DIPARTIMENTO DI MATEMATICA E INFORMATICA

Simulating the Energy Spectrum of Quantum Dots

7th IIC-EMTCCM
European Master in Theoretical Chemistry and Computational Modelling
7th International Intensive Course

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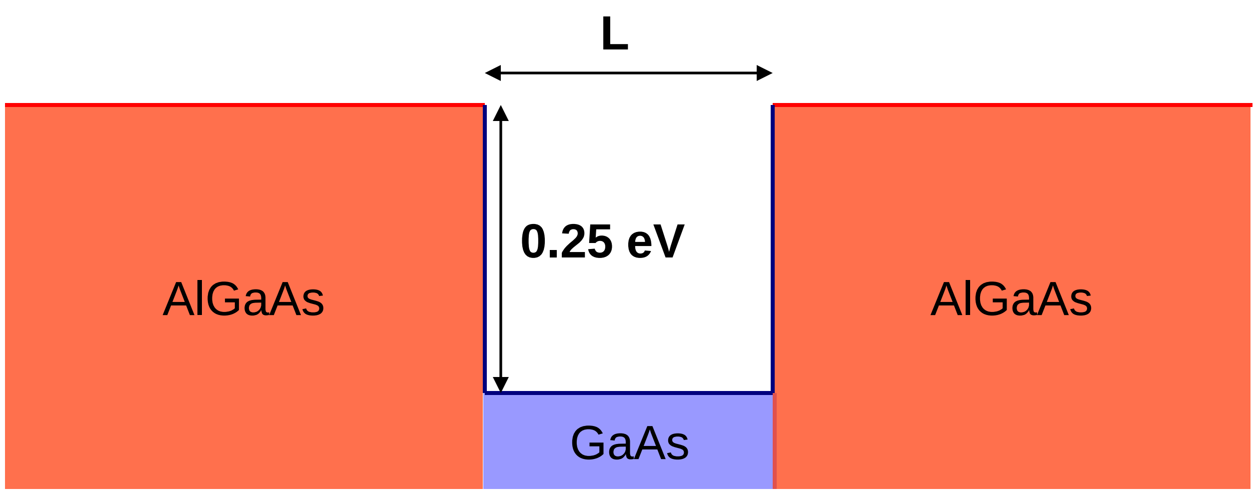
PROBLEM 1. Calculate the electron energy spectrum of a 1D GaAs/AlGaAs QD as a function of the size.

Hint: consider GaAs effective mass all over the structure.



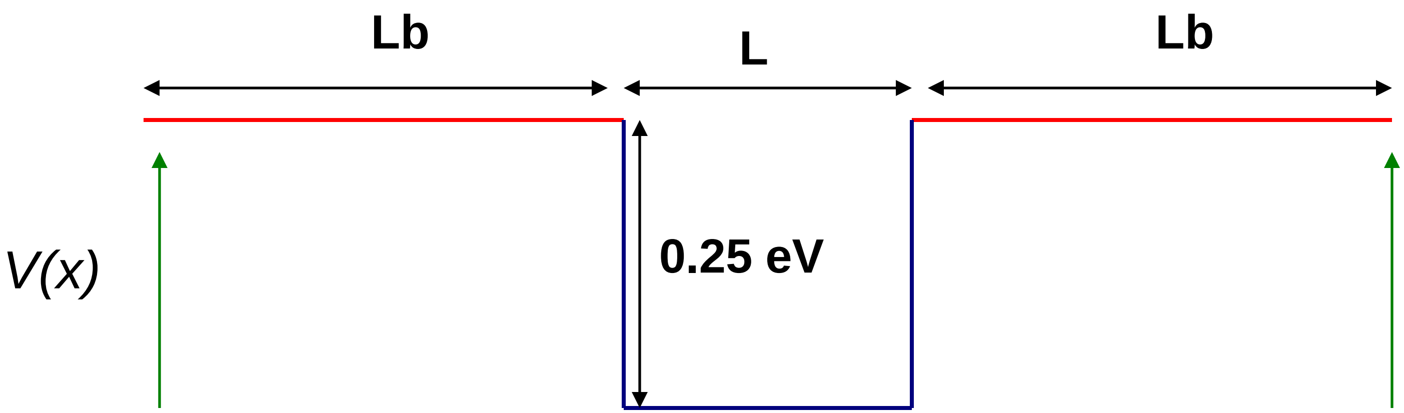
$m^*_{GaAs} = 0.05\ m_0$

The single-band effective mass equation:

$$[-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2}+V(x)]\,f(x)=E\,f(x)$$

