Numerical Modeling of Rectangular Quantum Dot

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Outline

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- Result
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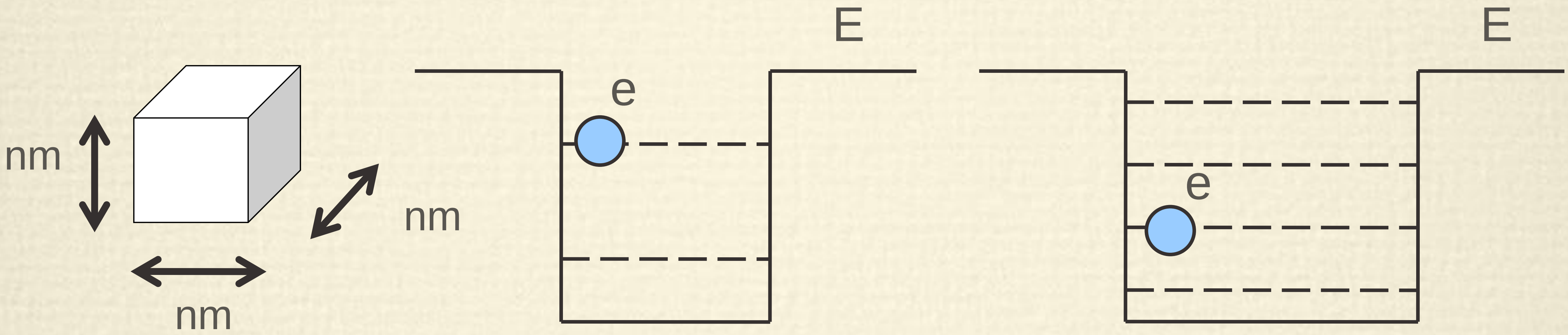
Introduction

- Quantum Dot



Introduction

- Schrödinger equation

$$\left[-\frac{\hbar^2}{2}\nabla\cdot\left(\frac{1}{m^*(\vec{r})}\nabla\right)+V(\vec{r})\right]\psi(\vec{r})=E\psi(\vec{r})$$

