TEACHING QUANTUM ATOMIC PHYSICS IN COLLEGE AND RESEARCH RESULTS ABOUT A LEARNING PATHWAY

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Abstract
Our approach is centered around the concepts of "state" and "orbital". Its primary aim is to explain and calculate phenomena and basic facts like size, spectra and energies of different atoms, molecules and solids. Our approach makes use of the analogy with standing waves and uses model building with the computer (STELLA) to avoid high mathematical difficulties.
Finally we give very short results of a case study of one student following this course. We show four different states of his learning pathway to a model of the atom, starting with a planetary model and coming to a model of a distributed electron cloud. A short characterization of his final cognitive state follows.

Introduction

Teaching atomic physics with a quantum approach still often is not leading to a sufficient understanding of students. On the basis of empirical investigations of students' conceptions (1) and of further trials in classes of advanced high school course as well as introductory physics courses in university we suggest an approach which is centered around the concepts of "state" and "orbital". Furthermore we changed our interpretation of the ψ-fuction in bound states from a probability interpretation to the electron cloud or even "electronium" interpretation (see below) to avoid student difficulties of the following type:

> *"The function you have is nothing but the probability of presence of an electron. ... you can't say it moves on an orbit. To explain - well, the motion cannot really be explained anymore ... It's however, not an orbit any more. .. The electron must move somehow - very strange, it is now here and then there .. That gets crazy .. Damned, it could theoretically move in between. Just that it moves in a strange zig-zag, but that would mean again something like an orbit. And that's crazy again. Well, somehow I can't get that clear."*

These concepts are familiarized by analogies from standing waves in one, two or three dimensions. These analogies are also used to introduce a powerful computer tool (STELLA) to deal with differential equations without being drowned in mathematics. We try to use this computer tool to model the Schroedinger equation for real atoms, molecules and solids.. This avoids overwhelming mathematical difficulties and helps to deal with even more interesting phenomena such as higher atoms with more electrons. We also foster student orientation by discussing students' own conceptions explicitly and by letting students develop their own models with STELLA.

Basic physics ideas of our approach

To come to a deeeper understanding of atomic physics two intentions seem crucial: to develop a better understanding of the underlying mathematics and to develop a clear spatial view of the atom. The first intention in our approach is done by working on the analogy between states of standing waves and stationary states in atoms (Table 1).

The analogy of standing waves

String	**Atom**
Standing waves	**Electron distribution**
Oscillating motion	**No motion**
STATE n	
Numbers n	**Quantum numbers n**
Frequency f_n	**Energy W_n**
Amplitude function $y_n(x)$	**Amplitude function $\psi_n(r)$**
Nodal points	**Nodal surfaces**
Boundary condition: node	**Bound. condition: ψ =>0**
Inhomogeneous string m' = f(x)	**Varying potential V =V(r)**
$y_n''(x) \sim -f_n^2 * m'(x) * y_n(x)$	**$\psi_n''(r) \sim -[W_n - V(r)] * \psi_n(r)$**

TABLE 1. Analogy of string and atom

Interpretations of the ψ-function

The second intention we try to achieve by guiding the students to a simpler interpretation of the ψ-function, along the lines of chemists ("electron clouds") or even more radical like Herrmann (2) thinking of an electron in bound states as of a kind of liquid ("electronium", interpretation 2, see Figure 1).

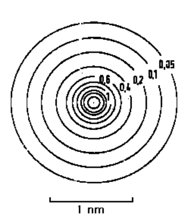
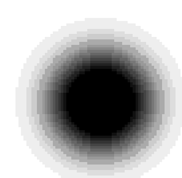
 Graph of ψ^2-function in ground state of H (repres. in 2 dimensions)	 **Interpretation 1** "Probability of localization" Born 1926	 **Interpretation 2** "Charge density", "electron cloud", Schrödinger 1926 "electronium", Herrmann 1991

FIGURE 1. Two different interpretations of the ψ-function

Outline of a possible course

"Atomic physics - quanta, states, orbitals"

(6 weeks, 6 labs and/or computer modeling tasks)

1) The free electron as a quantum

2) Introduction of the main idea: states in an atom like states in a standing wave (sound waves in a spherical glass bulb, standing waves on a tambourine, standing waves on a string)

3) Computer models and lab work with standing waves on an inhomogeneous string

4) Hydrogen atom: The SCHROEDINGER equation, the potential V(r)

5) Computer model of the hydrogen atom

6) Hydrogen atom: two interpretations; shape and size; experiments with spectra and Franck-Hertz; orbitals and their nodal surfaces; the periodic table of elements; the He+-atom

7) Equation for the hydrogen atom energy levels; application to x-rays

8) Computer models of higher atoms He, Li, Be,Na

9) Molecules: computer modeling with STELLA; binding energy and distance of the nuclei in the H2+ molecule

10) Band structure in solids with a computer model with 4 atoms; explaining optical properties of solids.