Let us use atomic units (*ħ=m₀=e=1*)

$$\boxed{[-\frac{1}{2(m^*/m_0)}\frac{d^2}{dx^2}+V(x)]\,f(x)=E\,f(x)}$$



BC: $f(0)=0$

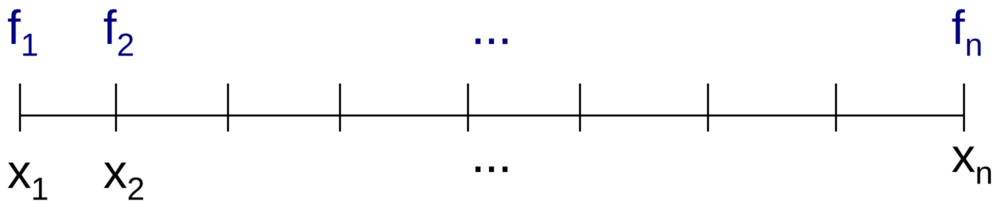
$m^*_{GaAs} = 0.05\ m_0$

$f(L_t)=0$

Numerical integration of the differential equation: *finite differences*

$$[-\frac{1}{2m^*}\frac{d^2}{dx^2}+V(x)]\,f(x)=E\;f(x)$$

Discretization grid

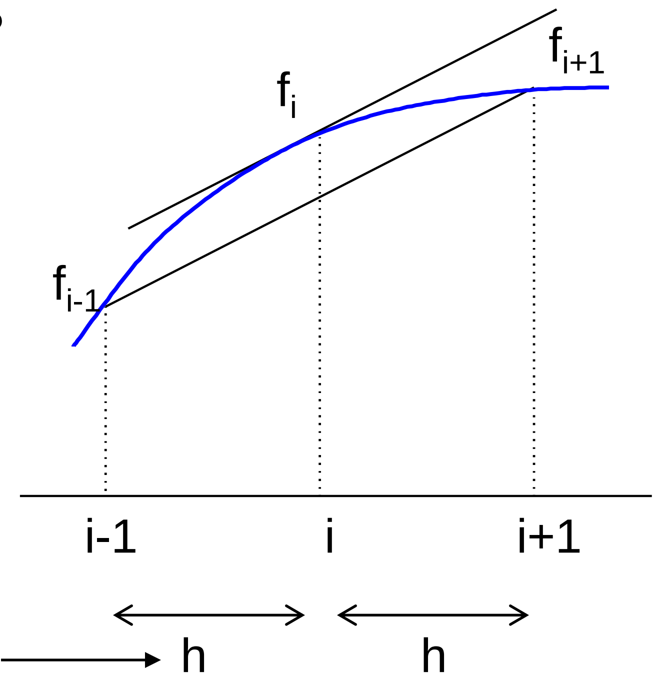


How do we approximate the derivatives at each point?

$$f^{'}(x_i)=f_i^{'}=\frac{f_{i+1}-f_{i-1}}{2h}$$

$$f^{''}(x_i)=f_i^{''}=\frac{f_{i+1}^{'}-f_{i-1}^{'}}{2h}=$$

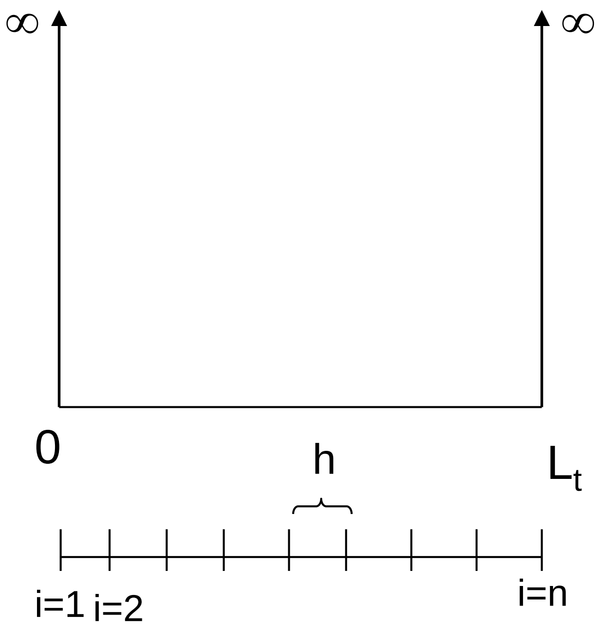
$$=\ldots=\frac{f_{i+1}-2f_i+f_{i-1}}{h^2}$$



Step of the grid → h

FINITE DIFFERENCES METHOD

$$[-\frac{1}{2m^*}\frac{d^2}{dx^2} + V(x)]\, f(x) = E\, f(x) \quad + \quad BCs: \left| \begin{array}{l} f(0)=0 \\ f(L_t)=0 \end{array} \right.$$



$$n = \frac{L_t}{h} + 1$$

1. Define discretization grid
2. Discretize the equation:

$$-\frac{1}{2m^*} f_i'' + V_i f_i = E\, f_i$$

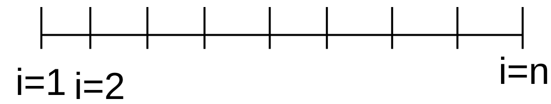
$$-\frac{1}{2m^* h^2}[\, f_{i+1} - 2 f_i + f_{i-1}] + V_i f_i = E\, f_i$$

3. Group coefficients of fwd/center/bwd points

$$\left(-\frac{1}{2m^* h^2}\right) f_{i-1} + \left(\frac{1}{m^* h^2} + V_i\right) f_i + \left(-\frac{1}{2m^* h^2}\right) f_{i+1} = E\, f_i$$

$$\boxed{b\, f_{i-1} + a_i\, f_i + b\, f_{i+1} = E\, f_i}$$

$$b\,f_{i-1} + a_i\,f_i + b\,f_{i+1} = E\,f_i$$



Trivial eqs: $f_1 = 0$, $f_n = 0$.

Extreme eqs:

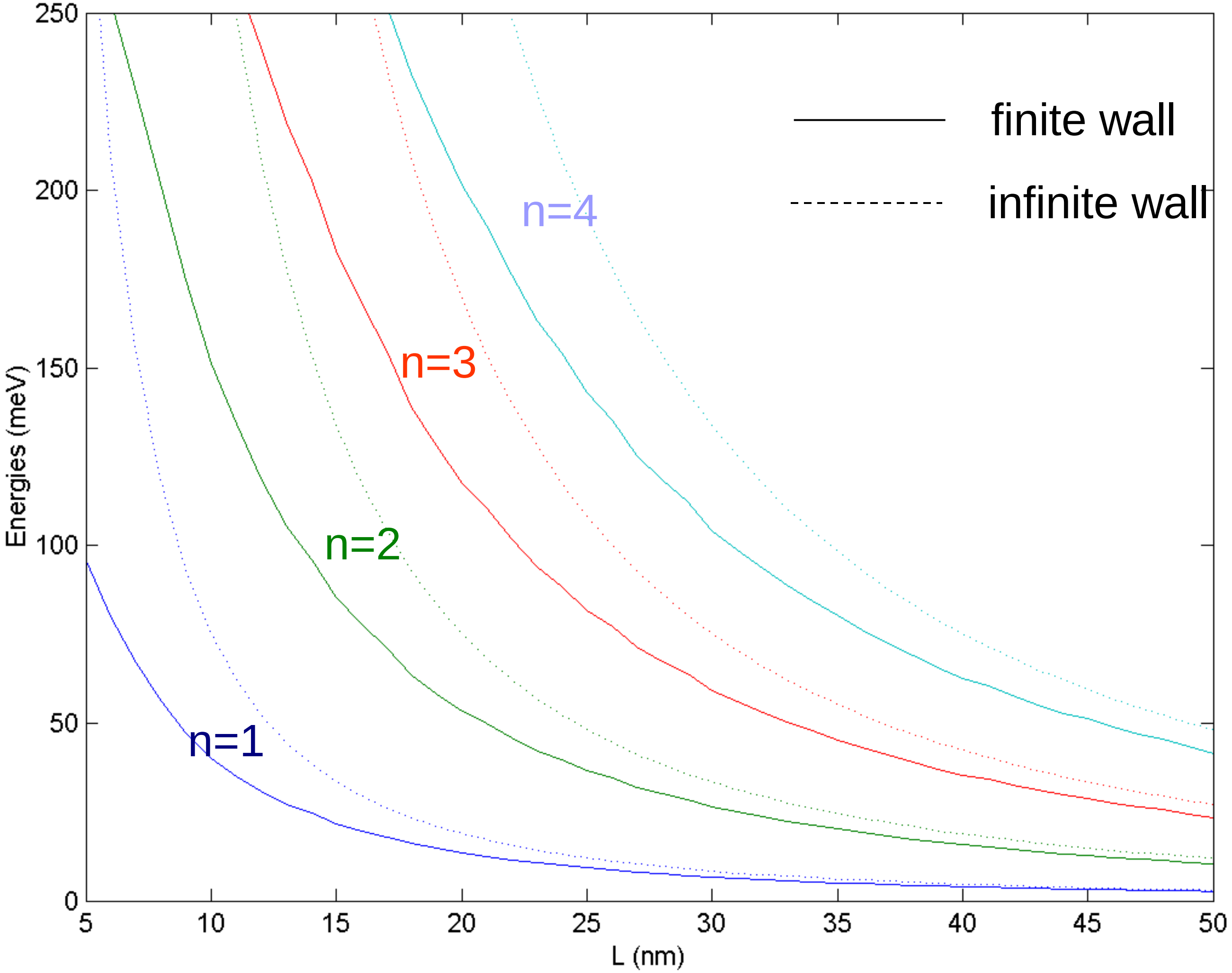
$$\begin{aligned} i = 2 &\;\rightarrow\; b\,\cancelto{0}{f_1} + a_2\,f_2 + b\,f_3 = E\,f_2 \\ i = n-1 &\;\rightarrow\; b\,f_{n-2} + a_{n-1}\,f_{n-1} + b\,\cancelto{0}{f_n} = E\,f_{n-1} \end{aligned}$$

Matriz (n-2) x (n-2) - sparse

We now have a standard diagonalization problem (dim n-2):

$$\begin{bmatrix} a_2 & b & & & \\ b & a_3 & b & & \\ & \ddots & \ddots & \ddots & \\ & & b & a_{n-2} & b \\ & & & b & a_{n-1} \end{bmatrix} \cdot \begin{bmatrix} f_2 \\ f_3 \\ \vdots \\ f_{n-2} \\ f_{n-1} \end{bmatrix} = E \begin{bmatrix} f_2 \\ f_3 \\ \vdots \\ f_{n-2} \\ f_{n-1} \end{bmatrix}$$

The result should look like this:



PROBLEM 1 – Additional questions

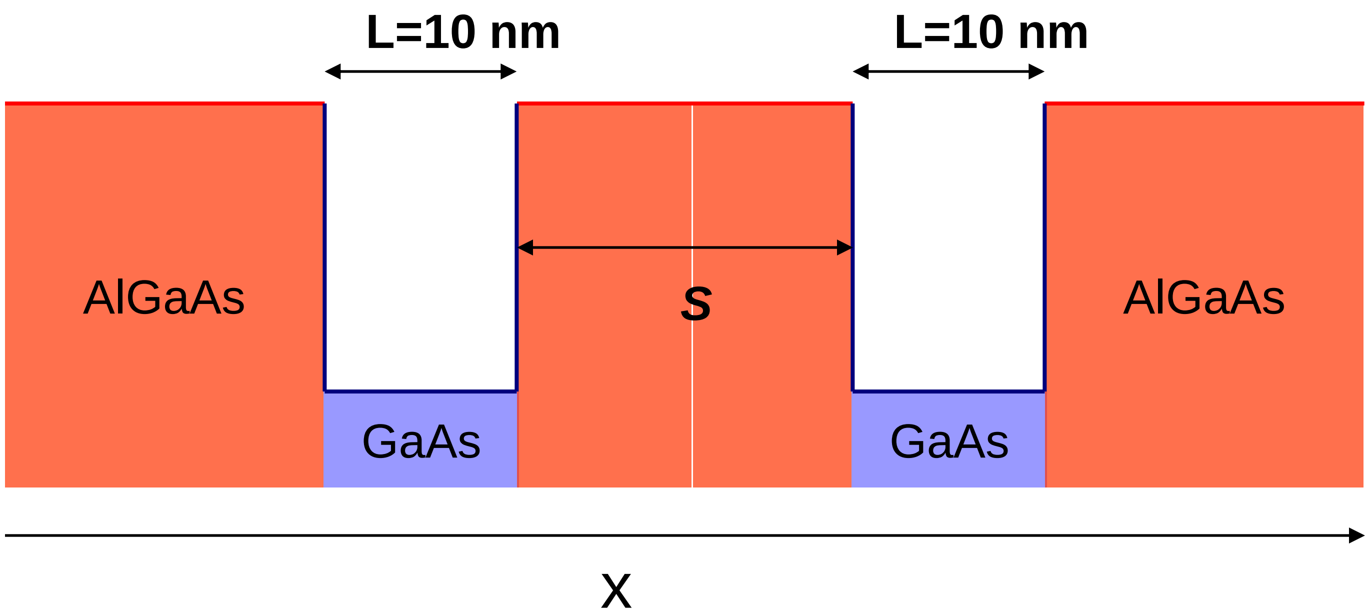
a) Compare the converged energies with those of the particle-in-the-box with infinite walls for the n=1,2,3 states.