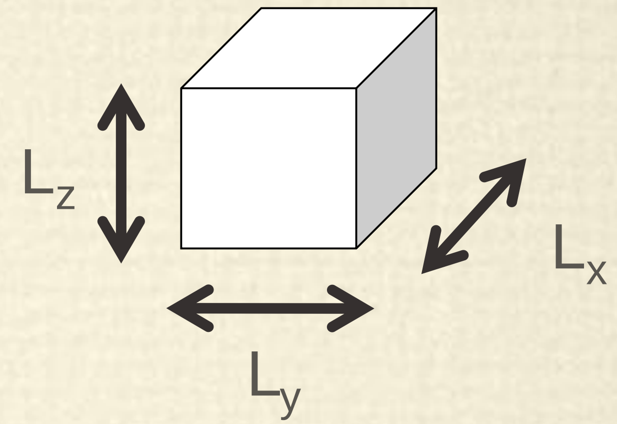
E

$\psi(\vec{r})$

$p(\vec{r})=\left|\psi(\vec{r})\right|^2$

Introduction

- Rectangular Quantum Dot



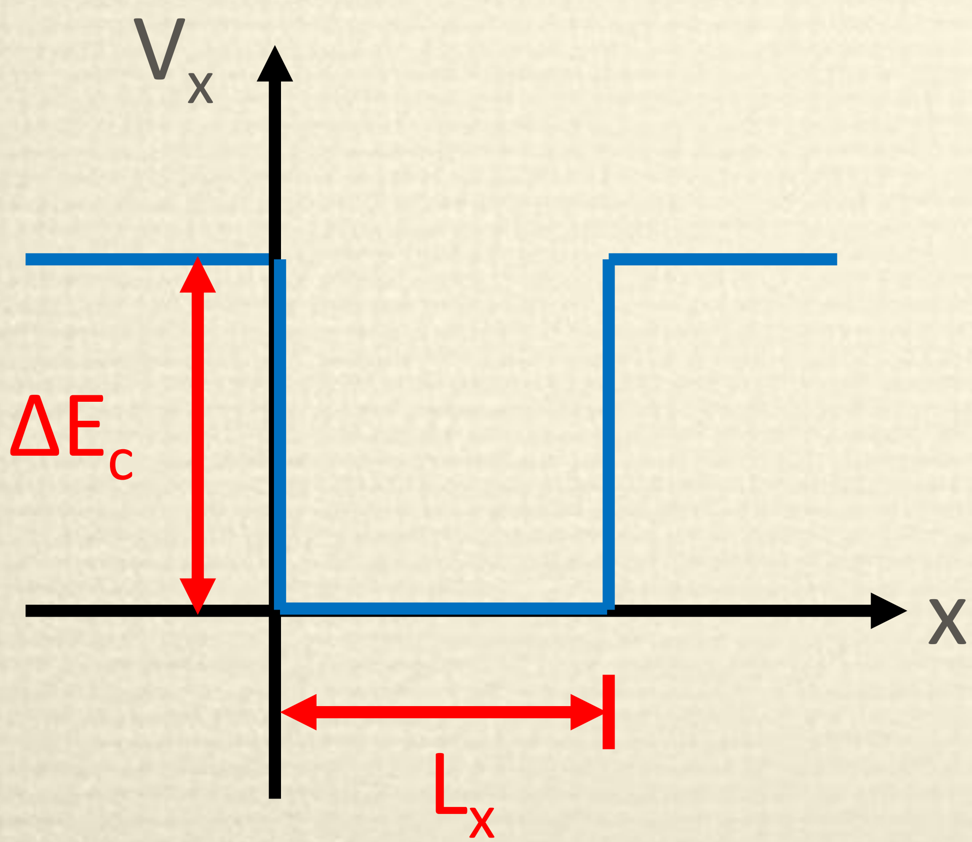
$$\left[-\frac{\hbar^2}{2}\nabla\cdot\left(\frac{1}{m^*(\vec{r})}\nabla\right)+V(\vec{r})\right]\psi(\vec{r})=E\psi(\vec{r})$$

$$E = E_x + E_y + E_z$$

$$\psi(\vec{r})=\psi_x(x)\psi_y(y)\psi_z(z)$$

$$V(\vec{r})\sim V_x(x)+V_y(y)+V_z(z)$$

$$\left[-\frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m^*}\frac{d}{dx}\right)+V_x\right]\psi_x = E_x\psi_x$$



Modeling

- Finite Difference Method

$$\left[-\frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m^*}\frac{d}{dx}\right)+V_x\right]\psi_x = E_x\psi_x$$

$$-\frac{\hbar^2}{2}\left[\frac{d}{dx}\left(\frac{1}{m^*}\right)\frac{d\psi}{dx}+\frac{1}{m^*}\frac{d^2\psi}{dx^2}\right]+V_x\psi_x = E_x\psi_x$$

$$f'(x)=\frac{f(x+\Delta x)-f(x-\Delta x)}{2\Delta x}$$

$$f''(x)=\frac{f(x+\Delta x)-2f(x)+f(x-\Delta x)}{\Delta x^2}$$

- Boundary condition for bound states

Modeling

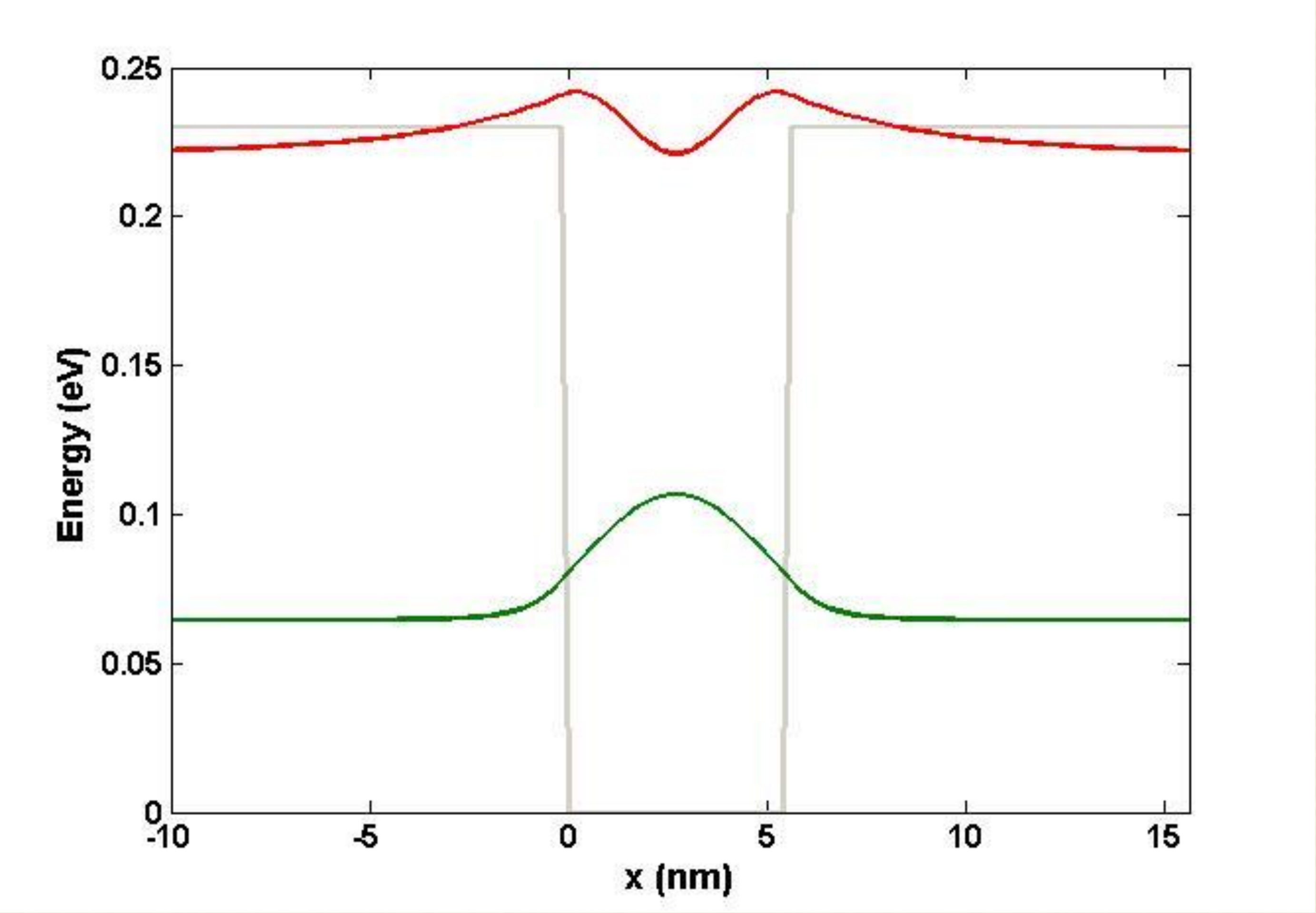
- Modified 1D Schrödinger equation

$$\overline{\overline{M}}\,\overline{\Psi} = E\overline{\Psi}$$

$$M_{ij} = -\frac{\hbar^2}{2}\begin{cases} -\frac{2}{m_i} - \frac{2}{\hbar^2}V_i & i = j \\ \frac{1}{m_i} + \frac{1}{4}\left(\frac{1}{m_{i+1}} - \frac{1}{m_{i-1}}\right) & i = j-1 \\ \frac{1}{m_i} - \frac{1}{4}\left(\frac{1}{m_{i+1}} - \frac{1}{m_{i-1}}\right) & i = j+1 \\ 0 & otherwise \end{cases}$$

Result (1D Schrödinger)

- GaAs/AlGaAs Quantum well*



Exact solutions (meV)*	Numerical solutions (meV)	Error (%)
64.2	64.6	0.62
220.8	221.1	0.14

*H. Tan, G. L. Snider, L. D. Chang, and E. L. Hu, J. Appl. Phys., vol.68, no.8, 1990.

Modeling: continue

- Quantum Dot (3D)

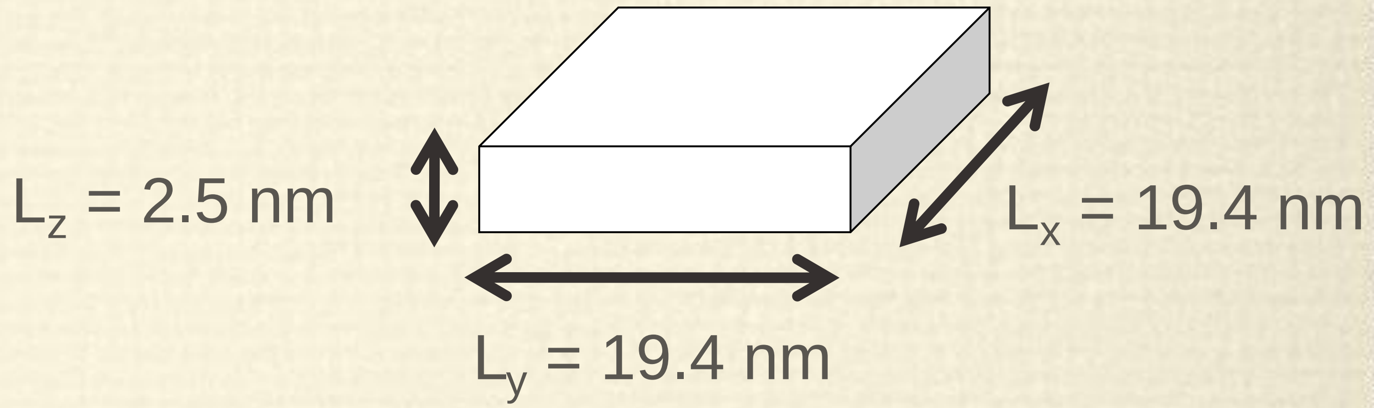
$$E = E_x + E_y + E_z$$

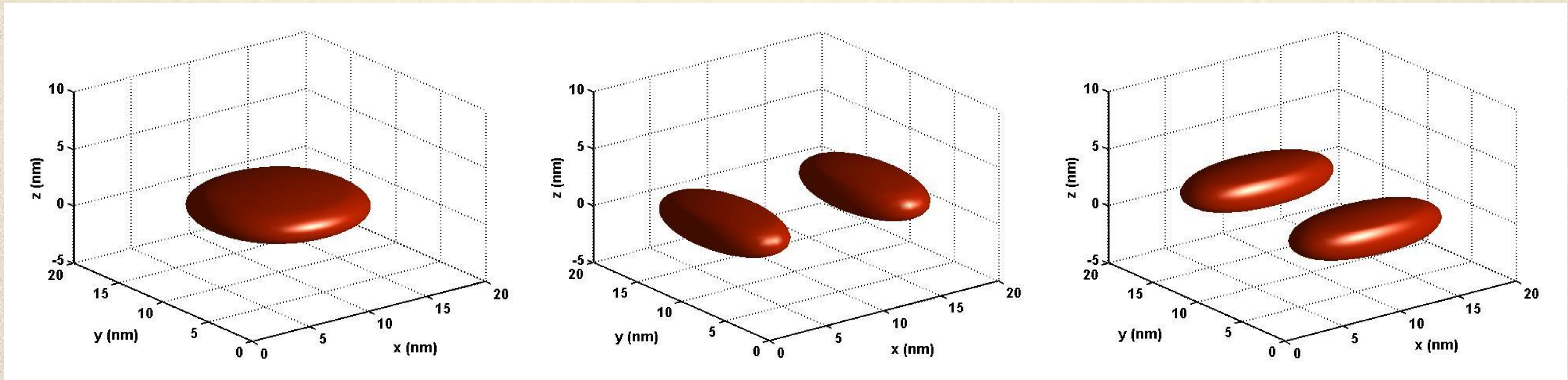
$$\psi(\vec{r}) = \psi_x(x)\psi_y(y)\psi_z(z)$$

$$p(\vec{r}) = \left|\psi(\vec{r})\right|^2$$

Result

- InGaAs/GaAs Quantum dot**
  - $\Delta E_c = 0.324$ eV

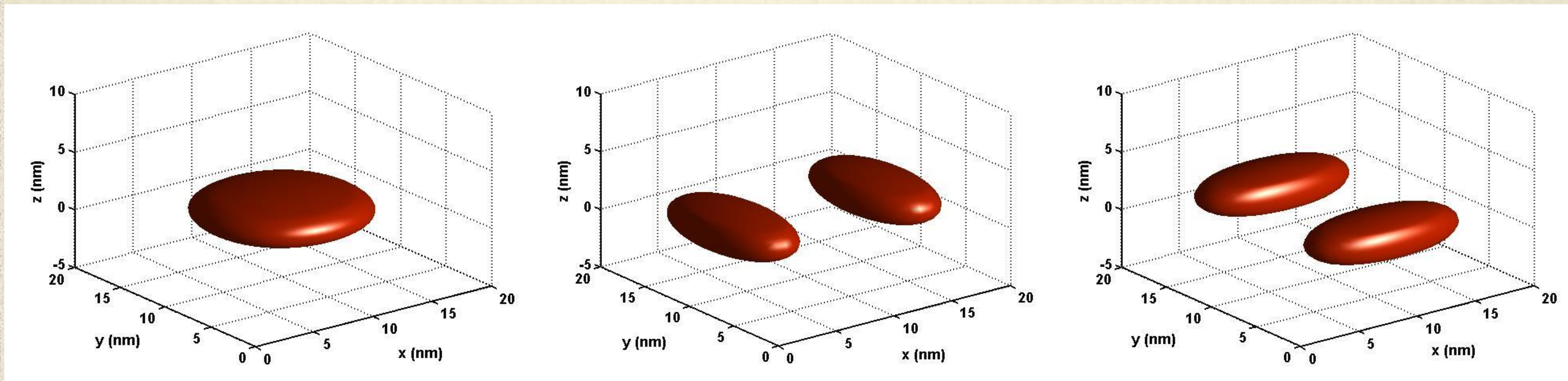




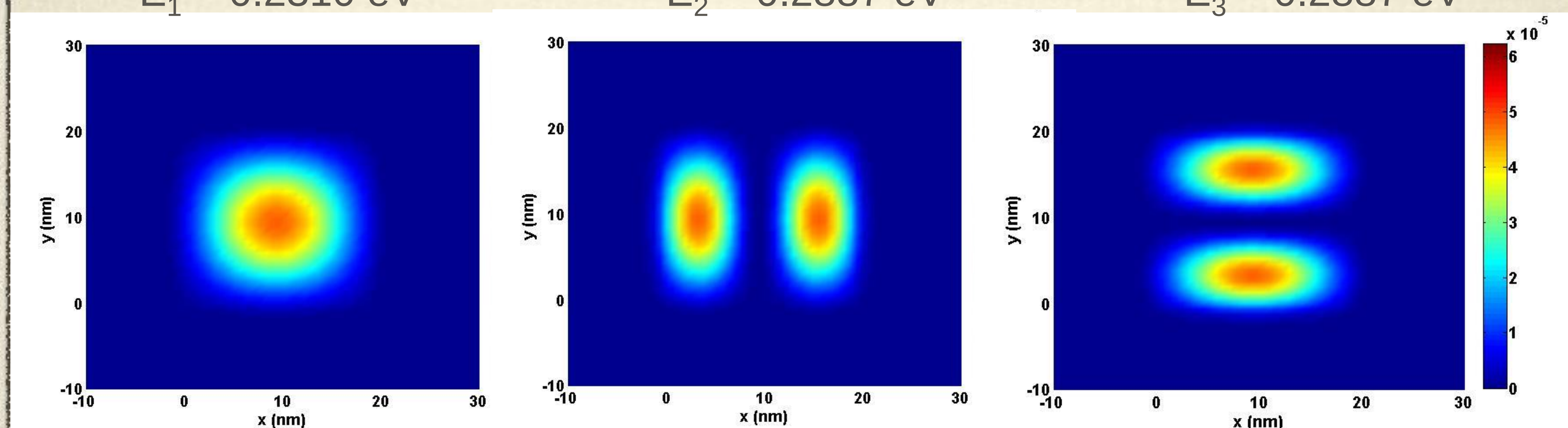
$E_1 = 0.2310$ eV $E_2 = 0.2887$ eV $E_3 = 0.2887$ eV

** N. Thudsalingkarnsakul, Master's Thesis, Faculty of Engineering, 2008.

Result



$E_1 = 0.2310$ eV $E_2 = 0.2887$ eV $E_3 = 0.2887$ eV



Conclusion

- The model can solve for
  - The energy states
  - The wave functions
  - The probability distributions
- Analytical tool for the electronic structure of a quantum dot

References

[1] G. W. Bryant and G. S. Solomon, *Optics of Quantum Dots and Wires*, 1st ed. Norwood, MA: Artech House, Inc., 2005.

[2] G. A. Narvaez, G. Bester, and A. Zunger, “Dependence of the electronic structure of self-assembled (In,Ga)As/GaAs quantum dots on height and composition,” J. Appl. Phys., vol. 98, 043708, 2005.

[3] O. L. Lazarenkova and A. A. Balandin, “Miniband formation in a quantum dot crystal,” J. Appl. Phys., vol. 89, no. 10, 2001.

[4] I. H. Tan, G. L. Snider, L. D. Chang, and E. L. Hu, “A Self-Consistent solution of Schrodinger-Poisson Equation Using a Nonuniform Mesh,” J. Appl. Phys., vol.68, no.8, 1990.

[5] N. Thudsalingkarnsakul, *Effective One-Dimensional Electronic Structure of InGaAs Quantum Dot Molecules*, Master’s Thesis, Department of Electrical Engineering, Faculty of Engineering, 2008.

Thank you

Q&A