Some selected materials

Standing waves on a beaded string

(see other paper from Niedderer in this volume)

Overview of standing waves in 1, 2 and 3 dimensions.

Standing waves in one, two and three dimensions provide a very good preparation on the concept of "state". Already in this classical phenomena there are states which can be defined by eigenvalues and amplitude functions. In addition to observe and calculate amplitude fuctions with one dimensional standing waves on beaded strings, in higher dimensions they are most easy to characterize by their nodes (points, lines or surfaces, see Table 2). This also helps for a spatial view of orbitals. From a mathematical point of view, angular functions of three dimensional standing waves of standing sound waves in a spherical tube are the same as of ψ-functions in a hydrogen atom.

Stand. Waves	**1 dimension**	**2 dimensions**	**Three dimensions**
Apparatus	Beaded string	Tambourine	Sound in spherical glass bulb
Type of Nodes	Points	Lines	Surfaces
Node Systems	One System	Two systems, e.g. circles and straight lines	Three systems, e.g. spherical surfaces, planes and double cones
"q-numbers"	one (n)	two (n , m)	three (n, m, l)

TABLE 2. Standing waves in one, two and three dimensions

A very helpful example are standing waves in two dimensions with a tambourine.

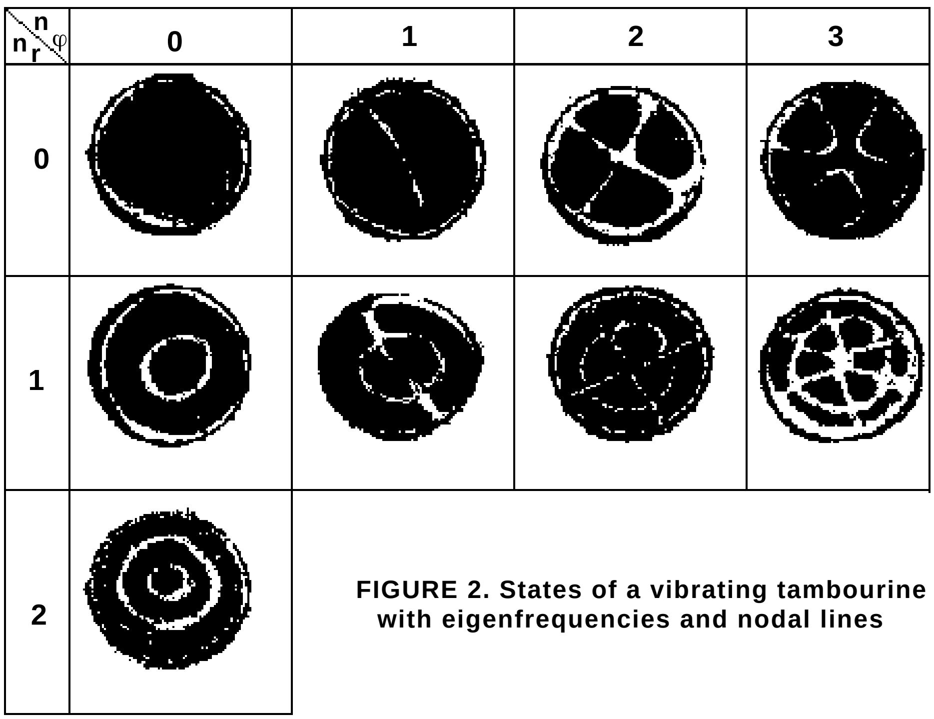


FIGURE 2. States of a vibrating tambourine with eigenfrequencies and nodal lines

Hydrogen atom: STELLA model

To come to a plausibility of the Schroedinger equation we start with free electrons and the de Broglie equation. Once the Schroedinger equation is explained and given, it is easy for students to build their own STELLA model of the hydrogen atom (Table 3). The graphical structure of the STELLA model then enforces to think of the Schroedinger equation as a relation which determines the curvature of the ψ-function from energy W_n, potential V(r) and the value of ψ already arrived at.

