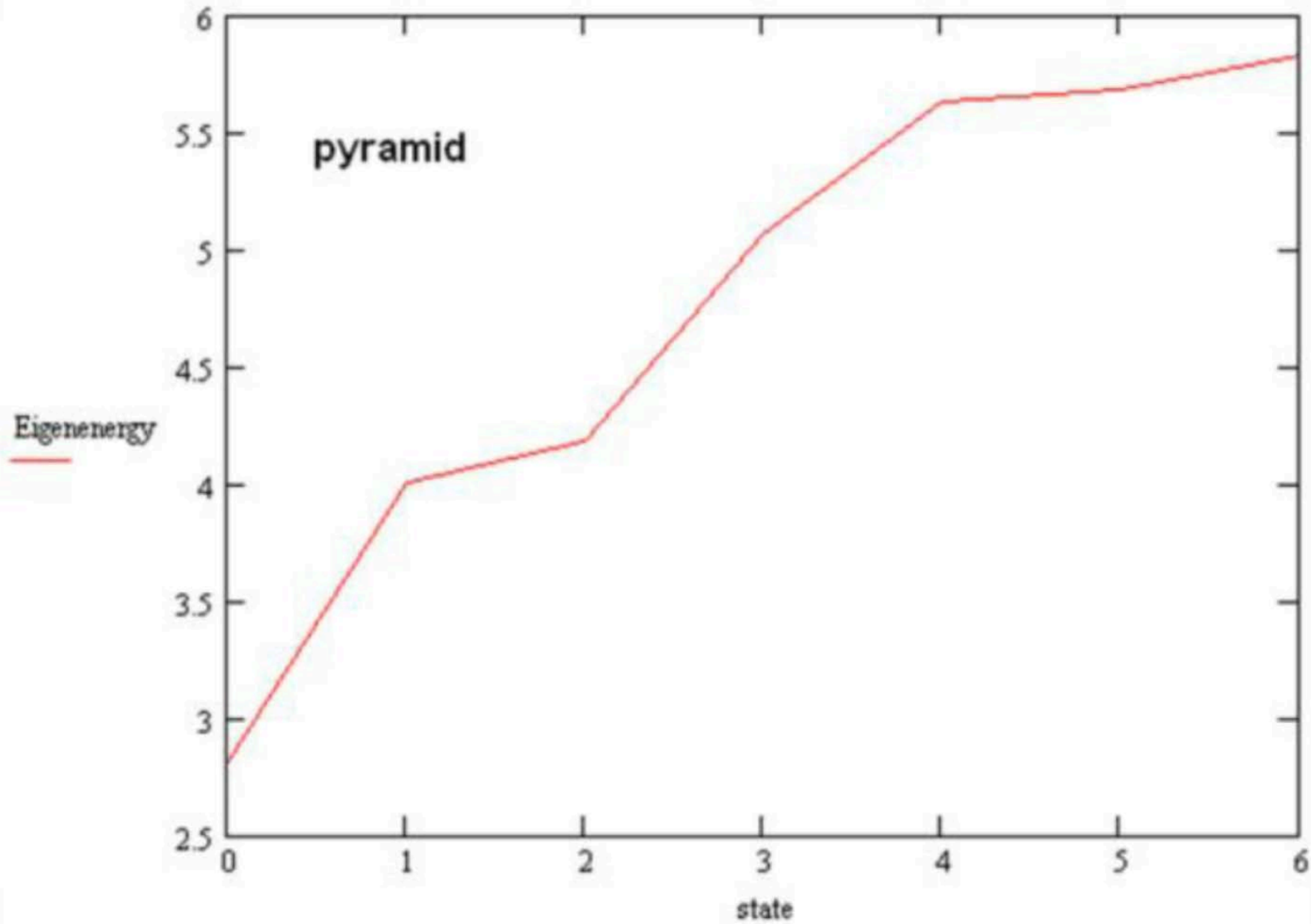
2a) Eigenenergy vs. State

Results:



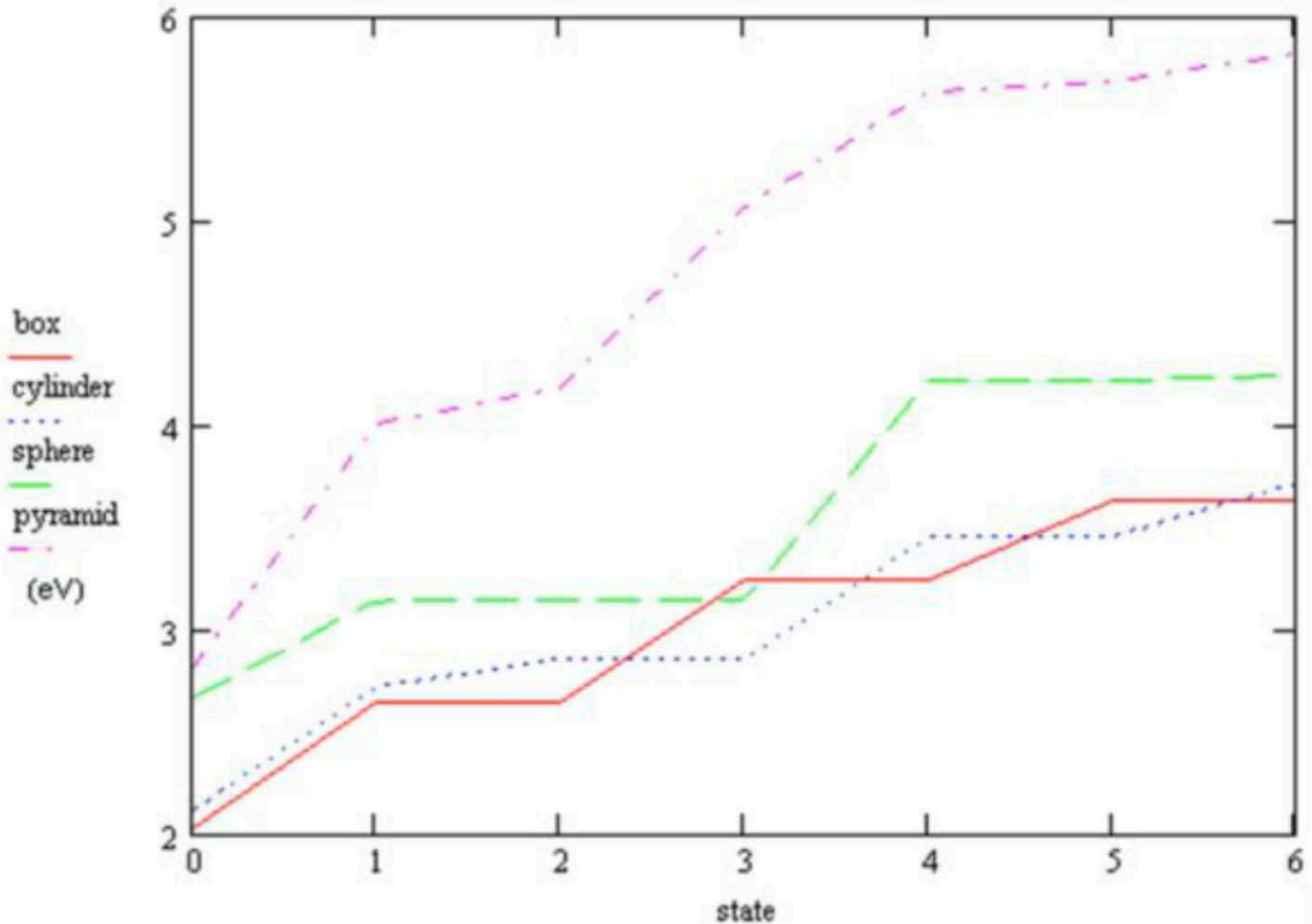
2a) Eigenenergy vs. State

Results:



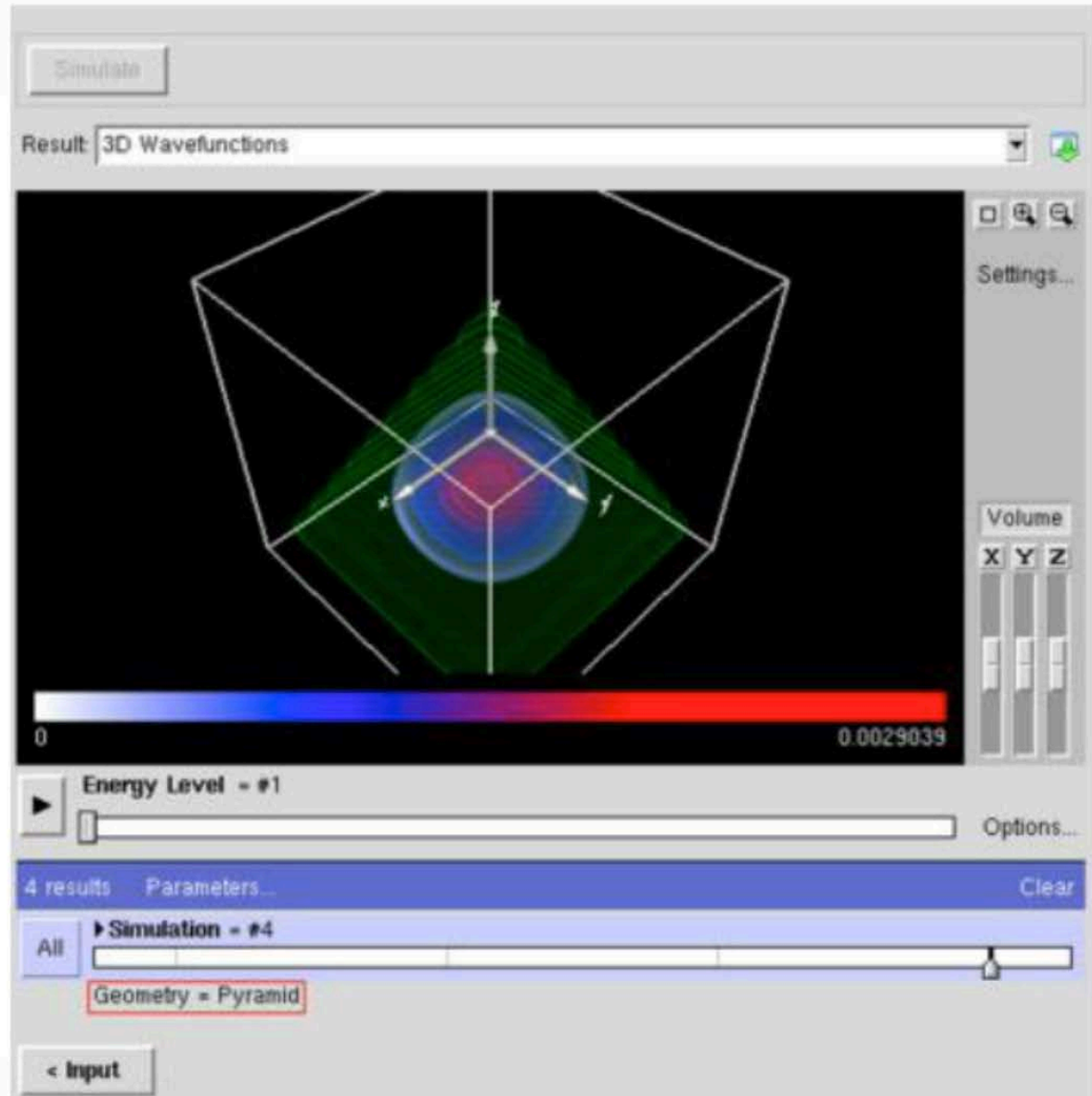
2a) Eigenenergy vs. State

Results:



2b) 3D Wave Function

Results:



Quantum Dot Lab Problem 3

Problem 3: Device material

- a) *Simulate a box quantum dot made of GaAs and a dot made of InAs. Plot and compare the eigenenergy as a function of the state number for the lowest 7 quantum states. Let $L_x = 12\text{nm}$, $L_y = 11\text{nm}$, and $L_z = 10\text{nm}$.*
- b) *Plot and compare the 3D wave functions of the lowest 3 quantum states for the GaAs and the InAs quantum dots.*

3a) Eigenenergy vs. State

Settings and Parameters:

Number of States: 7

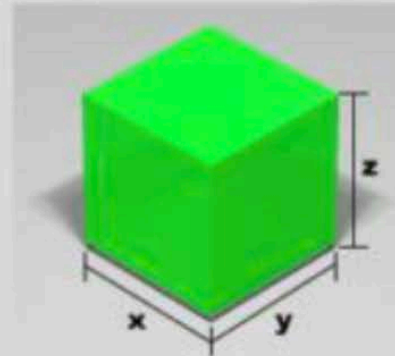
Device Structure | Light Source

Geometry: Box

X dimensions: 12.0nm

Y dimensions: 11.0nm

Z dimensions: 10.0nm



Material: InAs

Simulate >

3a) Eigenenergy vs. State

Results:

Result: Output Log

The number of OP*x is 304
The number of reorthogonalization steps is 304
The convergence criterion is 5e-07

Found eigval.

State	Eigval	Ritzval	Residual
0	2.03374 -7.4678e-17	2.03374 -7.4678e-17	2.654283e-27
1	2.63894 5.5155e-17	2.63894 5.5155e-17	3.800141e-27
2	2.63894 -1.84216e-16	2.63894 -1.84216e-16	2.416809e-27
3	3.24414 -1.82682e-16	3.24414 -1.82682e-16	5.419051e-27
4	3.24414 -1.8452e-17	3.24414 -1.8452e-17	1.319393e-19
5	3.63257 -8.66608e-17	3.63257 -8.66608e-17	2.280881e-16
6	3.63257 5.32426e-17	3.63257 5.32426e-17	2.264389e-13

of matrix-vector multiplies: 300

Memory usage: active: 8.56998 MB;max active: 12.3234 MB;freed: 6.59291 MB;total:
Memory usage: active: 8.52532 MB;max active: 12.3234 MB;freed: 6.63758 MB;total:

Exiting NEMO-3D

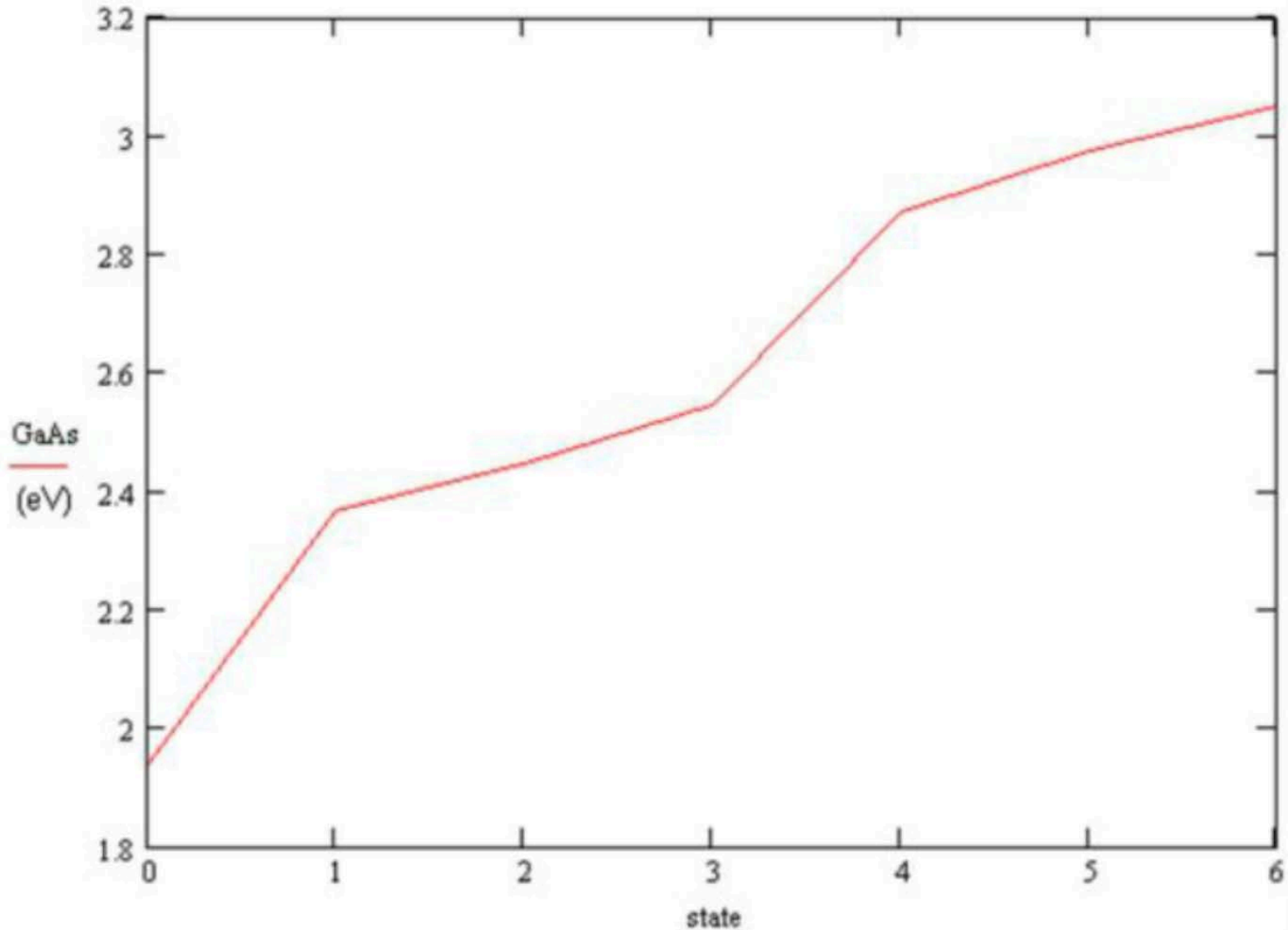
Memory usage: active: 8.52532 MB;max active: 12.3234 MB;freed: 6.63758 MB;total:
Memory usage: active: 0 MB;max active: 0 MB;freed: 0 MB;total: 0 MB; End of fmd:

Find:

1 result Parameters

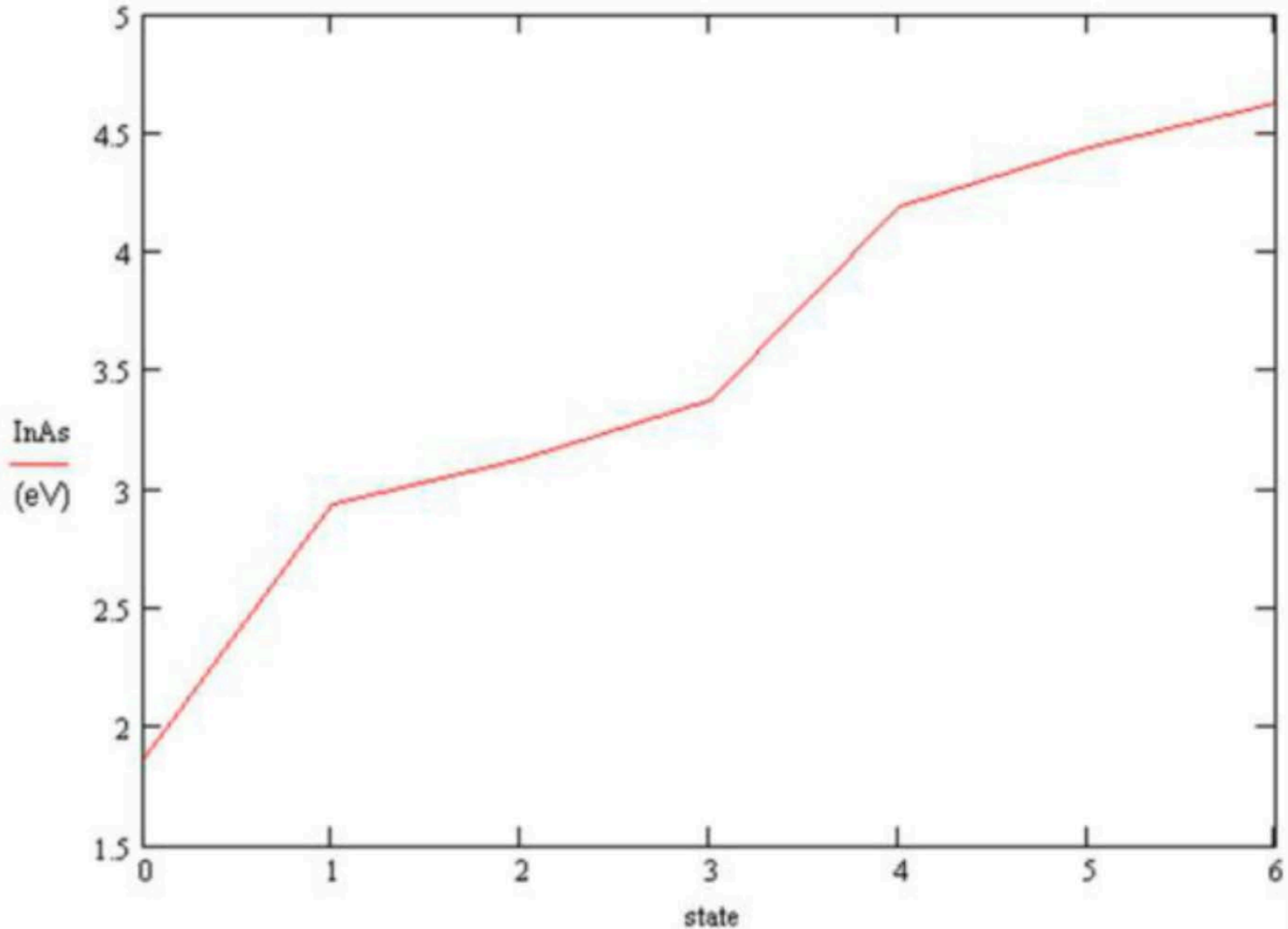
3a) Eigenenergy vs. State

Results:



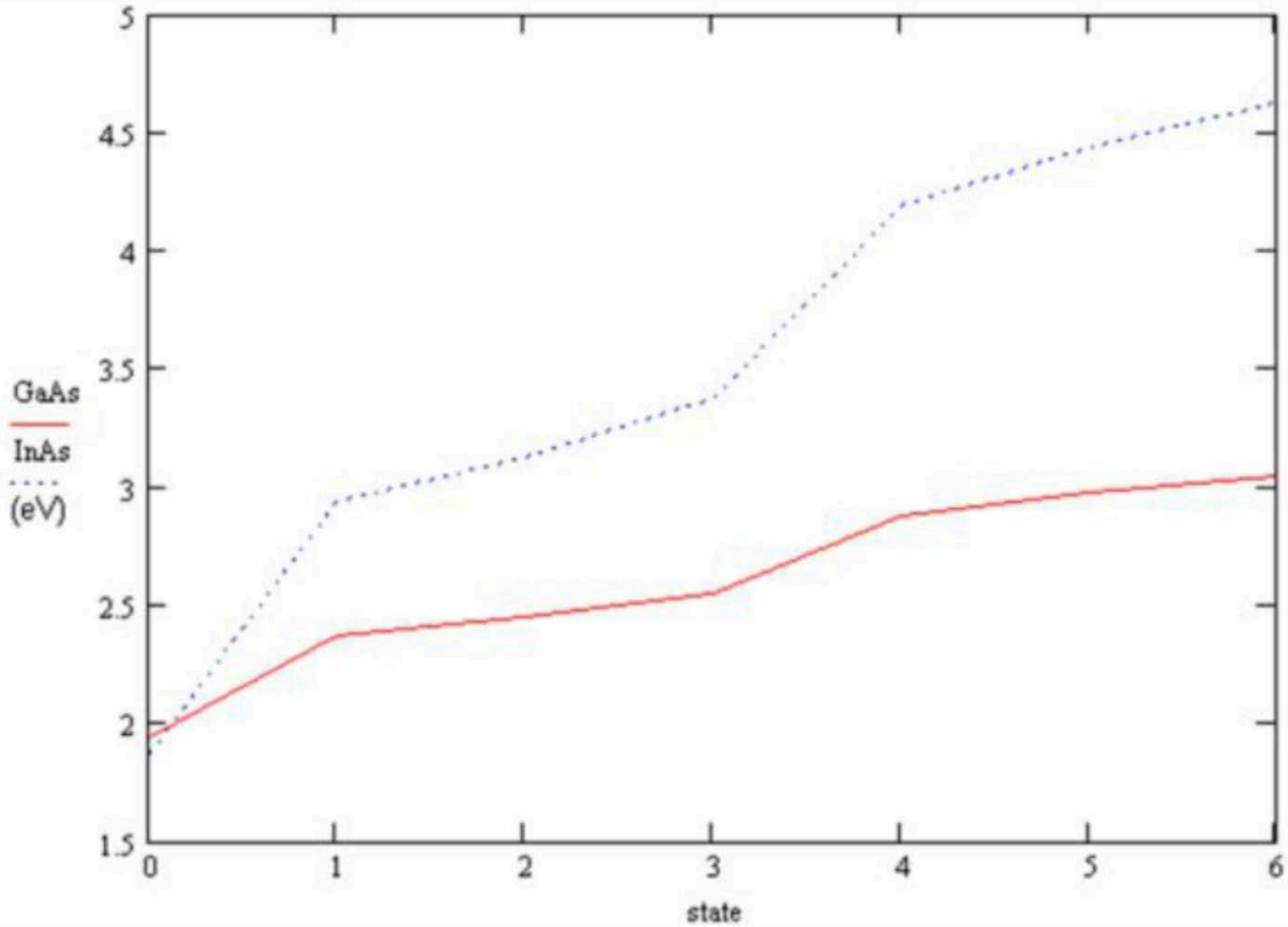
3a) Eigenenergy vs. State

Results:



3a) Eigenenergy vs. State

Results:



3b) 3D Wave Function

Results:

