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SELECTED PROBLEMS OF ELECTRONS  
CONFINED TO NANOSCALED SYSTEMS

Bachelor thesis

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March 20, 2009

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# 1 Introduction

This thesis will mathematically describe a few systems of electrons confined to a nanoscaled geometry.

It starts with a general discussion of finding the solution, the dispersion relation and density of states for electrons in 0, 1, 2 and 3 dimensional quantum systems in chapter 2.

Afterwards electrons confined to a square, the surface of a torus and the surface of a sphere will be described in chapters 3, 4, 5 and 6.

Programs to study the properties of those systems in Matlab are added in the appendix. There's a description at the end of the chapters.

The descriptions find application in theory and praxis.

For example are electrons on the surface of a torus a model crop circles. Those are nanotubes, that form stable rings at certain radii.

Electrons confined to a rectangle or a square describe electrons in transistor devices.

Electrons in a quantum dot are described by electrons confined to a 3-dimensional square well.

There's research on spherical gold shells with a silicon core. Electromagnetic waves cause the electrons in the shell to oscillate. The resonance frequencies reach from the blue end of the visible spectrum of light to the near infrared, depending on the ratio of the radii of core and shell.

Electrons in nanotubes are used as sensors or electrodes for example. There's research on nanotubes that detect visible light. They could be used in solar cells, to make them more efficient concerning light absorption. Other nanotubes are selective concerning light absorption.

Another application could be in artificial retinas or tiny cameras, that work in very low light (article [13]).

Other nanotubes are selective concerning light absorption.

## 2 Structure of calculation

### 2.1 Defining the dimension of the problem

**0 dimensional problem:** the electrons are confined to a 3-dimensional quantum well (small cube or quantum dot). It's motion is quantized in all directions.

**1 dimensional problem:** electrons confined to a quantum wire (f.e. polymers). The electrons are quasi free in one direction.

**2 dimensional problem:** electrons confined to a plane (f.e. in a transistor device).

**3 dimensional problem:** electrons in a bulk.

### 2.2 Finding the Solutions

In all the problems the electrons are considered as non interacting and free. This means they've zero potential inside the confinement area and infinite potential anywhere else.

The equation that has to be solved is the stationary and free Schrödinger equation. This type of differential equation is called the **Helmholtz equation**, for which the solutions are known for several geometries:

$$\frac{-\hbar^2}{2m}\Delta\psi = E\psi \quad (1)$$

$\psi$ ....wave function

$E$ ....energy eigenvalues

$m$ ...electron mass

$\hbar$ ....Planck's constant

### 2.3 Dispersion relation (DISP)

The Dispersion relation describes the dependence of the energy on momentum

$$E(\mathbf{p})$$

and because of the de Broglie relation

$$\mathbf{p} = \hbar\mathbf{k} \quad (2)$$

also the dependence of the energy on the wave vector  $\mathbf{k}$

$$E(\mathbf{k}).$$

It's found by inserting the solution  $\psi$  into the Helmholtz equation.

For free electrons the solutions are

$$\psi = C \cdot e^{i\mathbf{k}x}, \quad (3)$$

where the wave vector  $\mathbf{k}$  is not specified yet.

The energy is the expectation value of the Hamilton operator:

$$\begin{aligned} E = \langle \psi | \hat{H} | \psi \rangle &= \langle \psi | \frac{\hat{\mathbf{P}}^2}{2m} | \psi \rangle = \frac{1}{2m} \langle \psi | \sum_{i=1}^3 \hat{P}_i^2 | \psi \rangle \\ &\stackrel{(*)}{=} \frac{1}{2m} \sum_{i=1}^3 \int_0^{L_i} \psi(x_i) \cdot (-\hbar^2) \frac{\delta}{\delta x_i} \psi(x_i) dx_i \\ &= \frac{1}{2m} \sum_{i=1}^3 \hbar^2 k_i^2 \end{aligned} \quad (4)$$

(\*)....insert Identity operator

$$E(k) = \frac{\hbar^2}{2m} \cdot |\mathbf{k}|^2$$

(5)

The energy can also be written as a function of a quantum number, if  $\mathbf{k}$  is specified.

$\mathbf{k}$  is specified by the dimension and the geometry (boundary conditions) of the problem. Hence the DISP is characteristic for the geometry of the problem.

- For instance for a volume with sides  $L_1, L_2, L_3$ : The solution has to vanish at the boundary, which causes nodes in the wave function (solutions are sinusoidal). The allowed  $k$  values are

$$|\mathbf{k}| = k = \sum_{i=1}^3 k_i^2 \quad ; k_i = \frac{n_i \cdot \pi}{L_i} \quad ; n_i = 1, 2, 3\dots \quad (6)$$

$n_i$ ...quantum number

$n_i = 0$  is not allowed, because in this case the wave function would vanish independently from  $x$ .

- In case of periodic boundary conditions, the solutions are moving waves ( $e^{ikx}$ ), there are no nodes. The allowed  $k$  values are

$$|\mathbf{k}| = k = \sum_{i=1}^3 k_i^2 \quad ; k_i = \pm \frac{n_i \cdot 2\pi}{L_i} \quad ; n_i = 0, 1, 2, 3\dots \quad (7)$$

The energy can be expressed in terms of the quantum numbers  $n_1, n_2$  and  $n_3$ :

$$E_n = \frac{\hbar^2}{2m} \cdot \sum_{i=1}^3 \left( \frac{n_i \cdot 2\pi}{L_i} \right)^2 \quad (8)$$

$L_i$  influences the spacing of the  $k$  values and therefor also the spacing of the energy levels.

Small lengths cause large spacing and a discrete DISP.

For large  $L_i$  the DISP can be described by a continuous function.

From eq.(5) and(6) follows, that the DISP shows the  $E(\mathbf{k})$  dependence, where  $k$  represents a triple of  $n$  values implicitly

$$E(k) = E(n_1, n_2, n_3). \quad (9)$$

The  $E(n_i)$  dependences can be shown separately.

Then the influence of the different lengths  $L_i$ , and in some cases energy degeneracies, become obvious.

In one dimension, the energy depends on the square of  $n_1$  over  $L$ . The dependence is parabolic. It's shown in fig.(1). The energy dependence of the absolute value of  $\mathbf{k}$  is parabolic as well:  $E(|\mathbf{k}|)$  looks similar to  $E(n_1)$ .

In two dimensions, the energy dependence on the two quantum numbers  $n_1, n_2$  can be represented as in fig.(2). The degeneracy of the energy with respect to the number of n-tuples  $(n_1, n_2)$ , that belong to the same absolute value of  $k$ , can be seen as well.

It's the number of parabolas  $x$ , that reach the  $x$ - times degenerate energy.

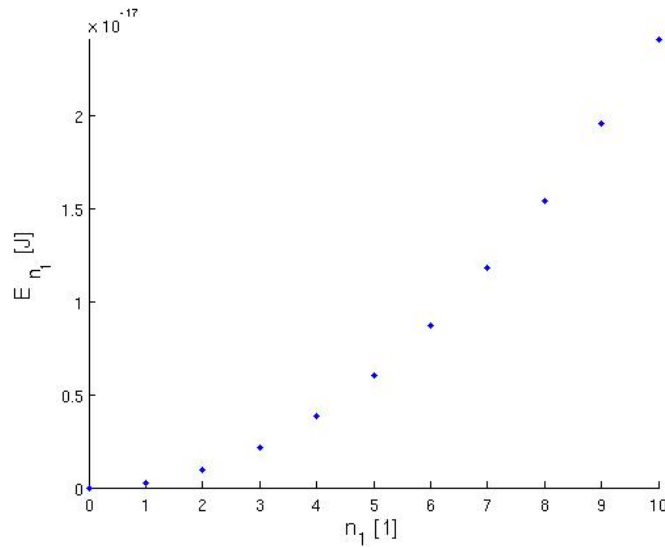


Figure 1: Dispersion relation of a 1-dimensional system with length  $L = 1 \text{ nm}$ . The energy depends on the square of quantum number  $n_1$  divided by  $L$ . The spacing of the energy states is defined by the length  $L$ .

## 2.4 Density of states (DOS)

The DOS gives the change in the number of possible energy states per energy range.

$$\frac{\Delta N}{\Delta E} \quad L \rightarrow \infty \quad \frac{dN}{dE}$$

N.....total number of states  $N$ , that exist for a given Fermi energy  
 E...energy eigenvalues

For the calculation of the DOS one needs to know  $N$  and the dispersion relation.

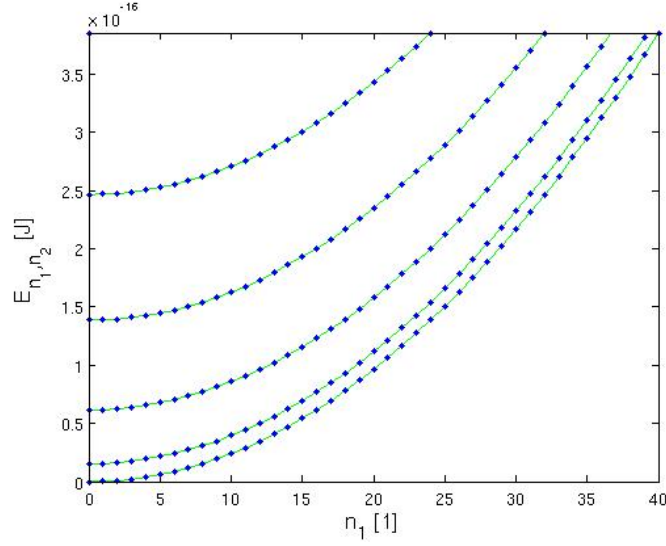


Figure 2: Dispersion relation of a 2-dimensional system with lengths  $L_1 = L_2 = 1 \text{ nm}$ . The values of one parabola are the eigenstates of the energy depending on quantum number  $n_1$  while  $n_2 = \text{const.}$ . The spacing of the energy states of each parabola is defined by  $L_1$ . The spacing between the bottoms of the parabolas is defined by  $L_2$ . The degeneracy of one energy state is given by the number of parabolas, that include this energy.

#### Discrete DOS:

If the spacing between the energy eigenvalues is large, the DOS is given by

$$\frac{\Delta N}{\Delta E} = \frac{N(E_2) - N(E_1)}{E_2 - E_1}. \quad (10)$$

Actually  $\Delta N$  is the degeneracy of  $E_2$  (except the spin degeneracy, because not only  $E_2$ , but all eigenstates are spin degenerate).

In one dimension this calculation is done very fast. In two or three dimensions it very quickly becomes computationally intensive, because all the  $n$ -tuples that satisfy eq.(8) for the concerned energy, would have to be found and divided by the proper  $\Delta E$ .

#### Continuous DOS:

It's easier to consider the DOS to be quasi continuous. If the spacing between the energy states is about  $k_B T$ , the DOS can be described by the continuous function



$$\frac{dN}{dE} \tag{11}$$

if the system is large in the dimension the electrons are considered to be quasi free.

In this case N can be calculated with the Fermi sphere.

The Fermi sphere is a model for the Fermi surface (k-space), which fits well, if the period L (real space) becomes large.

Large L causes small spacing of k. Hence the single state volumes are small enough to be almost completely adjusted into the Fermi sphere.

$$\begin{aligned}
 N(E) = & \quad 2 \sum_l \Theta(E - E_l) && n=0 \\
 & 2 \sum_l \Theta(E - E_l) \frac{V_k}{\Omega_k} + N^* && n=1,2 \\
 & 2 \frac{V_k}{\Omega_k} + N^* && n=3
 \end{aligned}
 \tag{12}$$

- n.....dimension of the system
- $\Theta$ .....Heavyside stepfunction
- k....wave vector
- $V_k$ ....Volume of the Fermi sphere (in k-space)
- $\Omega_k$ ....Volume, a single state takes in k-space
- $N^*$ ....extra states

The factor of two accounts for the spin degeneracy of a state.  
 $N^*$  takes extra states in account.

Using the dispersion relation, the fermivector in the equation above can be expressed in terms of energy.

The DOS is given by the derivation of N(E) with respect to E.

Notice, that the calculation of N is valid for both specifications of k (eq.(6) and (7)), even though there's a factor of two in  $k_2$  and  $k_2$  can be zero and negative.

$$\begin{aligned}
 k_1 &= \frac{n_1 \cdot \pi}{L_1} && n_1 = 1, 2, 3... \\
 k_2 &= \pm \frac{n_2 \cdot 2\pi}{L_2} && n_2 = 0, 1, 2, 3...
 \end{aligned}
 \tag{13}$$

For a given Fermi energy E

$$E = \frac{\hbar^2}{2m} \cdot \frac{n_1 \cdot \pi}{L} = \frac{\hbar^2}{2m} \cdot \frac{n_2 \cdot 2\pi}{L} \quad (14)$$

follows

$$n_2 = \frac{n_1}{2}$$

With eq.(12) follows

$$N_1 = 2 \cdot \frac{n_1 \frac{\pi}{L}}{\frac{\pi}{L}} = 2n_1 = 4n_2 = 2 \cdot \frac{n_2 \frac{2\pi}{L}}{\frac{2\pi}{L}} = N_2 \quad (15)$$

The two states at  $k = 0$  for  $N_2$  are not necessary to mention, because they don't influence the DOS, which is the derivation of N.

#### 2.4.1 0-dimensional DOS

Since the energy levels of systems, that are quantized in all three dimensions are discrete, the DOS is a couple of delta functions with peaks at discrete energies. The height of the peak is the total number of degeneracies of the energy level. The spin degeneracy causes a factor of two.

$$D_0(E) = 2 \cdot n_i \cdot \sum_l \delta(E - E_l) \quad (16)$$

$\delta$ ....Dirac delta function

$E_l$ ....discrete energies  $E_{n_1, n_2, n_3}$

$n_i$ .....degeneracy of the energy  $E_l$  besides the spin degeneracy

Exemplary values for  $n_i$  are listed in table (2.4.1).

#### 2.4.2 1-dimensional DOS

If a quantum dot is enlarged in one dimension to the length L the system becomes 1-dimensional.

Table 1: Degeneracy of the first six eigenstates of a 0-dimensional system.

Degenerate states	$n_i$
(1,1,1)	1
(1,1,2), (1,2,1), (2,1,1)	3
(1,2,2), (2,1,2), (2,2,1)	3
(1,1,3), (1,3,1), (3,1,1)	3
(2,2,2)	1
(3,2,1), (3,1,2), (2,3,1), (2,1,3), (1,3,2), (1,2,3)	6

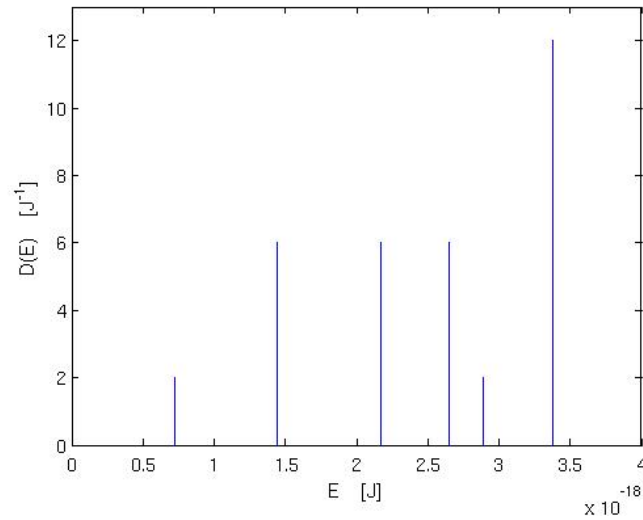


Figure 3: Exemplary DOS of a 0-dimensional system. Single peaks with defined height at the allowed energies. The lowest energy is  $E_{11} > 0$ .

The 1-d DOS is given by:

$$D_1(E) = 2 \cdot \frac{\sqrt{2mL}}{\hbar\pi} \cdot \sum_l \frac{\Theta(E-E_l)}{\sqrt{E-E_l}} \quad (17)$$

L....length of the 1-dimensional system

$\Theta$ ...Heaviside step function

$E_l$ ....discrete energies  $E_{n_2, n_3}$

### Derivation:

In  $k$  space the possible states for an energy  $E(k)$  lie in the interval  $[-k, +k]$ .

From equations (7) and (12) follows

$$N = 2 \cdot \frac{2 \cdot \frac{n \cdot 2\pi}{L}}{2\pi} + 2 = 4n + 2 \quad (18)$$

The plus 2 is for the two electron states at  $k = 0$ .

$4n + 2$ ,  $n = 0, 1, 2, 3, \dots$ , is known as **Hückl's rule**.

In organic chemistry ring molecules with such a number of  $\pi$  electrons have aromatic properties. It also gives the number of possible energy states for electrons in ring systems, like in quantum wires with periodic boundary conditions.

From equation (18) follows

$$\Delta N = 4..$$

And from equation (5) follows

$$\Delta E = \frac{2\pi^2 \hbar^2}{m} \left( \frac{2n+1}{L^2} \right). \quad (19)$$

Using the dispersion relation eq.(8) the 1-dimensional DOS in is given by:

$$\frac{\Delta N}{\Delta E} = \frac{\sqrt{2mL}}{\hbar\pi\sqrt{E} + \frac{\hbar^2\pi^2}{\sqrt{2mL}}} \quad (20)$$

If  $L$  becomes larger and the electrons are regarded as quasi free, the limit  $L \rightarrow \infty$  can be taken and eq.(20) becomes

$$D_1(E) = \frac{\sqrt{2mL}}{\hbar\pi\sqrt{E}}, \quad (21)$$

which is the derivation of

$$N = 4n + 2 \stackrel{(*)}{=} \frac{\sqrt{8mL}}{h} \cdot \sqrt{E} + 2 = N(E) \quad (22)$$

(\*)...using the dispersion relation eq.(8)

with respect to  $E$ .

If more than the first energy state is used, eq. (21) becomes eq.(17).

Equation (17) can be regarded as a discrete 2-dimensional DOS (transition to a 2-dimensional system).

The factor of two in the front accounts for the two extra degeneracies caused by the second quantum number  $n_2$ , the energy is now depending on. (The dependence of the third quantum number exists, but there will be considered the transition to two dimensions first, which means that the energy mainly changes with  $n_1$  and  $n_2$ .)

From the considerations above we know, that enlarging the energy from  $E_n$  to  $E_{n+1}$  causes four more states, the spin degeneracy included.

When making the transition from one to two dimensions there's no further spin degeneracy but only degeneracy caused by another quantum number, which is a factor of two.

Building the sum is only possible, because the summands are continuous functions of  $E$ .

It's not possible to do the same with discrete summands (eq.(20)).

$$\frac{\Delta N_3}{\Delta E_3} \neq \frac{\Delta N_1}{\Delta E_1} + \frac{\Delta N_2}{\Delta E_2} \quad (23)$$

Have a look at fig.(4):

The beginning of the green interval is called  $E_1$ ,  
the beginning of the red interval  $E_2$ ,  
the the end of the green interval  $E_3$   
and the the end of the red interval  $E_4$ .

$$\Delta E_1 = E_3 - E_1$$

$$\Delta E_2 = E_4 - E_2$$

$$\Delta E_3 = E_3 - E_2$$

$\Delta E_3$  is the difference between energies of two different 1-dimensional densities and the proper  $\Delta N$  is not  $\Delta N_1 + \Delta N_2$ .

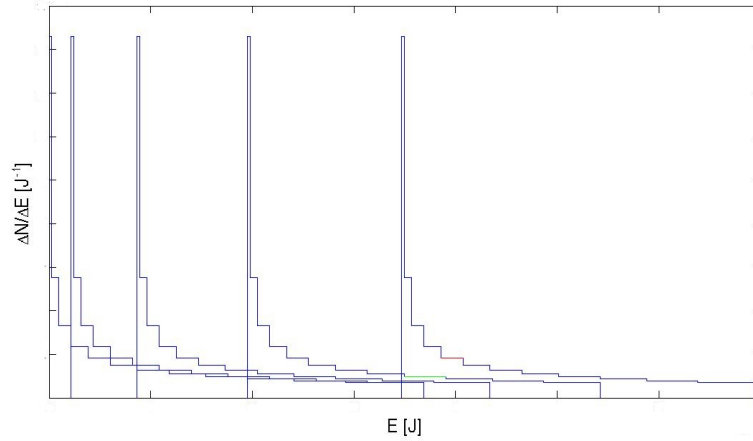


Figure 4: A couple of overlapping 1-dimensional densities of states.

### 2.4.3 2-dimensional DOS

If a quantum dot is enlarged to a plane, the system becomes 2-dimensional.

The 2-d DOS is given by:

$$D_2(E) = 2 \cdot \frac{mL_1L_2}{\hbar^2\pi} \cdot \sum_l \Theta(E - E_l) \quad (24)$$

$L_1, L_2$ ...size of the 2-dimensional system

$\Theta$ ...Heaviside step function

$E_l$ ...discrete energies  $E_{n_3}$

#### Derivation:

If the spacing of the energy eigenvalues is smaller than  $k_B T$  the van Hove singularities of the 1-dimensional DOS are that close together, that they are no longer distinguishable.

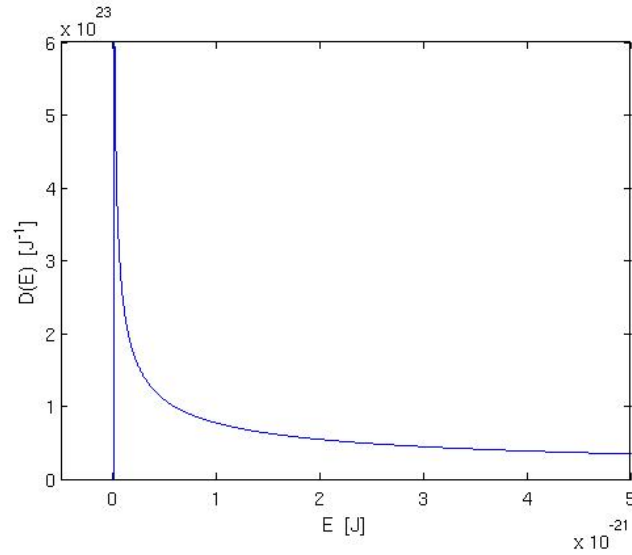


Figure 5: Exemplary DOS of a 1-dimensional system using the first energy state only, eq.(21).

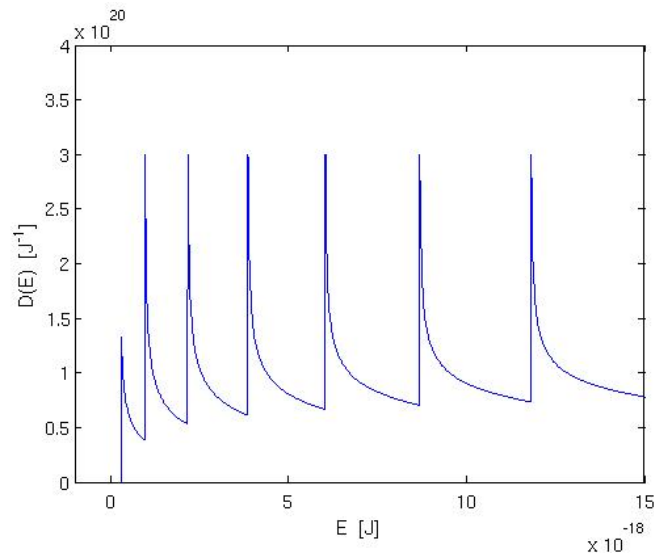


Figure 6: Exemplary DOS of a 1-dimensional system using more than the first energy state, eq.(17). The peaks are van Hove singularities. They appear if the quantum numbers  $n_2$  and  $n_3$  change. Between those states the energy changes with quantum number  $n_1$ . The change of energy with a single quantum number is described by the  $\frac{1}{\sqrt{E}}$ -dependence.

N is found by looking at  $k$  space.

In  $k$  space the possible states lie in a circle with radius

$$k = \frac{n_1 \cdot 2\pi}{L_1} = \frac{n_2 \cdot 2\pi}{L_2}. \quad (25)$$

From equation (12) follows

$$N = 2 \cdot \frac{k^2 \pi}{\left(\frac{(2\pi)^2}{L_1 L_2}\right)} + 2 \quad (26)$$

The plus 2 is for the two electron states at  $\mathbf{k} = (0, 0)$ .

Using the dispersion relation, equation (5), N can be expressed in terms of E

$$N(E) = \frac{4\pi m L_1 L_2}{h^2} \cdot E + 2 \quad (27)$$

Derivation with respect to E gives the 2-dimensional DOS:

$$D_2(E) = \frac{m L_1 L_2}{\pi \hbar^2} \quad (28)$$

Using more than the first energy state, the DOS is described by eq.(24). The factor of two in the front is again because of the transition to a higher dimensional system. This was already explained in the passage above eq.(23).

#### 2.4.4 3-dimensional DOS

If a quantum dot is enlarged to a bulk, the system becomes 3-dimensional.

The 3-d DOS is given by:

$$D_3(E) = \frac{4\pi L_1 L_2 L_3 (2m)^{3/2}}{h^3} \cdot \sqrt{E}. \quad (29)$$



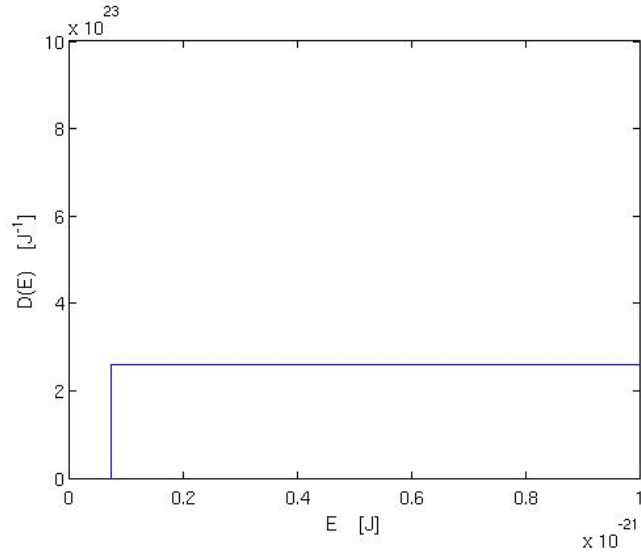


Figure 7: Exemplary DOS of a 2-dimensional system using the first energy state only, eq.(28).

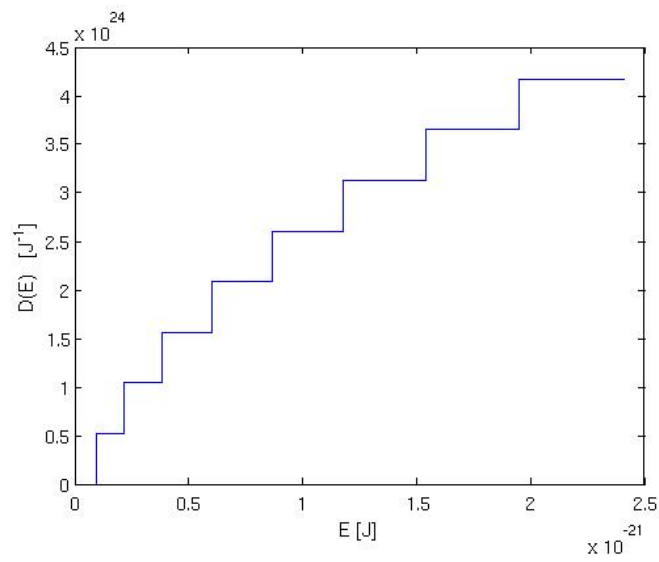


Figure 8: Exemplary DOS of a 2-dimensional system using more than the first energy state, eq.(24).

### Derivation:

The steps in the 2-dimensional DOS get smaller and finally almost vanish.  $N$  is found by looking at  $k$  space.

In  $k$  space the possible states lie in a sphere with radius

$$k = \frac{n_1 \cdot 2\pi}{L_1} = \frac{n_2 \cdot 2\pi}{L_2} = \frac{n_3 \cdot 2\pi}{L_3}. \quad (30)$$

From equation (12) follows

$$N = 2 \cdot \frac{\frac{4k^3\pi}{3}}{\left(\frac{(2\pi)^3}{L_1L_2L_3}\right)} + 2 \quad (31)$$

The plus 2 is for the two electron states at  $\mathbf{k} = (0, 0, 0)$ .

Using the dispersion relation, equation (5),  $N$  can be expressed in terms of  $E$

$$N(E) = \frac{8\pi L_1 L_2 L_3}{3h^3} (2m)^{3/2} \cdot E^{3/2} + 2 \quad (32)$$

After derivation with respect to  $E$ , we get eq.(29).

The ground state of 3-dimensional systems is  $E_{00} = 0$ , because it's possible to solve the bulk case with periodic boundary conditions and therefore  $n = 0, 1, 2, \dots$  (eq. (7)).

## 3 Electrons confined to a square

The potential energy is

$$V(x, y) = V(x) + V(y)$$

$$V(x, y) = \begin{cases} 0 & x, y \in [0, L] \\ \infty & \text{else} \end{cases}$$

The ansatz can be written as a product, because the potential is separable.

$$\Psi(x, y) = X(x)Y(y)$$

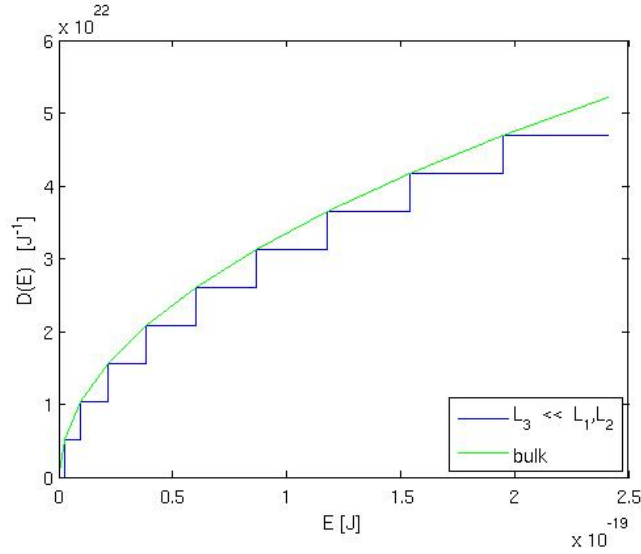


Figure 9: Exemplary DOS of a 3-dimensional system (bulk), eq.(29). A 2-dimensional DOS is shown as well (steps) to demonstrate the transition from two to three dimensions. The ground state in the bulk case is  $E_{00} = 0$ .

The Schrödinger equation for this problem reduces to Helmholtz equation, because there's zero potential, where solutions exist.

$$\hat{H}\Psi = \frac{-\hbar^2}{2m}\Delta\Psi = E\Psi \quad (33)$$

After the ansatz is put into eq.(33), the partial differential equation can be separated in the following two ordinary ones:

$$I) \quad \frac{X''}{X} = -A^2$$

$$II) \quad \frac{Y''}{Y} + \frac{2mE}{\hbar^2} = A^2$$

$A^2$ ....separation parameter

I) is solved by

$$X(x) = X_0 \cdot e^{iAx}$$

The constants A and  $X_0$  are determined by the boundary conditions.

Boundary conditions:

The square has finite side length L.

The boundary conditions in x and y are

$$\begin{aligned} X(0) &= X(L) = 0 \\ Y(0) &= Y(L) = 0. \end{aligned}$$

Only sinusoidal functions satisfy the demand of vanishing wavenfunctions at the edges of the square.

$$\sin(AL) = 0.$$

is a condition to the separation parameter.

$$A = \frac{n_x \pi}{L} \quad n_x = 1, 2, 3, \dots$$

Comment:  $n_x = 0$  is no physical solution, because the wavefunction would disappear independent from x.

$X_0$  is the scaling:

$$\begin{aligned} \int_0^L (X_0)^2 \sin^2(Ax) dx &= (X_0)^2 \left[ \frac{x}{2} - \frac{1}{4A} \sin(2Ax) \right]_0^L = (X_0)^2 \frac{L}{2} \stackrel{!}{=} 1 \\ \longrightarrow X_0 &= \sqrt{\frac{2}{L}} \end{aligned}$$

Hence

$$X(x) = \sqrt{\frac{2}{L}} \cdot \sin\left(\frac{n_x \pi}{L} x\right).$$

II) is solved by

$$Y(y) = Y_0 \cdot e^{i\sqrt{\frac{2mE}{\hbar^2} - A^2} y}$$

Again only the sinusoidal functions satisfy the boundary conditions.

$$\sin\left(\sqrt{\frac{2mE}{\hbar^2} - A^2} L\right) = 0$$

This is a condition to the energy.

$$\sqrt{\frac{2mE}{\hbar^2} - A^2} = \frac{n_y \pi}{L}$$

$$\text{with } A = \frac{n_x \pi}{L}$$

$$\left( \frac{n_y \pi^2}{L} + \frac{n_x \pi^2}{L} \right) \frac{\hbar^2}{2m} = E$$

Hence

$$Y(y) = Y_0 \cdot \sin\left(\frac{n_y \pi}{L} y\right).$$

$Y_0$  is found by calculating the scale.

$$\begin{aligned} \int_0^L (Y_0)^2 \sin^2\left(\frac{n_y \pi}{L} y\right) dx &= (Y_0)^2 \left[ \frac{y}{2} - \frac{1}{4\left(\frac{n_y \pi}{L}\right)} \sin\left(2\left(\frac{n_y \pi}{L}\right)y\right) \right]_0^L = (Y_0)^2 \frac{L}{2} = 1 \\ \longrightarrow Y_0 &= \sqrt{\frac{2}{L}} \end{aligned}$$

Finally the eigenfunctions and eigenvalues for electrons in a square of finite size  $L$  are:

$$\Psi(x, y) = \frac{2}{L} \cdot \sin\left(\frac{n_x \pi \cdot x}{L}\right) \cdot \sin\left(\frac{n_y \pi \cdot y}{L}\right) \quad (34)$$

$$E = \frac{\hbar^2}{2m} \cdot \left( \left(\frac{n_y \pi}{L}\right)^2 + \left(\frac{n_x \pi}{L}\right)^2 \right) \quad (35)$$

$$n_x, n_y = 1, 2, 3, \dots$$

### 3.1 Dispersion relation

$$\boxed{E = \frac{\hbar^2}{2m} \cdot \left( \left(\frac{n_y \pi}{L}\right)^2 + \left(\frac{n_x \pi}{L}\right)^2 \right)} \quad (36)$$

$$n_x, n_y = 1, 2, 3, \dots$$

The energy depends on the two quantum numbers  $n_x$  and  $n_y$  and the length of the square  $L$ .

### 3.2 Density of states

The length  $L$  of the square characterizes the DOS.

If  $L$  is very small, the energy states are widely spaced ( $\Delta E > k_B T$ ). The DOS is described by the delta peaks of the 0-dimensional system. Have a look at chapter (2.4.1) and figure (11).

If  $L$  becomes that large, that the spacing of the delta functions is about  $k_B T$  and the DOS can be described by the quasicontinuous 2-dimensional DOS, which is a constant (using the first energy state only).

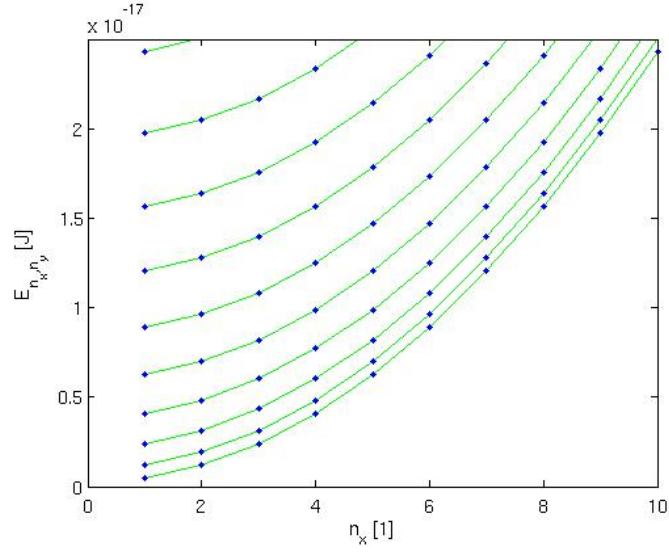


Figure 10: Dispersion relation for electrons in a square with side length  $L = 1 \text{ nm}$ . The ground state energy is  $E_{11}$ . There's no state underneath  $E_{11}$ .

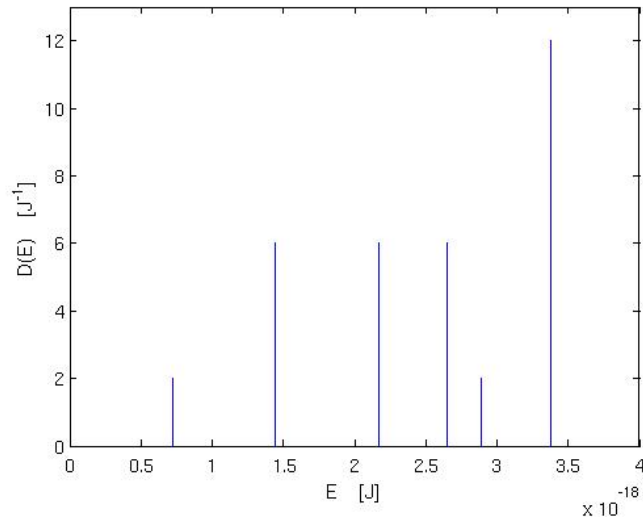


Figure 11: Dispersion relation of a square with  $L = 1 \text{ nm}$ . The spacing of the energy states is about  $10^{-19} \text{ J}$ , which is much larger than  $k_B T \simeq 10^{-21} \text{ J/K}$  at  $T = 300 \text{ K}$ . Hence the DOS is described by the one of a 0-dimensional system, eq. (16).

$$D_2(E) = \frac{mL^2}{\hbar^2\pi} \Theta(E - E_{11})$$

(37)

$L$ .....length of the square  
 $\Theta$ ...Heaviside step function

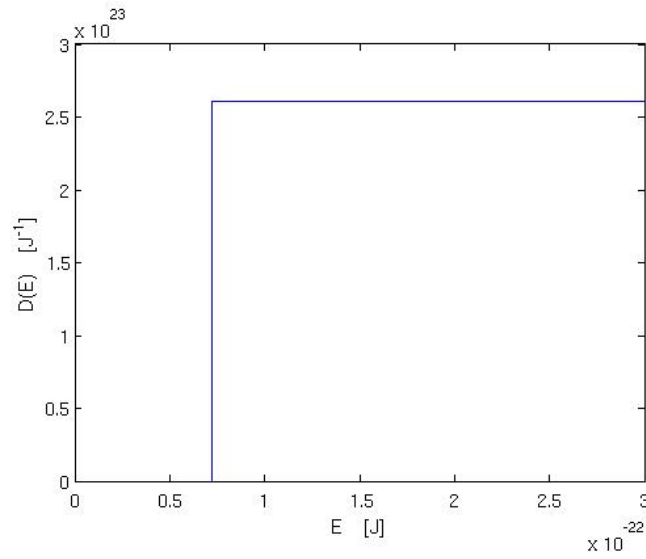


Figure 12: Dispersion relation of a square with  $L = 100 \text{ nm}$ . The spacing of the energy states is about  $10^{-24} \text{ J}$ , which is much smaller than  $k_B T \simeq 10^{-21} \text{ J/K}$  at  $T = 300 \text{ K}$ . Hence the DOS is to be described the one of a 2-dimensional system, eq.(37). There's no density below the ground state energy  $E_{11}$ .

The transition from the delta peaks to the constant value becomes clear, if the DOS of a rectangle is studied (next chapter).

If one side of the square becomes larger, while the other stays the same, van Hoven singularities, that characterize the energy dependence on a single quantum number, appear. With growing length of both sides, they get closer together until they finally fuse and the DOS approximates the constant value of the 2-dimensional DOS.

## 4 Electrons confined to a rectangle

This problem is solved just like the one for the electrons in a square. The results look similar:

Finally the eigenfunctions and eigenvalues for electrons in a rectangle of finite

size L are:

$$\Psi(x, y) = \frac{2}{\sqrt{L_x L_y}} \cdot \sin\left(\frac{n_x \pi \cdot x}{L_x}\right) \cdot \sin\left(\frac{n_y \pi \cdot y}{L_y}\right) \quad (38)$$

$$E = \frac{\hbar^2}{2m} \cdot \left( \left(\frac{n_y \pi}{L_y}\right)^2 + \left(\frac{n_x \pi}{L_x}\right)^2 \right) \quad (39)$$

$$n_x, n_y = 1, 2, 3, \dots$$

#### 4.1 Dispersion relation

$$E = \frac{\hbar^2}{2m} \cdot \left( \left(\frac{n_y \pi}{L_y}\right)^2 + \left(\frac{n_x \pi}{L_x}\right)^2 \right) \quad (40)$$

$$n_x, n_y = 1, 2, 3, \dots$$

The energy depends on the two quantum numbers  $n_x$  and  $n_y$  and the side lengths  $L_x$  and  $L_y$  of the rectangle (fig.(13)).

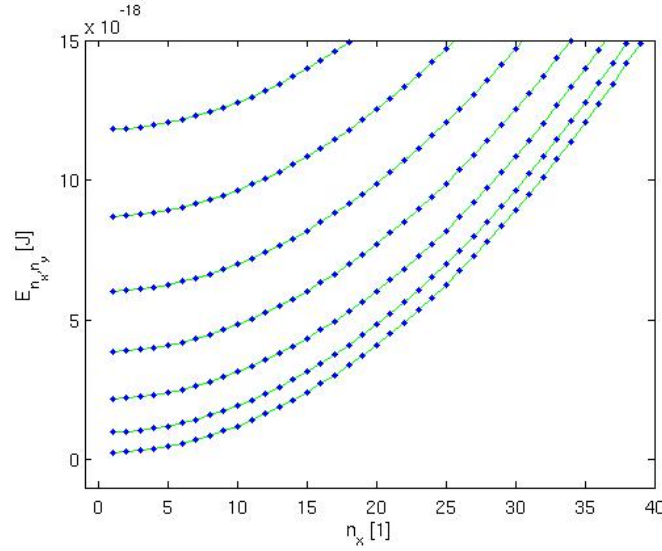


Figure 13: Dispersion relation for electrons in a square with side lengths  $L_x = 1 \text{ nm}$  and  $L_y = 5 \text{ nm}$ .



## 4.2 Density of states

The lengths of the sides of the rectangle characterize the DOS.

If both sides are very small, the energy states are widely spaced. The DOS is a combination of the 1-dimensional densities in  $n_x$  and  $n_y$  and shows van Hoven singularities.

The DOS is described by eq.(17):

$$D(E) = \frac{2 \cdot \sqrt{2m} L_x}{\hbar \pi} \cdot \sum_l \frac{\Theta(E - E_{n_y,0})}{\sqrt{E - E_{n_y,0}}} \quad (41)$$

$L_x$ ....length of the rectangle, the width  $L_y$  defines the distance between the van Hoven singularities. It's included in  $E_{n_y,0}$ .

$\Theta$ ...Heaviside step function

$E_{n_y,0}$ ....energy eigenstates of quantum number  $n_y$  while  $n_x = 0$

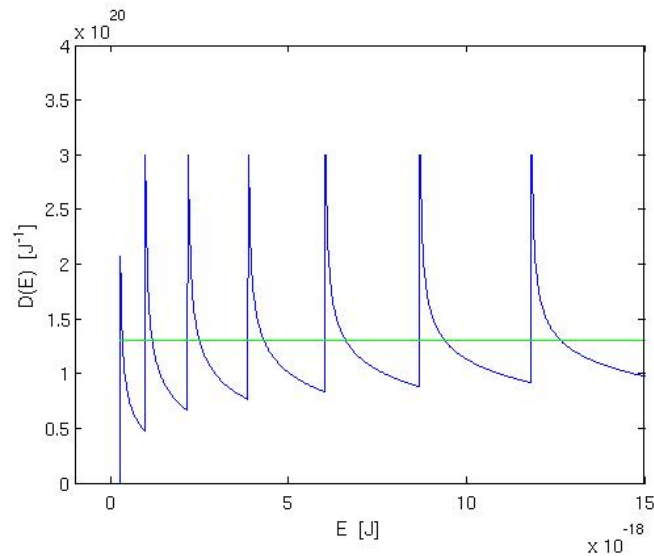


Figure 14: Density of states for electrons in a rectangle with  $L_x = 1 \text{ nm}$  and  $L_y = 5 \text{ nm}$ . There's no energy below the ground state energy  $E_{11} > 0$ . The green line is the value of the quasicontinuous 2-dimensional DOS. This value is approximated if the system becomes larger.

With growing  $L$ , the van Hoven singularities get closer together. The DOS is very sensitive to enlargement of  $L$ . Compare fig.(14) and (15). The van Hoven

singularities lie much closer together, if L is double as large.

If the spacing between the singularities is about  $kB_T$ , the system can be considered as two-dimensional and the DOS becomes a constant (green line in fig.(14)-(16)).

The DOS is described by eq.(24) with  $L_1 = L_x$  and  $L_2 = L_y$  :

$$D_2(E) = \frac{mL_xL_y}{\hbar^2\pi} \quad (42)$$

$L_x, L_y, \dots$  lengths of the rectangle  
 $\Theta$ ...Heaviside step function

The sum doesn't appear in this expression for the 2-dimensional DOS, because there's only the energy state with  $n_3 = 1$  taken.

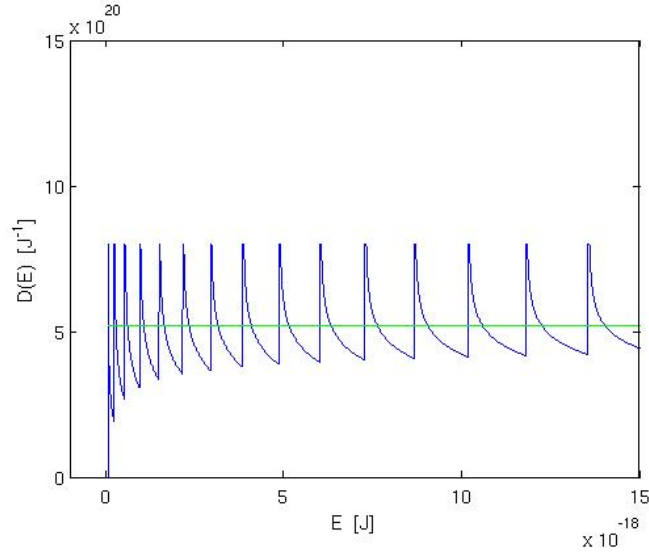


Figure 15: Density of states for electrons in a rectangle with  $L_x = 2 \text{ nm}$  and  $L_y = 10 \text{ nm}$ . The lengths of the sides is double of those in fig.(14), but the DOS looks much more like the one for a plane (green line).

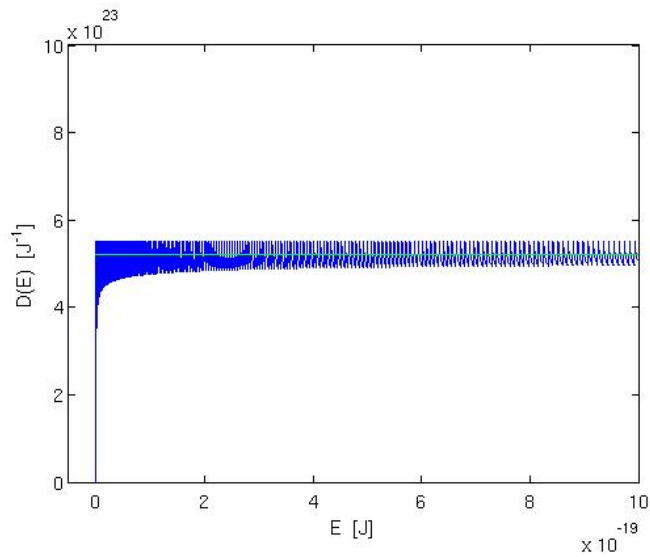


Figure 16: Density of states for electrons in a rectangle with  $L_x = 100 \text{ nm}$  and  $L_y = 200 \text{ nm}$ . Now the DOS can be approximated by the constant value of the 2-dimensional one (green line).

### 4.3 Program

The dispersion relation and the density of states were studied with Matlab: The program `rectangle.m` will ask for the side length  $L_x$  and a value for the ratio  $L_x/L_y$ . The program is added in the appendix.

Comment:

The Matlab plots show peaks of different height. Some almost exceed to infinity. This is an effect, caused by the approximation of the discrete analytic expression of the DOS by a continuous function  $\frac{1}{\sqrt{E}}$ . If the determinant is very small the function exceeds (van Hoven singularities). To prevent those singularities from dominating the whole density of states, I cut the peaks off to a reasonable height to be able to study the behaviour of the DOS.

## 5 Electrons confined to the surface of a torus

### 5.1 Finding Solutions

There is radial symmetry in the motion around the center  $0_R$  of the torus and the center  $0_\rho$  of the torus cross-section.

One can take the Helmholtz-equation in cylindrical coordinates, just like for electrons on a tube, but put periodic boundary conditions for the motion in  $z$  direction.

Because only noninterfering electrons are considered, it doesn't matter that

the inner circumference of the torus is smaller than the outer one. It's possible to transform the tube into a torus by calling the tube's length  $L$  the circumference through the center of the torus.

This ansatz will be discussed underneath. It is also possible to make a second transformation (rolling out the tube) and **treat the electrons in the torus like electrons in a rectangle, using periodic boundary conditions** ( $\mathbf{n}_x, \mathbf{n}_y = \mathbf{0}, \mathbf{1}, \mathbf{2}, \mathbf{3} \dots$ ).

**Tube with periodic boundary conditions (alternative discussion):**

$$L = 2R\pi \quad (43)$$

In the chosen coordinate system  $r, \varphi$  and  $z$  are independent from each other and the Hamilton Operator is separable. Therefore the solution can be written as a product of functions in the three cylindrical coordinates  $r, \varphi$  and  $z$ :

$$\psi(r, \varphi, z) = R(r)\Phi(\varphi)Z(z) \quad (44)$$

For a certain diameter  $\varrho$  the  $R(r)$  becomes a Dirac-Delta and the ansatz reduces to

$$\psi(r, \varphi, z) = \Phi(\varphi)Z(z) \cdot c \cdot \delta(r - \varrho) \quad (45)$$

where  $c$  is the scaling-factor.

The Nabla operator in the Helmholtz-equation has to be transformed to cylindrical coordinates (eq.(96)). The Nabla operating on  $R(r)$  is zero.

$$\Delta_r = \frac{\delta^2}{\delta r^2} + \frac{1}{r} \frac{\delta}{\delta r}$$

$$R(r) = c \cdot \delta(r - \varrho)$$

The derivation of the delta distribution is by definition deligated to the derivation of the function  $f(r)$ , which is described by the distribution.

$$\hat{\delta}(f) = \int_0^\infty \delta(r - \varrho) f(r) dr = f(\varrho) = 1$$

$$\hat{\delta}'(f) = -\hat{\delta}(f') = -f'(\varrho) = 0$$

In this case the  $f(r) = 1 = f(\varrho)$ . Therefore the derivation of  $f(\varrho)$  is zero and the whole radial part of the Nabla operating on the wavefunction cancels out.

This fact was to be expected. Electrons on the surface of a torus move in three dimensions, but define an only 2-dimensional mathematical problem. This is, because the electrons on the surface of the torus, which is defined by the two fixed radii  $R$  and  $\varrho$ , have only two degrees of freedom. One in  $\varphi$  and one in  $z$ . Therefore it's sufficient to consider a problem in two dimensions with the ansatz

$$\psi = \Phi(\varphi) \cdot Z(z). \quad (46)$$

The constant of the separation is chosen to be  $-m^2$ . The two differential equations are then

$$\begin{aligned} I) \quad & \frac{\Phi''}{\Phi} = -m^2 \\ II) \quad & \frac{Z''}{Z} = \frac{m^2}{\varrho^2} - \frac{2mE}{\hbar^2} \end{aligned} \quad (47)$$

The right side of equation II) is constant as well and will be called  $-k^2$ .

Ad I): Equation (47,I) is solved by a solution of the following kind:

$$\Phi(\varphi) = Ae^{im\varphi} + Be^{-im\varphi} \quad (48)$$

There are two conditions that have to be satisfied by this solution:

- 1) Uniqueness on the surface, concerning the motion in phi
- 2) The probability to find the electron at any angular  $\phi$  has to be one, which is a standardisation condition to the solution.

Those conditions determine the paramaters  $m$  and  $\Phi_0$ .

1) can be expressed as

$$\Phi(\varphi) = \Phi(\varphi + 2\pi) \quad (49)$$

meaning

$$\begin{aligned} Ae^{im\varphi} + Be^{-im\varphi} &= Ae^{im(\varphi+2\pi)} + Be^{-im(\varphi+2\pi)} \\ &= Ae^{im\varphi} e^{im2\pi} + Be^{-im\varphi} e^{-im2\pi} \end{aligned}$$

It is only true, if

$$e^{im2\pi} = e^{-im2\pi} = 1$$

which can be achieved by  $m \in N_0$ .

A more compact and common way to write the ansatz equation (48) is the following, in which  $m \in Z$ .

$$\Phi(\varphi) = \Phi_0 e^{im\varphi} \quad (50)$$

The factor  $\Phi_0$  is determined by the second condition, the scaling.

$$\begin{aligned} \int_0^{2\pi} |\Phi(\varphi)|^2 d\varphi &= \int_0^{2\pi} \Phi \cdot \Phi^* d\varphi = 1 \\ \int_0^{2\pi} \Phi_0^2 e^{im\varphi} e^{-im\varphi} d\varphi &= \Phi_0^2 \cdot \varphi|_0^{2\pi} = \Phi_0^2 \cdot 2\pi = 1 \\ \Phi_0 &= \frac{1}{\sqrt{2\pi}} \end{aligned}$$

The solutions in  $\varphi$  then are

$$\Phi(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}, \quad m \in Z \quad (51)$$

Ad II): Equation (47,II) can be solved with a similar ansatz like the one for  $\Phi(\varphi)$ . Compare it with equation (50).

$$Z(z) = Ae^{ikz} \quad (52)$$

A....constant real coefficient

$$k = \sqrt{\frac{2mE}{\hbar^2} - \frac{m^2}{r^2}} \quad (53)$$

For the solution in  $Z$  there are two similar conditions as there are for the  $\phi$  part:

- 1) Uniqueness concerning the motion in  $z$  direction (around the origin)
- 2) The probability to find the electron anywhere between  $z = 0$  and  $z = 2R\pi$  has to be 1, which is a standardization condition to the solution in  $Z$ .

In analogy to  $m$ ,  $k$  has to be chosen properly, so that  $Z(z)$  is periodic in  $L$  and thus unique concerning the motion around the center of the torus.

$$\begin{aligned} Z(z) &= Z(z + L) \\ Ae^{ikz} &= Ae^{ik(z+L)} = Ae^{ikz} Ae^{ikL} \\ e^{ikL} &= 1 \end{aligned}$$

This is satisfied if

$$k = n \cdot \frac{2\pi}{L} \quad n \in Z \quad (54)$$

$A$  is the scaling factor. Since the wavefunction disappears for  $z \in (-\infty, 0)$  and  $z \in (L, \infty)$ , the limits of the scaling integral can be set from 0 to  $L$ .

$$\begin{aligned} \int_0^L |Z(z)|^2 dz &= \int_0^L A^2 e^{ikz} e^{-ikz} dz \\ A^2 \cdot L &= 1 \\ A &= \frac{1}{\sqrt{L}} \end{aligned}$$

Finally the radial part is scaled too:

$$\begin{aligned} \int_0^\infty c^2 \delta^2(r - \varrho) r dr &= \int_0^\infty c^2 \delta(r - \varrho) \varrho dr = c^2 \varrho = 1 \\ c &= \frac{1}{\sqrt{\varrho}} \end{aligned} \quad (55)$$

The solution  $\psi$  is then

$$\psi(\varphi, z) = \frac{1}{\sqrt{2\pi \cdot L}} \frac{1}{\sqrt{\varrho}} \cdot e^{im\varphi} \cdot e^{ikz} \cdot \delta(r - \varrho)$$

$$k = n \cdot \frac{2\pi}{L} \qquad L = 2R\pi \qquad n, m \in Z \quad (56)$$

## 5.2 Dispersion relation

The energy is the expectation value of the Hamilton operator:

$$E = \langle \psi | \hat{H} | \psi \rangle \quad (57)$$

For the solution eq.(56) a tube was taken and periodic boundary conditions put in.

If the torus was treated as a rectangle with periodic boundary conditions, the two degrees of freedom would be x and z.

And the wavefunction:

$$\begin{aligned} \psi_2(x, z) &= \frac{1}{\sqrt{L_x L_z}} e^{ik_x x} e^{ik_z z} \\ k_x &= n_x \frac{2\pi}{L_x} & k_z &= n_z \frac{2\pi}{L_z} & n_x, n_z &\in Z \\ L_x &\hat{=} 2\varrho\pi & L_z &\hat{=} 2R\pi \end{aligned} \quad (58)$$

The solutions can also be found, if the ansatz is a product of two independent movements in the angulars  $\vartheta$  and  $\varphi$ . (Actually the momenta aren't linear, but torsional.)

$$\psi_3(\varphi, \theta) = C \cdot e^{im\varphi} \cdot e^{in\theta} \cdot \delta(r - \varrho) \qquad n, m \in Z \quad (59)$$

For calculating the dispersion relation it's equal to use eq.(56), (58) or (59).



Using (58), the Hamilton operator is

$$\hat{H} = \frac{\hat{\mathbf{P}}^2}{2m} = \frac{-\hbar^2}{2m} \Delta \quad (60)$$

and the dispersion relation is

$$E = \frac{\hbar^2}{2m} \left( \left( \frac{n_x 2\pi}{L_x} \right)^2 + \left( \frac{n_z 2\pi}{L_z} \right)^2 \right). \quad (61)$$

Using (59), the Hamilton operator is the sum of torque operators in the two angulars  $\varphi$  and  $\vartheta$  (there's no radial component, because the torus has a fixed geometry):

$$\hat{H} = \frac{\hat{L}_\vartheta^2}{2mR^2} + \frac{\hat{L}_\varphi^2}{2m\varrho^2} \quad (62)$$

$$\begin{aligned} \langle \psi | \hat{H} | \psi \rangle &= \langle \psi | \frac{\hat{L}_\vartheta^2}{2mR^2} + \frac{\hat{L}_\varphi^2}{2m\varrho^2} | \psi \rangle \\ &= \frac{1}{2mR^2} \int_0^{2\pi} \psi(\vartheta) \cdot (-\hbar^2) \frac{\delta}{\delta\vartheta^2} \psi(\vartheta) d\vartheta + \frac{1}{2m\varrho^2} \int_0^{2\pi} \psi(\varphi) \cdot (-\hbar^2) \frac{\delta}{\delta\varphi^2} \psi(\varphi) d\varphi \\ &= \frac{\hbar^2}{2m} \frac{n_\varphi^2}{\varrho^2} + \frac{\hbar^2}{2m} \frac{n_\vartheta^2}{R^2} \end{aligned} \quad (63)$$

And the dispersion relation is

$$E = \frac{\hbar^2}{2m} \left( \left( \frac{n_\varphi}{\varrho} \right)^2 + \left( \frac{n_\vartheta}{R} \right)^2 \right). \quad (64)$$

Using eq.(56) the dispersion relation is a mixture of eqs. (61) and (64) .

But since

$$L_x \doteq 2\varrho\pi \quad L_z \doteq 2R\pi \quad (65)$$

the solutions  $\psi$ ,  $\psi_2$  and  $\psi_3$  as well as the dispersion relations  $E(n_x, n_z)$  and  $E(n_\varphi, n_\theta)$  are equal.

Because the significant parameters  $\varphi$  and  $R$  are used, eq.(64) is called the

DISP of a torus

$$E = \frac{\hbar^2}{2m} \left( \left( \frac{n_\varphi}{\varrho} \right)^2 + \left( \frac{n_\theta}{R} \right)^2 \right). \quad (66)$$

$$n_\theta, n_\varphi = 0, 1, 2, 3, \dots \quad (67)$$

Because of the discussion above it's clear, that the DISP and DOS of a torus are very similar to the one of the rectangle. The only differences are

$$L = 2R\pi \quad (68)$$

and

$$n = 0 \rightarrow E_0 = 0. \quad (69)$$

### 5.3 Density of states

The electrons on the surface of a torus is a two dimensional problem. The energy depends on the two quantum numbers  $n_\varphi$  and  $n_\theta$  and on the two radii  $R$  and  $\varrho$ .

The total number of states  $N$  is calculated using eq.(12) and  $k$  from the dispersion relation eq.(66).

$$\Delta k_\varphi = \frac{1}{\varrho} \quad \text{and} \quad \Delta k_R = \frac{1}{R}. \quad (70)$$

$$N = 2 \cdot \frac{k^2 \cdot \pi}{\left( \frac{1}{\varrho \cdot R} \right)} + 2. \quad (71)$$

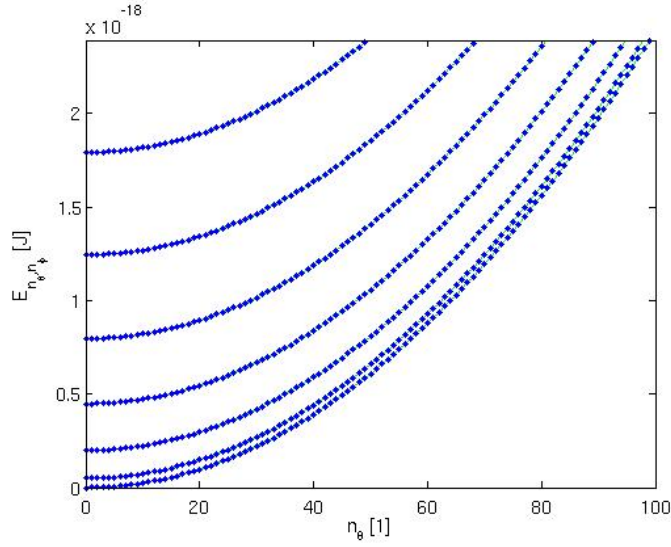


Figure 17: Dispersion relation for electrons in a torus with  $\varrho = 0.35 \text{ nm}$  and  $R = 5 \text{ nm}$ . The ground state is  $E_{00} = 0 \text{ J}$ .

The ratio  $\frac{R}{\varrho}$  and the total value of  $R$  and  $\varrho$  is characteristic for the DOS.

$$\frac{R}{\varrho} \geq 1. \quad (72)$$

The minimum value of the ratio is reached, when the radius  $\varrho$  of the torus cross-section equals the radius of the torus ring  $R$ .

**If both radii are very small** (at about  $1 \text{ nm}$ ), the DOS shows the van Hoven singularities of the 1-dimensional DOS (see eq.(17)).

$$D(E) = \frac{4R \cdot \sqrt{2m}}{\hbar} \cdot \sum_{n_\varphi} \frac{\Theta(E - E_{n_\varphi, 0})}{\sqrt{E - E_{n_\varphi, 0}}} \quad (73)$$

$R$ .....radius of the torus

$E_{n_\varphi, 0}$ .....energy eigenstates of quantum number  $n_\varphi$  while  $n_\theta = 0$

The distance between the van Hoven singularities depends on the ratio of the two radii. It becomes larger the larger the ratio is.

**If the radii become larger**, the van Hoven singularities flatten and get closer. The DOS becomes quasicontinuous and approximates the constant value of the 2-dimensional DOS (see eq.(24)) if the spacing between the van Hoven singularities is smaller than  $k_B T$ :

$$D(E) = \frac{m \cdot 4\pi \cdot R \cdot \varrho}{\hbar^2}$$

The sum doesn't appear in this expression for the 2-dimensional DOS, because there's only the first energy level ( $n_3 = 1$ ) taken.

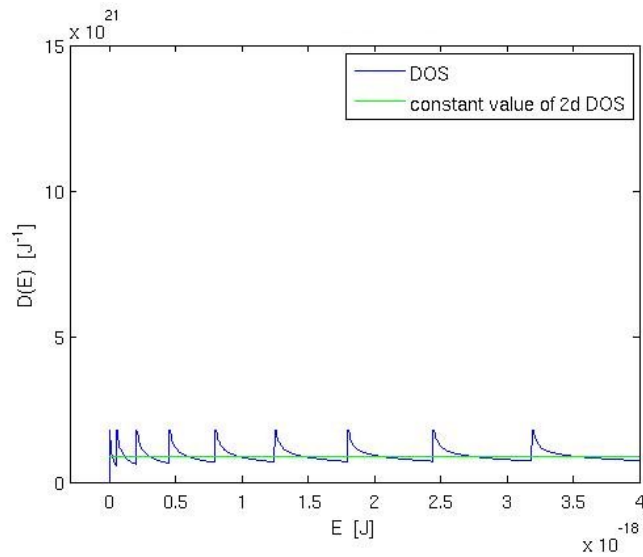


Figure 18: Density of states for electrons in a torus with  $\varrho = 0.35 \text{ nm}$  and  $R = 5 \text{ nm}$ . The ground state is  $E_{00} = 0 \text{ J}$ .

## 5.4 Program

The dispersion relation and the density of states can be studied in Matlab: The program `torus.m` will ask for the radius of the torus cross-section  $\varrho$  and a value for the ratio  $\frac{R}{\varrho}$ .

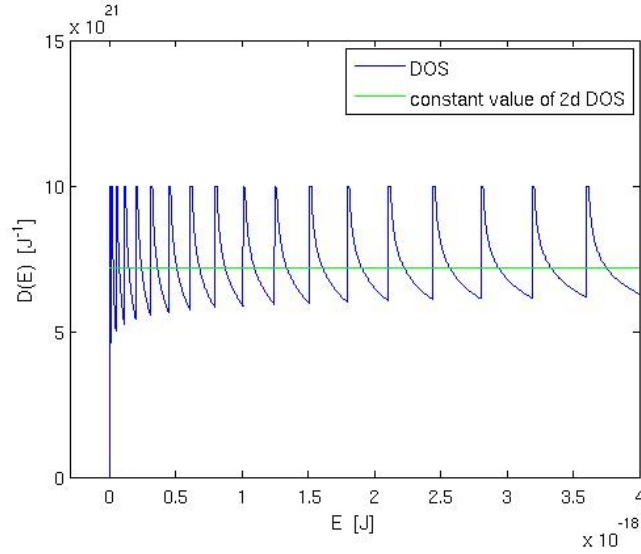


Figure 19: Density of states for electrons in a torus with  $\varrho = 0.7 \text{ nm}$  and  $R = 20 \text{ nm}$ . The ground state is  $E_{00} = 0 \text{ J}$ .

Interesting values for modern investigation are diameters of  $2R = (10 - 100) \text{ nm}$  and  $2\varrho = (1 - 1,5) \text{ nm}$ .

Those values are taken from papers (chapt.(8), [9] and [10]).

The studies say, that tori grown from tubes with diameter  $0.7 \text{ nm}$ ,  $1.1 \text{ nm}$  and  $1.4 \text{ nm}$  become circular and stable at diameters  $2R > 10 \text{ nm}$ ,  $2R > 20 \text{ nm}$  and  $2R > 40 \text{ nm}$ , respectively. The strain per atom in a the torus behaves like  $\frac{1}{(2R)^2}$ . In a perfect circular torus the strain per atom is  $< 0.03eV$ .

The figures in this section refer to  $2\varrho = 1.4 \text{ nm}$ ,  $2R = 40 \text{ nm}$  and  $2\varrho = 0.7 \text{ nm}$ ,  $2R = 10 \text{ nm}$ .

## 6 Electrons confined to the surface of a sphere

The following part until chapter (6.4) includes background information taken from references [1],[2] and [3].

The following section will discuss in the most general way the solutions of the Schrödinger equation in spherical coordinates. The radius will be varied from classical values to nanoscale. And there will be some discussion about the deformation of the sphere to an ellipse and, at the limit, to a tube.

The confinement to the surface can be expressed as a potential, that is zero right at the surface and infinite anywhere else. Therefore the problem can be reduced to a two dimensional one in  $\vartheta$  and  $\varphi$  and a constant radial part. Right at the surface, where solutions exist, the Schrödinger equation reduces to the

Helmholtz-equation (eq.(1)) with the Nabla of eq.(97).

Since the spherical coordinates are independent for this problem, the ansatz can be written as a product with a delta function for the radial part:

$$\psi(r, \varphi, \vartheta) = \Phi(\varphi) \cdot \Theta(\vartheta) \cdot c \cdot \delta(r - \varrho). \quad (74)$$

The Schrödinger equation for this problem is the Helmholtz equation, because we concentrate on the surface, where the potential is zero.

$$\hat{H}\Psi(r, \varphi, \vartheta) = \frac{\mathbf{p}^2}{2m}\Psi(r, \varphi, \vartheta) = \frac{-\hbar^2}{2m}\Delta_{\vartheta\varphi}\Psi = E \cdot \Psi(r, \varphi, \vartheta) \quad (75)$$

$\Delta_{\vartheta\varphi}$  is the angular part of the Nabla operator.

There's no radial part, because  $r = const.$ .

The Nabla operator doesn't affect the radial part of the ansatz.

The differential equation that has to be solved for that problem is:

$$\begin{aligned} \frac{-\hbar^2}{2m}\Delta_{\vartheta\varphi}\Psi &= E \cdot \Psi(r, \varphi, \vartheta) \\ \frac{-\hbar^2}{2m} \cdot \frac{1}{r^2} \cdot \left[ \frac{1}{\sin(\vartheta)} \cdot \frac{\delta}{\delta\vartheta} (\sin(\vartheta) \cdot \Phi\Theta') + \frac{1}{\sin^2(\vartheta)} \cdot \Phi''\Theta \right] &= E \cdot \Psi \end{aligned} \quad (76)$$

## 6.1 Background for radial symmetric problems

In radial symmetric potentials, it's often useful to transform the Cartesian coordinates to spherical ones. The Nabla operator has to be transformed too.

In the following section it will be shown, that the angular part of the Nabla is closely connected to the square of the operator of the angular momentum  $\hat{\mathbf{L}}$ .

And further that the radial symmetric problem is solved, if the eigenvalues for  $\hat{\mathbf{L}}$  and  $\hat{\mathbf{L}}^2$  are found.

$$[\hat{\mathbf{L}}^2, L_i] = [\hat{\mathbf{P}}^2, L_i] = [\hat{\mathbf{r}}^2, L_i] = 0 \quad (77)$$

Since  $\hat{\mathbf{L}}^2$  as well as  $\hat{\mathbf{P}}^2$  and  $\hat{\mathbf{r}}^2$  commute with one component of the operator of angular momentum, they are all invariant with respect to rotation.

Thus in radial symmetric problems, where  $V(\mathbf{r}) = V(r)$ , the whole Hamiltonian is invariant with respect to rotation.

This means that  $\hat{H}$ ,  $\hat{\mathbf{L}}^2$ ,  $\hat{\mathbf{P}}^2$ ,  $\hat{\mathbf{r}}^2$  and  $L_i$  have a common set of eigenfunctions.

The eigenvalue problem for  $\hat{\mathbf{L}}^2$  and  $L_i$  can be analytically solved and the eigenvalues of the Hamiltonian for the electrons on the surface of a sphere are the eigenvalues of  $\hat{\mathbf{L}}^2$  times a constant, because

$$\frac{-\hbar^2}{2m}\Delta_{\vartheta,\varphi}\Psi = \frac{\hat{\mathbf{L}}^2}{2mr^2}\Psi, \quad r = const. \quad (78)$$

as we will see.

The following section will concentrate on the eigenvalue problem of  $\hat{\mathbf{L}}^2$ . The way of solving the eigenvalue problem will be sketched. In the end the solutions for the angular part of a radial symmetric problem will be presented.

## 6.2 Operators of angular momentum:

Each operator that has hermetian (see chapter 7) components  $J_i$  and satisfies

$$[J_i, J_j] = i\hbar \sum_k \varepsilon_{ijk} J_k, \quad \forall i, j \quad (79)$$

describes an operator of angular momentum.

If two operators don't commute, e.g.

$$L_1 L_2 - L_2 L_1 = i\hbar L_3, \quad (80)$$

their expectation values can't be measured sharply at the same time. They oscillate around the  $x_3$  axis. The factor  $i\hbar$  has its origin in the uncertainty relation

$$[x_i, p_j] = i\hbar \delta_{ij}. \quad (81)$$

If two operators commute,

$$[\hat{\mathbf{J}}^2, J_i] = 0 \quad (82)$$

they build a system of observables, that can be measured sharply at the same time. Without restriction  $J_i$  is chosen to be  $J_z$ .

$\hat{\mathbf{J}}^2$  and  $\hat{J}_z$  satisfy the following eigenvalue equations:

$$\begin{aligned} \hat{\mathbf{J}}^2 |\alpha_j m\rangle &= \hbar^2 \alpha_j |\alpha_j m\rangle \\ J_z |\alpha_j m\rangle &= \hbar m |\alpha_j m\rangle \end{aligned} \quad (83)$$

$\hbar$  was pulled out of the eigenvalues, so that  $\alpha_j$  and  $m$  are dimensionless values. This is, because the expectation value of a linear momentum operator can be expressed in multiples of  $\hbar$ . Since  $\hat{\mathbf{J}}^2$  and  $\hat{J}_z$  are hermetian (see chapter ??) the eigenfunctions build a basis and the eigenvalues are real.

The solution is found by introducing step operators  $J_{\pm} = L_x \pm iL_y$  that work similar like  $a^+$  and  $a^-$  for the harmonic oscillator. It can be shown, that  $J_{\pm}$  working on the eigenfunctions, the eigenvalues for  $\hat{\mathbf{J}}^2$  stay the same and the eigenvalues of  $J_z$  raise or fall about 1.

$$\begin{aligned} \hat{\mathbf{J}}^2 (J_{\pm} |\alpha_j m\rangle) &= \hbar^2 \alpha_j (J_{\pm} |\alpha_j m\rangle) \\ J_z (J_{\pm} |\alpha_j m\rangle) &= \hbar(m \pm 1) (J_{\pm} |\alpha_j m\rangle) \end{aligned} \quad (84)$$

**Properties of the eigenvalues:**

- $-\sqrt{\alpha_j} \leq m \leq \sqrt{\alpha_j}$

Since  $J_i$  is hermetian, the expectation values of  $J_x^2$  and  $J_y^2$  are never negative. Consequently  $\hat{\mathbf{J}}^2 - J_z^2 = J_x^2 + J_y^2$  has also a not negative expectation-value in any state. For  $|\alpha_j m\rangle$  the expectation value was  $\hbar^2(\alpha_j - m^2) \geq 0$ , which verifies the first property.

- **There's a maximum and a minimum for m and they are unique.**

Existence:

$\alpha_j$  stays the same when  $J_{\pm}$  is applied on  $|\alpha_j m\rangle$  and encloses m, which rises or lowers with the number n of applications

$$J_z(J_{\pm}^n |\alpha_j m\rangle) = \hbar(m \pm n)(J_{\pm}^n |\alpha_j m\rangle).$$

Uniqueness:

Application of  $J_-^n$  decreases the maximum of m to the minimum in n steps. Therefore

$$m_{max} - m_{min} = n, \quad n \in N.$$

- $\alpha_j$  is defined by  $m_{max}$  and  $m_{max}$  also defines  $m_{min}$ .

Application of  $J_- J_+$  on  $|\alpha_j m_{max}\rangle$  gives an expression for  $\alpha_j$ :

$$\alpha_j = m_{max}(m_{max} + 1) = j(j + 1)$$

Application of  $J_+ J_-$  on  $|\alpha_j m_{min}\rangle$  leads to an expression for  $m_{min}$ :

$$j(j + 1) = m_{min}(m_{min} - 1)$$

Solutions are  $m_{min} = j + 1$  and  $m_{min} = -j$ . The first one drops out, because j is already the maximum.

- **j are half integers**, because of the results above:  $j - m_{min} = n$  and  $m_{min} = -j$ .

**Summarized results:**

- Eigenvalues of  $\hat{\mathbf{J}}^2$ :  $\hbar^2 j(j + 1)$ ,  $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$
- Eigenvalues of  $J_z$  are  $\hbar m$ ,  $m = -j, -j + 1, \dots, j - 1, j$
- lets call the eigenstates  $|\alpha_j m\rangle = |jm\rangle$



### 6.3 The orbital angular momentum operator $\hat{\mathbf{L}}$ in real space:

Trough the correspondence principle  $\hat{\mathbf{L}}$  is defined by

$$\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}.$$

The eigenvalue problem eq.(83) for

$$\begin{aligned} \hat{J} &\longrightarrow \hat{L} \\ \text{and} & \\ j &\longrightarrow l \end{aligned}$$

in real space becomes:

$$\begin{aligned} \mathbf{L}^2 \Psi_{lm}(r) &= -\hbar^2 (\mathbf{r} \times \nabla)^2 \Psi_{lm}(r) = \hbar^2 l(l+1) \Psi_{lm}(r) \\ L_z \Psi_{lm}(r) &= \frac{\hbar}{i} (\mathbf{r} \times \nabla)_z \Psi_{lm}(r) = \hbar m \Psi_{lm}(r) \end{aligned} \quad (85)$$

The components of  $\mathbf{L}$  are

$$L_i = \frac{\hbar}{i} \sum_{m,n} \varepsilon_{imn} x_m \frac{\delta}{\delta x_n}$$

When  $\mathbf{L}$  is transformed in spherical coordinates, the z component is simply

$$L_z = \frac{\hbar}{i} \frac{\delta}{\delta \varphi} \quad (86)$$

The square of  $\mathbf{L}$  in spherical coordinates is

$$\mathbf{L}^2 = -\frac{\hbar^2}{\sin^2(\vartheta)} \left\{ \sin(\vartheta) \frac{\delta}{\delta \vartheta} \left( \sin(\vartheta) \frac{\delta}{\delta \vartheta} \right) + \frac{\delta^2}{\delta \varphi^2} \right\} \quad (87)$$

Compared to the angular part of the Nabla operator in spherical coordinates

$$\Delta_{\vartheta, \varphi} = -\frac{\mathbf{L}^2}{r^2 \hbar^2} \quad (88)$$

it becomes clear that the angular part of the kinetic energy in the Hamiltonian is

$$T_{\vartheta, \varphi} = \frac{\mathbf{L}^2}{2mr^2}. \quad (89)$$

With eq.(86) and (87) eq.(85) becomes:

$$\begin{aligned} -\frac{1}{\sin^2(\vartheta)} \left\{ \sin(\vartheta) \frac{\delta}{\delta \vartheta} \left( \sin(\vartheta) \frac{\delta}{\delta \vartheta} \right) + \frac{\delta^2}{\delta \varphi^2} \right\} \Psi_{lm}(r) &= l(l+1) \Psi_{lm}(r) \\ -i \frac{\delta}{\delta \varphi} \Psi_{lm}(r) &= m \Psi_{lm}(r) \end{aligned} \quad (90)$$

With the ansatz eq. (74) the  $\varphi$ -part is determined to be

$$\Phi(\varphi) = \Phi_0 e^{im\varphi}. \quad (91)$$

$\Phi(\varphi)$  has to be scaled and unique with respect to rotation over  $2\pi$ . (Compare it with eq.(49) and following) which means, that  $\Phi_0 = \frac{1}{\sqrt{2\pi}}$  and  $m \in \mathbb{Z}$ .

And because of the properties of the eigenvalues of  $L_z$ , discussed above:  $l \in \mathbb{Z}_0^+$ .

For the quantum numbers follows:

- $l = 0, 1, 2, 3, \dots$  called the **orbital angular momentum quantum numbers** and quantizes  $\hat{\mathbf{L}}^2$
- $m = -l, -l+1, \dots, l-1, l$  called the **magnetic quantum numbers** and quantizes  $L_z$ .

Comment:

The half integer values, that were found for a generalized angular momentum operator  $J$  are eigenvalues of the spin operator.

$\Phi(\varphi)$  is put in eq.(90), which leads to a differential equation in  $\vartheta$ .

$$-\frac{1}{\sin^2(\vartheta)} \left\{ \sin(\vartheta) \frac{\delta}{\delta\vartheta} \left( \sin(\vartheta) \frac{\delta}{\delta\vartheta} \right) - m^2 \right\} \Theta(\vartheta) = l(l+1)\Theta(\vartheta) \quad (92)$$

With the substitution

$$t = \cos\vartheta$$

it becomes

$$\frac{d}{dt} \left[ (1-t^2) \frac{d\Theta}{dt} \right] + \left( l(l+1) - \frac{m^2}{(1-t^2)} \right) \Theta = 0$$

called the **generalized Legendre-Differential-Equation**.

It is singular at  $t = \pm 1$ .

Solutions that are regular at  $t = \pm 1$  behave like  $(1 - t^2)^{m/2}$ .

Thus an ansatz

$$\Theta(\vartheta) = (1 - t^2)^{m/2} \cdot v_m(t)$$

is made and the following relation is found:

$$v_m(t)' = v_{m+1}$$

alternatively

$$v_m(t) = \frac{d^m v_0(t)}{dt^m}$$

with  $v_0$ , the solution of the ordinary Legendre differential equation:

$$(1 - t^2)v_0'' - 2tv_0' + l(l + 1)v_0 = 0$$

A potential series at  $t = 0$  leads to its solutions the **ordinary Legendre-Polynomials  $P_l(\cos\vartheta)$** .

Finally the **solutions for a radial symmetric problem are**

$$\Psi(r, \vartheta, \varphi) = \frac{1}{N} \cdot f(r) \cdot e^{\pm im\varphi} \sin^m(\vartheta) \frac{d^m}{(d\cos\vartheta)^m} P_l(\cos\vartheta)$$

(93)

N...scaling

$m = 0, 1, 2, 3, \dots, l$

$l = 0, 1, 2, 3, \dots$

$$N = \int_{-1}^1 P_l^m(t) P_l^m(t) dt = \frac{2}{2l + 2} \frac{(l + m)!}{(l - m)!}$$

With

$$P_l^m(\vartheta) = (-1)^m \sin^m(\vartheta) \frac{d^m}{(d \cos \vartheta)^m} P_l(\cos \vartheta)$$

the solution can be written in a more compact way:

$$\Psi(r, \vartheta, \varphi) = \sqrt{\frac{2l+2}{4\pi} \frac{(l-m)!}{(l+m)!}} \cdot e^{\pm im\varphi} \cdot P_l^{|m|}(\vartheta) \cdot f(r)$$

$$m = 0, \pm 1, \pm 2, \pm 3, \dots \pm l$$

$$l = 0, 1, 2, 3, \dots$$

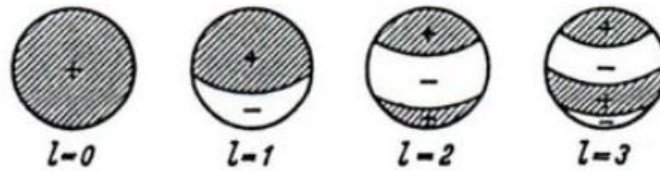


Figure 20: Spherical Harmonics  $P_l^m(\vartheta)$  for  $m=0$  and  $l=0,1,2,3$ . 2)



Figure 21: Spherical Harmonics  $P_l^m(\vartheta)$  for  $m=0,1,2$  and  $l=2$ . 2)

**Comment:**

An alternative way to finding  $\Theta(\vartheta)$  was solving the eigenvalue problem for  $L_+$  and  $L_z$  instead of the one for  $\hat{L}^2$  and  $\hat{L}_z$ . This is possible, because  $\hat{L}^2$  and  $\hat{L}_+$  commute

$$[\hat{L}^2, L_{\pm}] = 0$$

and therefor have a common set of eigenfunctions.

**Back to equation (76):**

Comparison of  $\hat{\mathbf{L}}^2$  and  $\Delta_{\vartheta\varphi}$  in spherical coordinates shows, that eq.(76) can be written as

$$\frac{\hat{\mathbf{L}}^2}{2mr^2}\Psi(r, \vartheta, \varphi) = E\Psi(r, \vartheta, \varphi)$$

Since the eigenvalue problem for  $\hat{\mathbf{L}}^2$  was solved above and  $\frac{1}{2mr^2} = \text{const.}$ , the **wavefunction and energy eigenvalues** for electrons on the surface of a sphere are

$$\Psi(r, \vartheta, \varphi) = \sqrt{\frac{2l+2}{4\pi\sqrt{\varrho}} \frac{(l-m)!}{(l+m)!}} \cdot e^{\pm im\varphi} \cdot P_l^{|m|}(\vartheta) \cdot \delta(r - \varrho)$$

$$E = \frac{\hbar^2}{2mr^2}l(l+1)$$

## 6.4 Dispersion relation

The energy eigenvalues are given by

$$E_l = \frac{\hbar^2}{2mr^2}l(l+1) \quad l = 0, 1, 2, 3\dots \quad (94)$$

$$(95)$$

The energy depends on the quantum number  $l$ .  $l$  quantizes the absolute value of the angular momentum.

$$|\mathbf{L}| = \hbar \cdot \sqrt{l(l+1)}$$

## 6.5 Density of states

Each energy eigenvalue  $E_l$  is

$$g_l = 2 \cdot (2l + 1)$$

times degenerated.

The invariance of  $|\mathbf{L}|$  with respect to rotation (magnetic quantum number  $m$ )

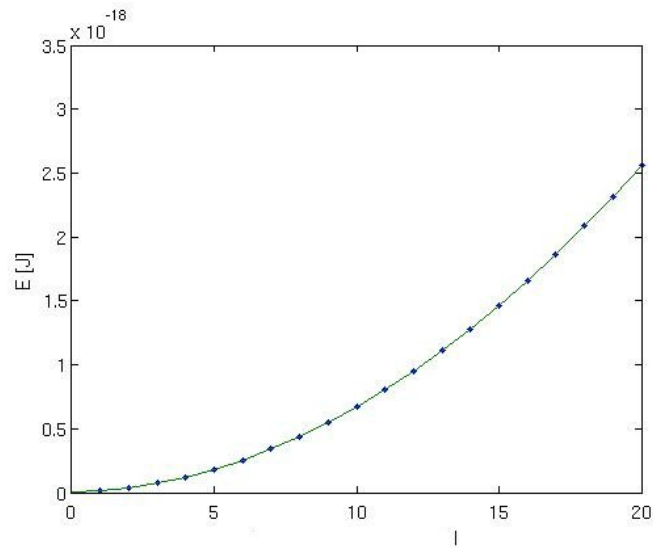


Figure 22: Dispersion relation for electrons on the surface of a sphere with  $R = 1 \text{ nm}$ .  $l$  is the quantum number of angular momentum.

leads to the factor  $2l + 2$ .

Besides that each state is two times spin degenerated.

The total number of states  $N_l$  for a Fermi-energy  $E_l$  is given by

$$\begin{aligned}
 N_l &= \sum_{k=0}^l 2(2k + 1). \\
 &= 2(l + 1)^2
 \end{aligned}$$

**Discrete density:**  $\frac{\Delta N}{\Delta E}$

$$\Delta N = N_{l+1} - N_l = 4l + 6$$

$$\Delta E = \frac{\hbar^2}{2mr^2} \cdot 2(l + 1)$$

$$\frac{\Delta N}{\Delta E} = \frac{4l + 6}{\frac{\hbar^2}{2mr^2} \cdot 2(l + 1)}$$

$$\stackrel{(94)}{=} \frac{l}{E_l} + \frac{4mr^2}{\hbar^2}$$

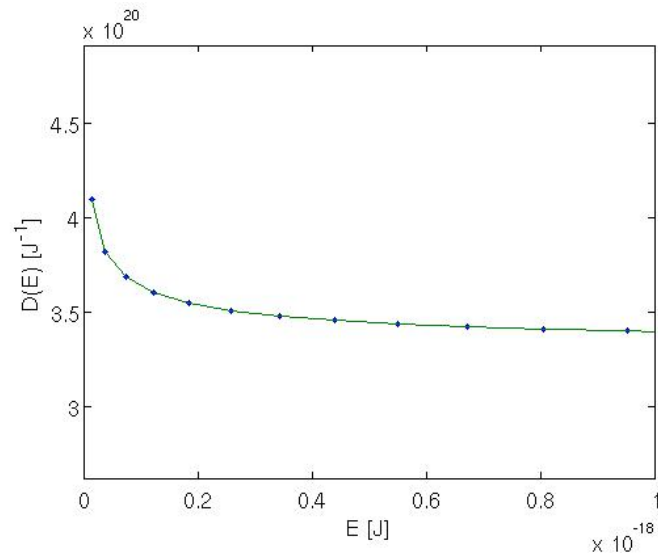


Figure 23: Density of states for a sphere with  $r = 1 \text{ nm}$ .

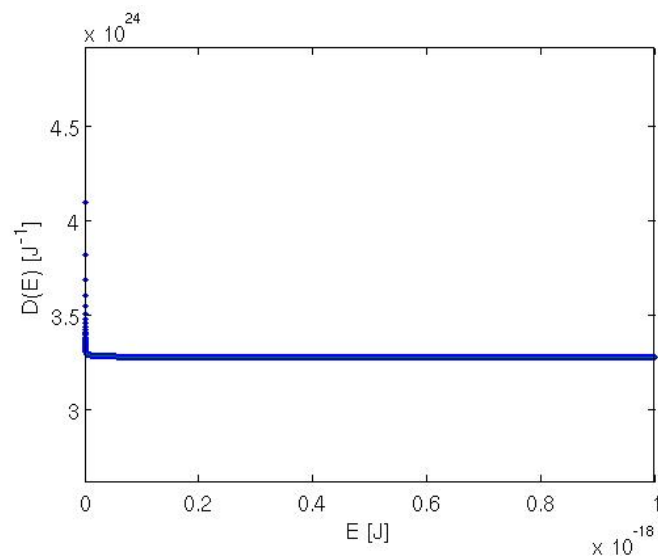


Figure 24: Density of states for a sphere with  $r = 100 \text{ nm}$ . Except for the first energy states, the DOS is quasi constant (2-dimensional DOS).

## 6.6 Program

The dispersion relation and the density of states were studied with Matlab: the program sphere.m will ask for the radius and show the dispersion relation and the density of states for the chosen radius.

### Large surfaces:

Figures (25)-(27) show the density of states for a large sphere, rectangle or torus. Surface, respectively area are that large (about  $40\,000\text{ nm}^2$ ), that they can be considered as a plane. The DOS has the same value (green line). It's the constant value of the 2-dimensional DOS.

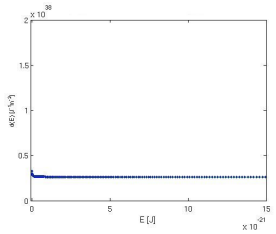


Figure 25: Specific density of states for electrons on the surface of a sphere with  $R = 100\text{ nm}$ .

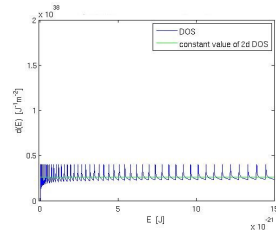


Figure 26: Specific density of states for electrons in a rectangle with  $L_x = 200\text{ nm}$  and  $L_y = 200\pi\text{ nm}$ .

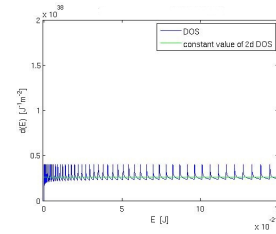


Figure 27: Specific density of states for electrons on the surface of a torus with  $r = 100/\pi\text{ nm}$  and  $R = 100\text{ nm}$ .



## 7 Appendix

### Nabla operator in cylindrical coordinates:

$$\begin{aligned}\Delta &= \frac{1}{r} \frac{\delta}{\delta r} \left( r \frac{\delta}{\delta r} \right) + \frac{1}{r^2} \frac{\delta^2}{\delta \varphi^2} + \frac{\delta^2}{\delta z^2} \\ &= \frac{\delta^2}{\delta r^2} + \frac{1}{r} \frac{\delta}{\delta r} + \frac{1}{r^2} \frac{\delta^2}{\delta \varphi^2} + \frac{\delta^2}{\delta z^2}\end{aligned}\quad (96)$$

### Nabla operator in spherical coordinates:

$$\Delta = \frac{1}{r^2} \frac{\delta}{\delta r} \left( r^2 \frac{\delta}{\delta r} \right) + \frac{1}{r^2 \sin \theta} \frac{\delta}{\delta \vartheta} \left( \sin \theta \frac{\delta}{\delta \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\delta^2}{\delta \varphi^2} \quad (97)$$

### hermetian:

A matrix is hermetian if

$$A = A^\dagger \quad (98)$$

$A^\dagger$  means to transpose and complex conjugate (or vice versa) the matrix:

$$A^\dagger = (A^T)^* = (A^*)^T$$

It's the analogy of a real space symmetric matrix but in complex space. Hermitesh matrices are square, normal and diagonalisable.

Since each Operator in an  $n$  dimensional vector space can be described by an  $n \times n$  matrix, one can also call an operator hermetian:

$$\hat{A} = \hat{A}^\dagger$$

A quantum mechanical postulate says, that each physical observable (f. i. energy, position, angular momentum) formally corresponds to a hermetian operator:

$$\hat{A} = \sum_j a_j |a_j\rangle\langle a_j| \quad (99)$$

Hermitesh operators

- work the same way on Bra- and Ket-vectors.
- have real eigenvalues
- eigenvectors to different eigenvalues are orthogonal
- if the eigenvalues are degenerated it's always possible to chose them to be orthogonal
- the eigenvectors build a basis, a complete set of eigenstates.

## 8 Literature

[1] Nolting, Wolfgang: Grundkurs theoretische Physik 5/2, Quantenmechanik-Methoden und Anwendungen,4.Auflage, Springer Berlin [u.a.], 2004,ISBN:3-540-4211-4

[2] Flügge, Siegfried: Rechenmethoden der Quantenmechanik,6.Auflage, Springer Berlin [u.a.], 1999, ISBN:3-540-65599-9

[3] Claude Cohen-Tannoudji, Bernard Diu, Franck Laloe: Quantum Mechanics,vol.1 and 2, 2.edition, Hermann and John Wiley and Sons, Paris, New York [a.o.] 1977, ISBN: vol.1: 2-7056-5833-5 (Hermann), vol.2: 2-7056-5834-3

[4] Kittel, Charles: Introduction to solid state physics, 8.edition, Wiley, New York [a.o.] 2005, ISBN:978-0-471-41526-8

[5] Bartsch, Hans-Jochen: Taschenbuch mathematischer Formeln, 20.Auflage, Fachbuchverlag Leipzig im Carl Hanser Verlag, München Wien 2004, ISBN:3-446-22891-8

[6] Moon P., Spencer D. : Field theory handbook, Springer, Berlin [u.a.] 1961

[7] Morse Ph., Feshbach : Methods of theoretical physics,vol.1 and 2,McGraw-Hill Book Company, Inc., New York [a.o] 1953 ISBN: vol.1: 0-07-043316-X, vol.2: 0-07-043317-8

[8] Arfken, George B.: Mathematical methods for physicists, 4. edition, Acad. Press, San Diego, California [u.a.] 1999, ISBN:0-12-059816-7

### Articles:

[9] Han, Jie: Toroidal Single Wall Carbon Nanotubes in Fullerene Crop Circles  
<http://www.nas.nasa.gov/News/Techreports/1997/PDF/nas-97-015.pdf>, 31.05.2008

[10] Liu, Jie [a.o.]:'Fullerene Crop Circles', In: Scientific Correspondence  
<http://www.nas.nasa.gov/News/Techreports/1997/PDF/nas-97-015.pdf>

**Articles from the Internet:**

[11] <http://de.wikipedia.org/wiki/Zustandsdichte>, 03/03/2009

[12] <http://britneyspears.ac/physics/dos/dos.htm>, 03/03/2009

[13] <http://www.technologyreview.com/computing/22257>, 19/03/2009

## %RECTANGLE

%dispersionrelation and density of states

```
clc
clear all
close all
```

```
h=6.6261*10^(-34);    %in Js
m=9.11*10^(-31);    %in kg
```

```
F=(h/2/pi).^2./(2*m);
```

```
disp('Choose a length Lx in meters');
Lx=input('Lx=');
```

```
if isempty(Lx)
Lx=1e-9;
fprintf('%e',Lx)
end
```

```
r=Lx/(2*pi);
```

```
fprintf('\n')
fprintf('\n')
fprintf('\n')
disp('Choose a ratio Ly/Lx>1');
fprintf('\n')
```

```
ratio=input('Ly/Lx=');
fprintf('\n')
```

```
if ratio<1          %necessary for the formula of the DOS
disp('Invalid value for the ratio! Choose Ly/Lx>1')
fprintf('\n')
ratio=input('Ly/Lx=')
end
```

```
if isempty(ratio)
ratio=2;
fprintf('%e',ratio)
end
```

```
R=ratio*r;
```

```

Ly=2*R*pi;

A=Lx*Ly;           %Area of the rectangle

nR=[1:ratio*50];
nphi=[1:50];

[nR,nphi ]=meshgrid(nR,nphi);
E_nR=nR.^2./R.^2.*F;           %eigenvalues for nphi=0
E_nphi= nphi.^2./r.^2.*F;      %eigenvalue for nR=0

En=E_nR +E_nphi;              %energy eigenvalues

figure(1)
set(0,'DefaultAxesFontSize',12)
z_par=5;                       %number of parabolas
subplot(1,2,1)

for i=1:z_par
plot([0,1],[E_nphi(i,1),E_nphi(i,1)])
hold on
end
hold off
title('E_{n_x}','FontSize', 12)
xlabel('[1]','FontSize', 12)
ylabel('E_{n_x} [J]','FontSize', 12)
axis([0 1 -1/8*E_nphi(z_par,1) (9/8)*E_nphi(z_par,1)])

subplot(1,2,2)

for i=1:z_par
plot([0,1],[E_nR(1,i),E_nR(1,i)])
hold on
end
hold off

title('E_{n_y}','FontSize', 12)
xlabel('[1]','FontSize', 12)
ylabel('E_{n_y} [J]','FontSize', 12)

axis([0 1 -1/8*E_nphi(z_par,1) (9/8)*E_nphi(z_par,1)])

```

```

%DISP

figure(2)

%dispersionsrelation E(n_phi,n_R) over n_R
x=nR(1,:);
y=En;

for i=1:size(En,1)
plot(x,y(i,:), 'Color',[0,1,0])
hold on
plot(x,y(i,:), '.')
hold on
end
hold off

title('dispersion relation for a rectangle','FontSize', 12)
xlabel('n_x [1]','FontSize', 12)
ylabel('E_{n_x,n_y} [J]','FontSize', 12)

%DOS

nR=nR(1,:);
nphi=nphi(:,1);
E_nR=E_nR(1,:);
E_nphi=E_nphi(:,1);

%quasicontinuous 1d-single-DOS

E=linspace(En(1,2),En(end,end),90000);
[E,EI]=meshgrid(E,E_nphi);

D_1=(sqrt(2*m)*8*pi*R/h).*heaviside(E-EI)./(sqrt(E-EI));
D_1((E-EI)==0)=0; %problem:1/0

plotend=sum(D_1(end,:)==0);

if plotend==size(E,2)
plotend=0
end

```

```
D_1sum=sum(D_1,1);
```

```
%quasicontinuous 2d-DOS
```

```
D_2=16*pi^3*m*R*r/(h^2);
```

```
figure(3)
```

```
set(0,'DefaultAxesFontSize',12)
```

```
%D_1sum(D_1sum> c)=c ; %c= cut off the infinite values
```

```
plot([E(1,1),E(1,1:(end-plotend))],[0,D_1sum(1:(end-plotend))])
```

```
hold on
```

```
plot([E(1,1),E(1,end-plotend)],[D_2,D_2], 'Color',[0,1,0])
```

```
hold off
```

```
legend('DOS','constant value of 2d DOS','FontSize',20)
```

```
title('Density of states for a rectangle','FontSize', 14)
```

```
xlabel('E [J]','FontSize', 12 )
```

```
ylabel('D(E) [J^{-1}]','FontSize', 12)
```

```
%specific density of states (DOS per unit area)
```

```
d=D_1sum./A;
```

```
d2=D_2./A;
```

```
figure(4)
```

```
set(0,'DefaultAxesFontSize',12)
```

```
%d(d> c)= c; %c= cut off the infinite values
```

```
plot([E(1,1),E(1,1:(end-plotend))],[0,d(1:(end-plotend))])
```

```
hold on
```

```
plot([E(1,1),E(1,end-plotend)],[d2,d2], 'Color',[0,1,0])
```

```
hold off
```

```
legend('DOS','constant value of 2d DOS','FontSize',20)
```

```
title('Specific density of states for a rectangle','FontSize', 14)
```

```
xlabel('E [J]','FontSize', 12 )
```

```
ylabel('d(E) [J^{-1}m^{-2}]','FontSize', 12)
```





## **%TORUS**

%dispersionrelation and density of states

clc

clear all

close all

h=6.6261\*10<sup>-34</sup>; %in Js

m=9.11\*10<sup>-31</sup>; %in kg

F=(h/2/pi).^2./(2\*m);

disp('Choose a radius r for the torus cross section in meters');

r=input('r='); %radius of the torusring

if isempty(r)

r=0.7e-9;

fprintf('%e',r)

end

fprintf('\n')

fprintf('\n')

fprintf('\n')

disp('Choose the ratio R/r >= 1');

fprintf('\n')

ratio=input('ratio=');

if ratio<1

disp('Invalid choice of ratio, ratio has to be >=1')

r=input('r=');

end

if isempty(ratio)

ratio=2;

fprintf('%e',ratio)

end

R=ratio\*r;

nR=[0:ratio\*70];

nphi=[0:70];

```

A=4*pi^2*R*r;           % surface of the torus

%DISP

[nR,nphi ]=meshgrid(nR,nphi);
E_nR=nR.^2./R.^2.*F;    %eigenvalues for nphi=0
E_nphi= nphi.^2./r.^2.*F; %eigenvalues for nR=0

En=E_nR +E_nphi;       %energy eigenvalues

figure(1)
set(0,'DefaultAxesFontSize',12)
z_par=5;                % number of parabolas
subplot(1,2,1)

for i=1:z_par
plot([0,1],[E_nphi(i,1),E_nphi(i,1)])
hold on
end
hold off
title('E_{n_{\phi}}','FontSize', 12)
xlabel('[1]','FontSize', 12)
ylabel('E_{n_{\phi}} [J]','FontSize', 12)
axis([0 1 -1/8*E_nphi(z_par,1) (9/8)*E_nphi(z_par,1)])

subplot(1,2,2)

for i=1:z_par
plot([0,1],[E_nR(1,i),E_nR(1,i)])
hold on
end
hold off

title('E_{n_{\theta}}','FontSize', 12)
xlabel('[1]','FontSize', 12)
ylabel('E_{n_{\theta}} [J]','FontSize', 12)

axis([0 1 -1/8*E_nphi(z_par,1) (9/8)*E_nphi(z_par,1)])

%DISP

```

```
figure(2) %dispersionsrelation E(n_phi,n_R) over n_R
set(0,'DefaultAxesFontSize',12)
```

```
x=nR(1,:);
y=En;
```

```
for i=1:size(En,1)
plot(x,y(i,:), 'Color',[0,1,0])
hold on
plot(x,y(i,:), '.')
hold on
end
hold off
```

```
title('dispersion relation for a torus','FontSize', 12)
xlabel('n_{\theta} [1]','FontSize', 12)
ylabel('E_{n_{\theta},n_{\phi}} [J]','FontSize', 12)
axis([x(1) 100 En(1,1) En(1,100) ])
```

```
%DOS
```

```
nR=nR(1,:);
nphi=nphi(:,1);
```

```
E_nR=E_nR(1,:);
E_nphi=E_nphi(:,1);
```

```
%quasicontinuous 1d-single-DOS
```

```
E=linspace(En(1,2),En(end,end),90000);
[E,E1]=meshgrid(E,E_nphi);
```

```
D_1=(sqrt(2*m)*8*pi*R/h).*heaviside(E-E1)./(sqrt(E-E1));
D_1((E-E1)==0)=0; %problem: 1/0
```

```
plotend=sum(D_1(end,:)==0);
```

```
if plotend==size(E,2)
plotend=0
end
```

```
D_1sum=sum(D_1,1);
```

```
%(quasicontinuous DOS) 2d-DOS
```

```
D_2=16*pi^3*m*R*r/(h^2);
```

```
figure(3)
```

```
set(0,'DefaultAxesFontSize',12)
```

```
%D_1sum(D_1sum> c)=c; %c= cut off the infinite values
```

```
plot([E(1,1),E(1,1:end-plotend)],[0,D_1sum(1:end-plotend)])
```

```
hold on
```

```
plot([E(1,1),E(1,end-plotend)],[D_2,D_2], 'Color',[0,1,0])
```

```
hold off
```

```
legend('DOS','constant value of 2d DOS','FontSize',12)
```

```
title('Density of states for a torus','FontSize', 12)
```

```
xlabel('E [J]','FontSize', 12 )
```

```
ylabel('D(E) [J^{-1}]','FontSize', 12)
```

```
%specific density of states
```

```
d=D_1sum ./A;
```

```
d2=D_2 ./A;
```

```
figure(4)
```

```
set(0,'DefaultAxesFontSize',12)
```

```
%d(d>c)=c; %c= cut off the infinite values
```

```
plot([E(1,1),E(1,1:end-plotend)],[0,d(1:end-plotend)])
```

```
hold on
```

```
plot([E(1,1),E(1,end-plotend)],[d2,d2], 'Color',[0,1,0])
```

```
hold off
```

```
legend('DOS','constant value of 2d DOS','FontSize',12)
```

```
title('Specific density of states for a torus','FontSize', 12)
```

```
xlabel('E [J]','FontSize', 12 )
```

```
ylabel('d(E) [J^{-1}]m^{-2}','FontSize', 12)
```

## %SPHERE

%dispersionrelation and density of states

clc

clear all

close all

$h=6.6261 \cdot 10^{-34}$ ; %in Js

$m=9.11 \cdot 10^{-31}$ ; %in kg

$l=[0:400]$ ;

$R=input('Value for the radius R=')$ ;

if isempty(R)

$R=1e-9$

end

$F=(h/(2 \cdot \pi))^2/(2 \cdot m \cdot R.^2)$ ;

$E=F \cdot l \cdot (l+1)$ ; %energy eigenvalues

$A=4 \cdot \pi \cdot R^2$ ; %surface of a sphere

%DISP

figure(1)

set(0,'DefaultAxesFontSize',12)

plot(l,E,'.',l,E)

title('Dispersion relation')

xlabel('Drehimpulsquantenzahl l','FontSize', 12)

ylabel('E [J]','FontSize', 12)

%DOS

$D=l./E+(16 \cdot \pi^2 \cdot m \cdot R^2/h^2)$ ;

figure(2)

set(0,'DefaultAxesFontSize',12)

plot(E,D,'.',E,D)

title('Density of states','FontSize', 12)

xlabel('E [J]')

ylabel('D(E) [J^{-1}]','FontSize', 1)

```
%specific density of states (DOS per unit area)
```

```
d=D./A;
```

```
figure(3)
```

```
set(0,'DefaultAxesFontSize',12)
```

```
plot(E,d,'.',E,d)
```

```
title('Specific density of states for a spherical shell','FontSize', 12)
```

```
xlabel('E [J]')
```

```
ylabel('d(E) [J-1m-2]', 'FontSize', 1)
```