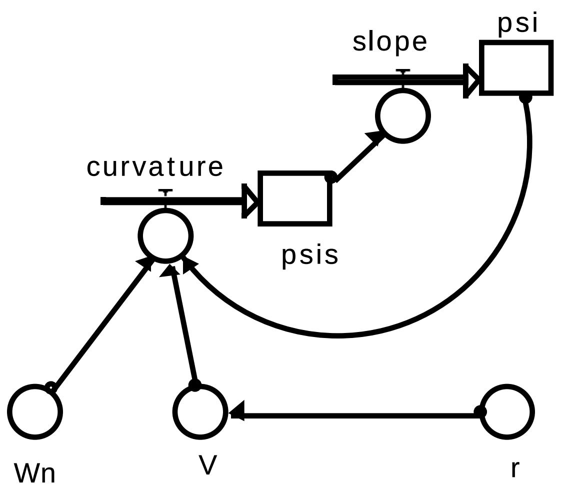
STELLA model	Model equations
	Model equations r = time {nm} psi = psi + dt * (slope) INIT (psi) = 0 psis = psis + dt * (curvature) INIT (psis) = 1 curvature = - 26.25*(Wn-V)*psi V = - 1.44 / r {eV} Wn = - 13.6 {eV}

TABLE 3. STELLA model for hydrogen

With this model we get the results in Figure 3 and Table 4.

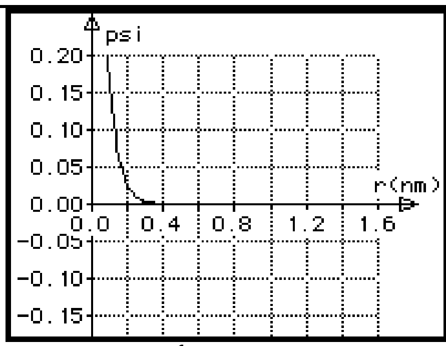
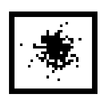
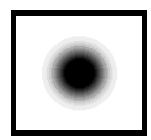
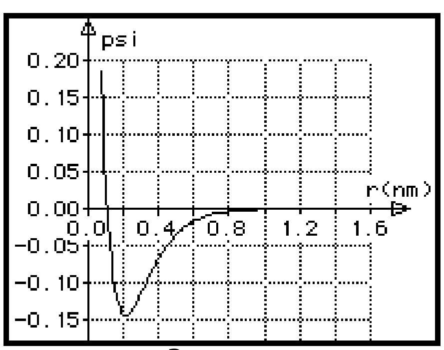
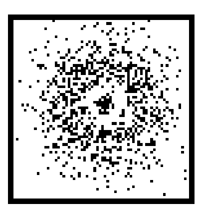
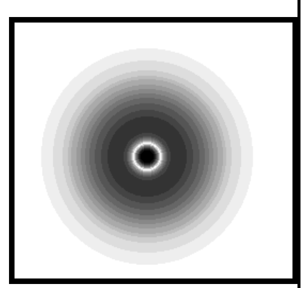
ψ-Function	probability of localization	distribution of density
 1s state	Wn= -13.6 eV  1s state	 1s state
 2s state	Wn= -3.4 eV  2s state	 2s state

FIGURE 3. The first two states of hydrogen

Measurement (from literature)	Theory/model calculation
Covalent radius of H: 0.032 nm	maximum of r*ψ at 0.053 nm
Radius from kinetic theory: 0.126 nm	68% at 0.093 nm; 90% at 0.136 nm

TABLE 4. Size of the hydrogen atom (ground state)

A simplified model for the lithium atom

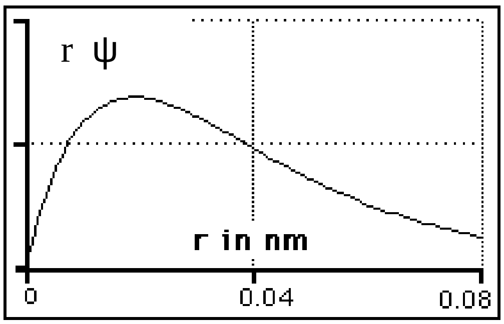


FIGURE 4. r*ψ of first electron

The first approach is based on the idea to put one electron after the other into the field of the nucleus. So we start with one electron around a lithium nucleus with a charge of +3e. Then the ground state of this single electron is calculated in the same manner as in hydrogen. From the maximum of the resulting r ψ-graph - in this case at 0.02 nm (see Figure 4) - it is roughly determined where the screening effect of this first electron to a next to build in second electron would be most effective.

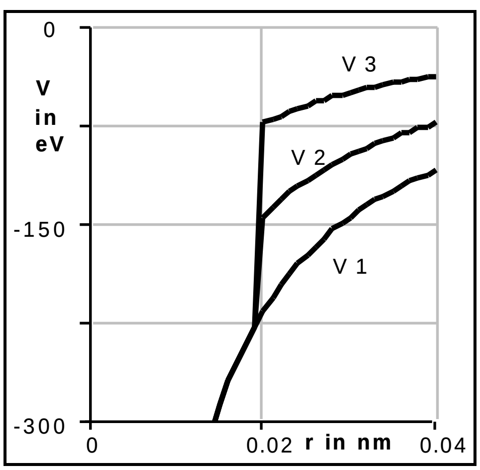


FIGURE 5.
Potential for all three electrons

For simplicity, we then assume the potential at this point to jump from $V_3=3*V_{hydrogen}$ to $V_2= 2*V_{hydrogen}$ (see Figure 5). We then calculate the ψ-function for the second electron with this potential V_2 to be also in an 1s state. It turns out, that its ψ-function is very similar to the first electron (see Figure 6). For the third electron we then assume the potential at r=0.02 nm to jump from $V_3=3*V_{hydrogen}$ to $V_1= V_{hydrogen}$ (see Figure 5). The resulting STELLA model and the model equations are shown in Table 5.

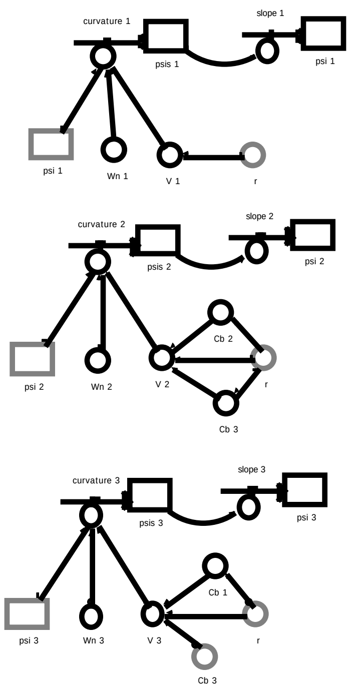
STELLA model	Model equations
	1. General definition r = time {nm} (space changes instead of time changes) 2. Equations for iteration psi_1(t) = psi_1(t - dt) + (slope_1) * dt INIT psi_1 = 0 psis_1(t) = psis_1(t - dt) + (curvature_1) * dt INIT psis_1 = 1 curvature_1 = -26.25*(Wn_1-V_1)*psi_1 These are the crucial equations for electron 1. The same equations for electron 2 and 3 come into play. 3. Equations for potentials Cb_1 = -1.44/r Cb_2 = -2*1.44/r Cb_3 = -3*1.44/r V_1 = -3*1.44/r V_2 = If r<.02 then Cb_3 else Cb_2 V_3 = If r<.02 then Cb_3 else Cb_1 4. Energy eigenvalues Wn_1 = -120.57 Wn_2 = -93.35 Wn_3 = -5.85 Wtot = -219.9 eV

TABLE 5. Simplified STELLA model and model equations for Li atom

The STELLA model (Table 5) shows the same principle structure for all three electrons, but with different potentials. The equations more precisely show what we did with the potential, as it was described above. The different values for Wn_1 and Wn_2 are due to the fact, that this is not a self consistent approach, which takes into account the full interaction between different electrons.

The resulting r ψgraphs of all three electrons are shown in Figure 6. The results, compared to measurement values from literature, are shown in Table 6.

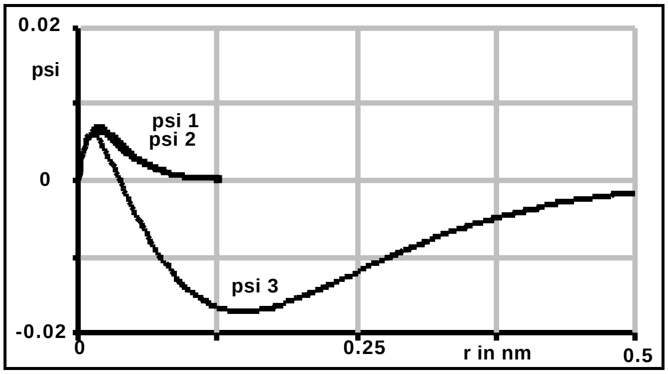


FIGURE 6.

Resulting r∗ψ-graph of all three electrons in Li

With similar simplified approaches students have also calculated He, Be and Na. Students in university courses have also developed STELLA models with a self consistent calculation of these atoms, both of ground states and excited states.

Measurement (from literature)	Theory/model calculation
Total energy of ground state (all 3 electrons) Wtot = 203.5 eV	Wtot = -219.9 eV
Atom radius: r= 0,152 nm (covalent binding or cristal lattice)	max of 2s-psi-function r ≈ 0,15 nm last turning p.: r ≈ 0.25 nm

TABLE 6. Energy and size of the Li atom (ground state)

The H_2^+ molecule - the most simple molecular system

By choosing an adequate simple rectangular potential, the effects of binding can be shown an calculated (Figure 7 and 8). Results are compared to measurement in Table 7.

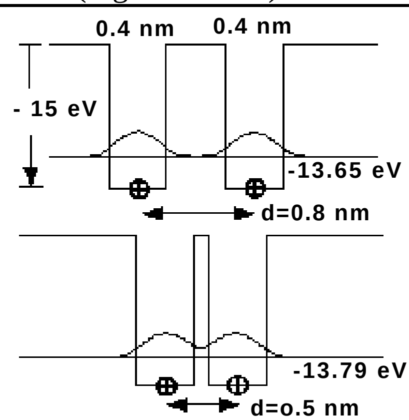


FIGURE 7.

Different Distance of Nuclei .

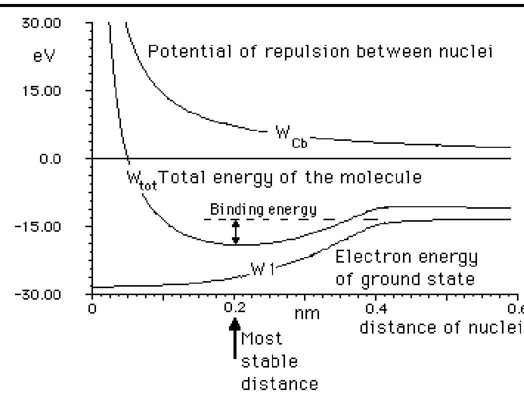


FIGURE 8.

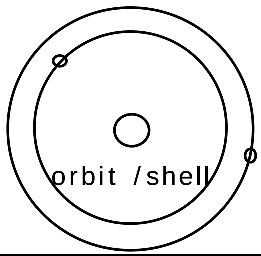
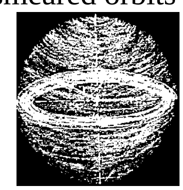
Total Energy of the Molecule

Measurement (from literature)	Theory/model calculation
Stable distance of nuclei: 0.1 nm	Stable distance of nuclei: 0.2 nm
Binding energy: 1.3 eV	Binding energy: about 3 eV

TABLE 7. Stable distance of nuclei and binding energy in H_2^+ molecule

5. Results about a learning pathway

According to results of Juergen Petri (6), one student Carl in a course like this in grade 13 (age 19) in a German gymnasium follows a learning pathway roughly characterized by the following steps:

Carl's **first conception** of the atom ("Planetary model")  	Carl's **second conception** of the atom ("Probability-orbits model", "smeared orbits") 
Carl's **third conception** of the atom ("Quantum model") 	Carl's **fourth conception** of the atom ("Orbital model") 

The **final state** of Carl's cognitive element "atom" consists of a **"federation"** of the conceptions 1, 2, and 4. These conceptions are connected, they don't exist isolated in their different generating contexts. Carl is able to reflect on differences, problems and advantages of each model. The cognitive element contains an **"internal administration level".** The most powerful "member" still is the first conception (planetary model), it first "raises its voice" (high **"strength"**), but the "prestige and influence of the other members" - espcially the fourth conception (orbital model) - is much higher (high **"status"**).

6. References

(1) Bethge, T., *Aspekte des Schülervorverständnisses zu grundlegenden Begriffen der Atomphysik (Aspects of students' ideas about basic concepts of atomic physics)*. Doctoral dissertation, University of Bremen, 1988, 251 pages.

(2) Herrmann, F., Laukenmann, H., *Der Karlsruher Physikkurs, Band III*, Universitaet Karlsruhe, Fachbereich Physik, 1994

(3) Niedderer, H., Bethge, T. & Cassens, H., "A Simplified Quantum Model: A Teaching Approach and Evaluation of Understanding", in: Lijnse, P.L., Licht, P. , de Vos, W. & Waarlo, A.J. (Eds.): *Relating Macroscopic Phenomena to Microscopic Particles - A*

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(5) Petri, J., Der Lernpfad eines Schülers in der Atomphysik - Eine Fallstudie in der Sekundarstufe II - (The learning pathway of one student in atomic physics - A case study in upper high school). Doctoral dissertation, University of Bremen. Published Aachen, Mainz, 1996 (ISBN3-89653-048-8) 365 pages