$$E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2$$

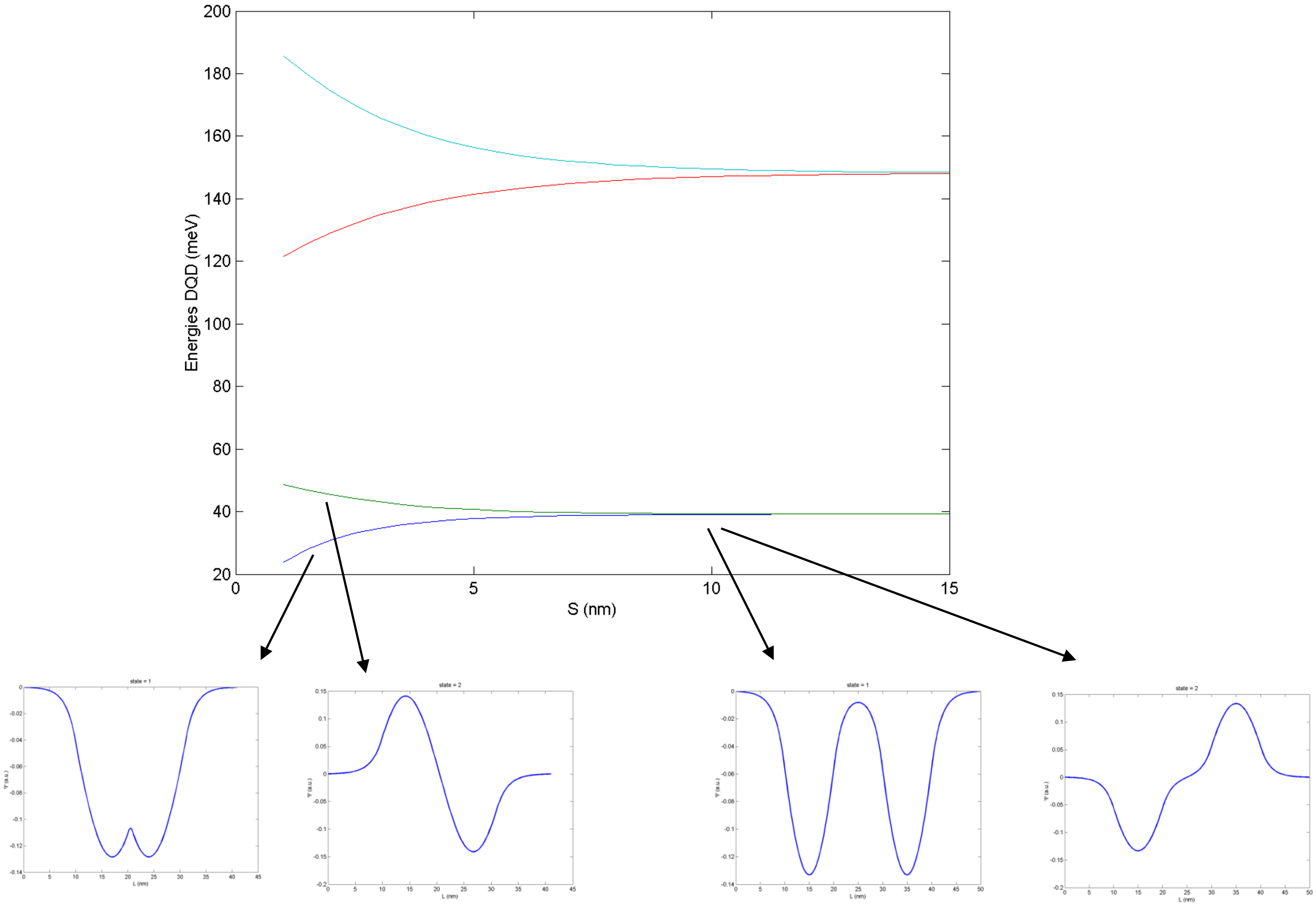
b) Use the routine plotwf.m to visualize the 3 lowest eigenstates for L=15 nm, L_b=10 nm. What is different from the infinite wall eigenstates?

PROBLEM 2. Calculate the electron energy spectrum of two coupled QDs as a function of their separation *S*.

Plot the two lowest states for S=1 nm and S=10 nm.



The result should look like this:

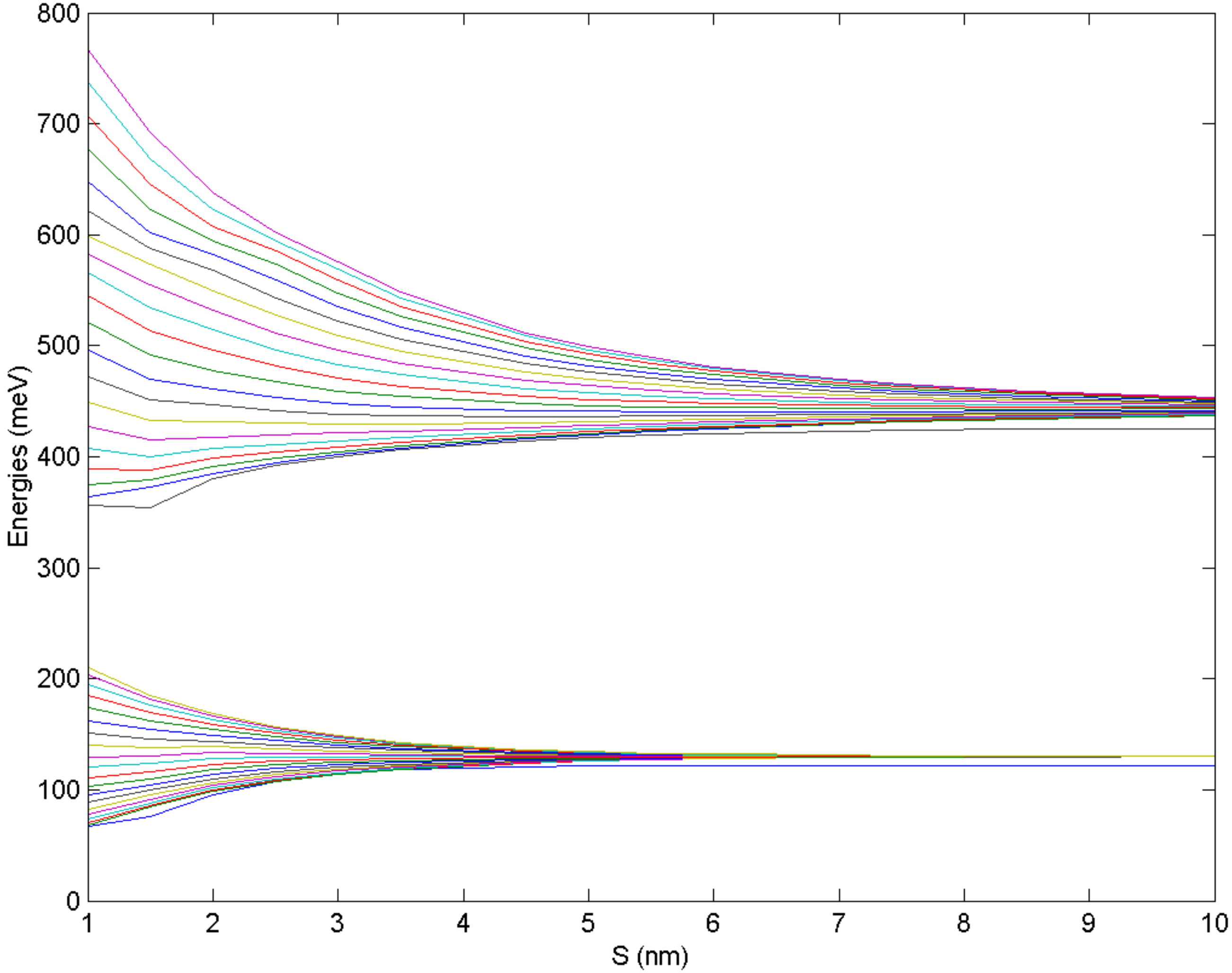


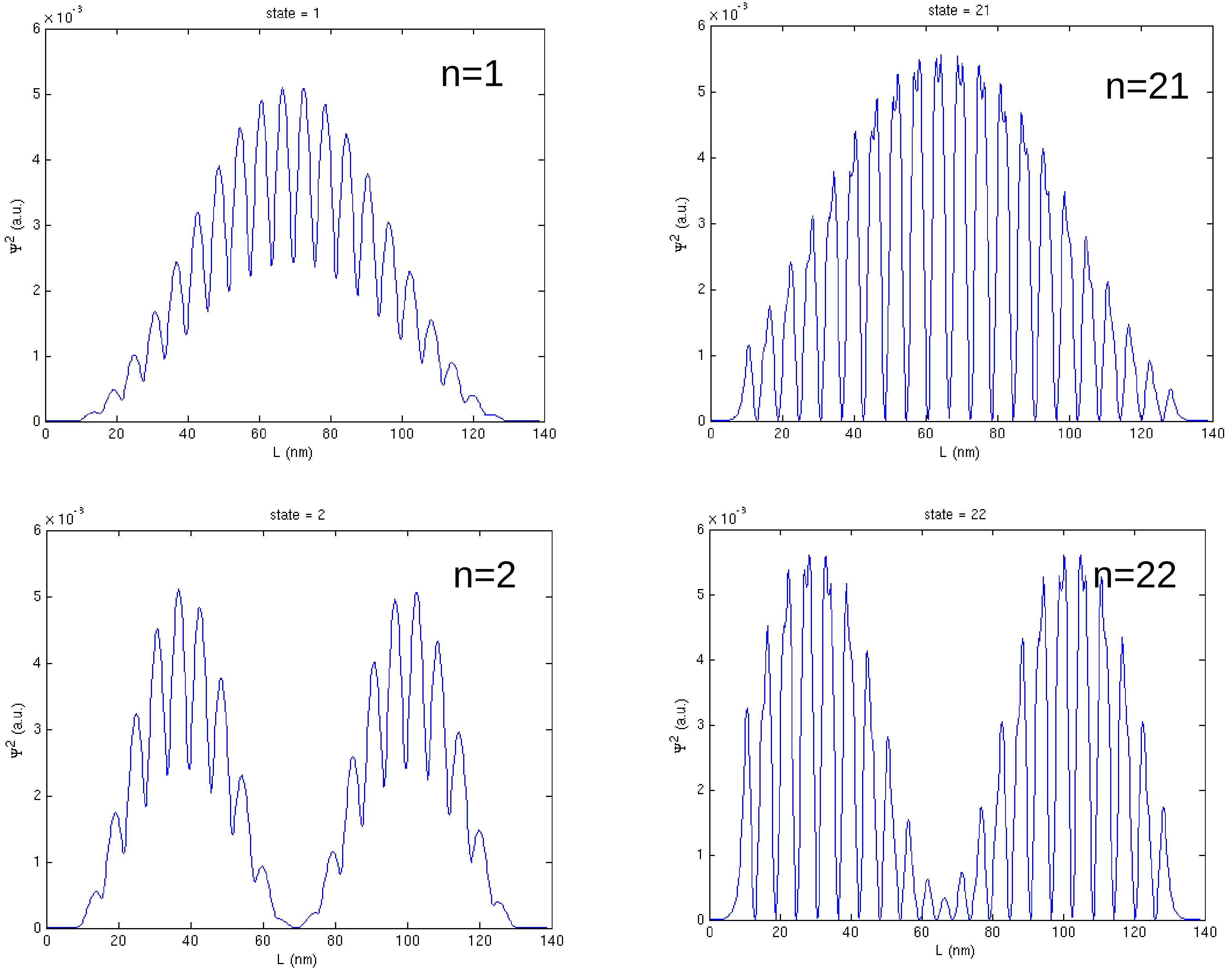
bonding antibonding bonding antibonding

PROBLEM 3. Calculate the electron energy spectrum of N=20 coupled QDs as a function of their separation *S*.

Plot the charge density of the n=1,2 and n=21,22 states for S=1 nm and L=5 nm.

The result should look like this (numerical instabilities aside):

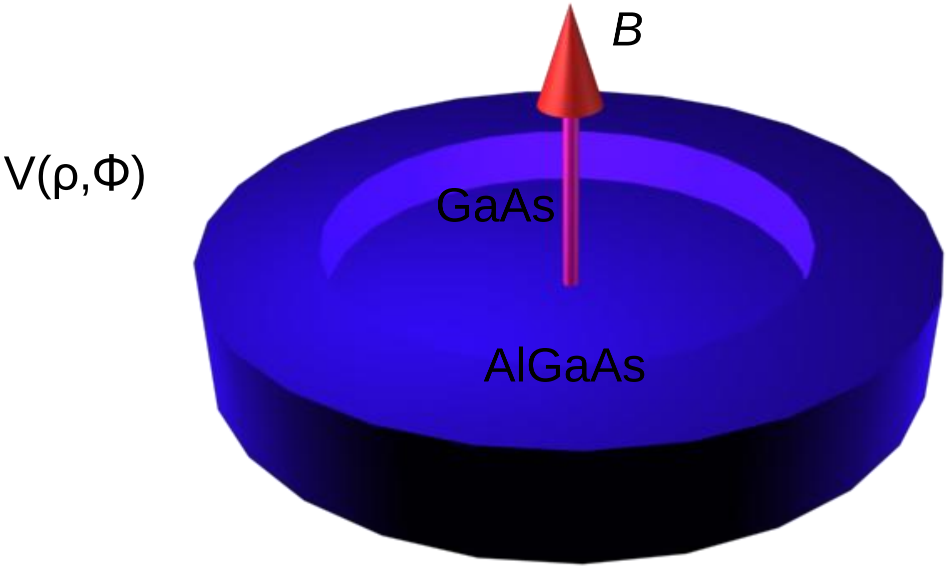


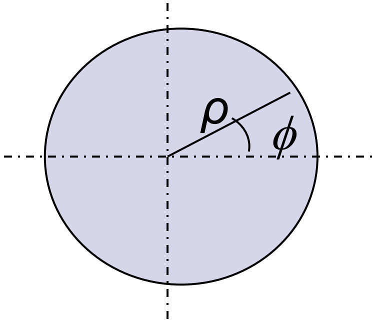


state = 1
n=1
state = 21
n=21
state = 2
n=2
state = 22
n=22
× 10^-3
Ψ^2 (a.u.)
L (nm)
0
20
40
60
80
100
120
140
0
1
2
3
4
5
6

PROBLEM 4. Write a code to calculate the energies of an electron in a 2D cylindrical quantum ring with inner radius R_{in} and outer radius R_{out}, subject to an axial magnetic field *B*.

Calculate the energies as a function of *B*=0-20 T for a structure with (R_{in},R_{out})=(0,30) nm –i.e. a quantum disk- and for (3,30) nm –a quantum ring-. L_b=10 nm. Discuss the role of the linear and quadratic magnetic terms in each case.





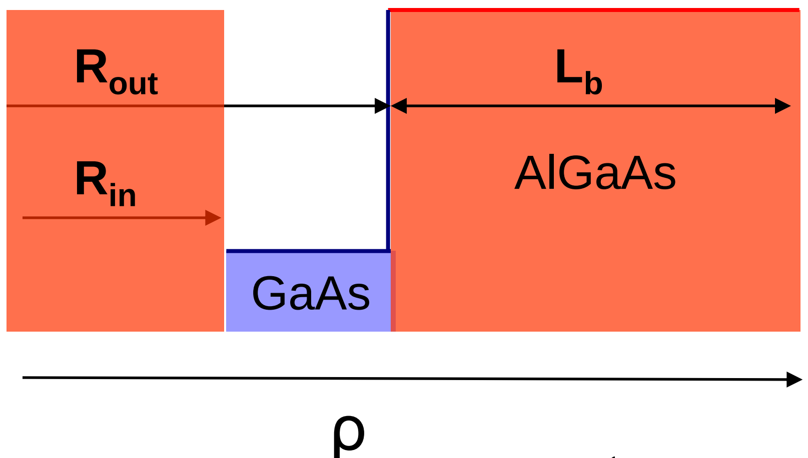
Hint 1: after integrating Φ, the Hamiltonian reads (atomic units):

$$\left[-\frac{1}{2m^*}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{M_z^{\ 2}}{\rho^2}+BM_z\right)+\frac{B^2\rho^2}{8}+V(\rho)\right]f(\rho)=E\,f(\rho)$$

with M_z =0, ±1, ±2... the angular momentum z-projection.

1 atomic unit of magnetic field = 235054 Tesla.

Hint 2: describe the radial potential as



where ρ=0 is the *center* of the ring

Hint 3: use the following BC

$$\begin{cases} f(L_t)=0 \text{ (i.e. } f_n=0) \\ \text{If } M_z=0, \text{ then } f'(0)=0 \text{ (i.e. } f_1=f_2) \\ \text{If } M_z\neq 0, \text{ then } f(0)=0 \text{ (i.e. } f_1=0) \end{cases}$$

The results should look like this: