An Approach for Second Year Quantum Atomic Physics based on the Schrödinger equation

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In this paper we describe the core concepts of the quantum atomic physics course we teach in introductory physics for second year teacher students. The approach has been developed over nearly twenty years based on results of several empirical studies on student understanding and student learning and an evaluation of the whole approach. The basic concept used to discriminate quantum mechanics from classical mechanics is the concept of state, especially that of stationary state . Stationary states are quantitatively determined in many interesting cases by finding graphical solutions of the Schrödinger equation (ψ-functions) and corresponding energy eigenvalues with modeling software on the computer.
The main goal of our approach is to develop a quantum mechanical understanding of atoms, molecules and solids, which allows to visualize atoms in a more appropriate way (compared to planetary models) and is able to explain essential features such as e.g. size and spectra of atoms, or binding energy of molecules.

I. INTRODUCTION

Our atomic physics approach was developed at the university of Bremen over about 20 years[1]. In addition, it has been taught and evaluated in German secondary schools in advanced physics courses in grade thirteen (age nineteen). Three manuscripts, two in German[2] and one in English language[3] can be downloaded from our home page.

From a physics point of view, we use the one-dimensional stationary Schrödinger equation to understand and calculate spherically symmetric eigenstates in atoms (s states, e.g. in H, He and Li), covalent binding in molecules and the explanation of energy bands in solids.

From a physics education point of view based on empirical research [4], we prefer an electron cloud conception of the orbital without any movement of the electron in its stationary state . The interpretation of $e*\psi^2$ as a continuous charge density[5] is preferred over ψ^2 as localization probability density usually depicted by discrete tiny dots to visualize the shape of the orbital.

II. BASIC INSTRUCTIONAL IDEAS AND PHYSICS CONCEPTS

A. Basic instructional ideas

One of our basic decisions is to put more emphasis on understanding fundamental features of matter as determined by quantum physics rather than to discuss problems of quantum philosophy in depth. Such features are the size, ionization energy and spectra of atoms, stable

distance and binding energy of molecules, energy bands explaining light and electricity in solids. We therefore focus on stationary states of electrons in atoms, molecules and solids. Our aim is to better link theory and experiment and to encourage students to see quantum physics as an ordinary part of physics, i.e. a part of physics where fundamental features of atoms, molecules and solids can be predicted, calculated and measured as precisely as in classical physics.

As a further result of the course, we want students to have the competence feeling that they themselves can do such calculations even in more complex and relevant applications, using computer tools for modeling physics (not simply for ready made simulations).

The second important idea is to provide a better intuitive understanding of the Schrödinger equation for stationary states. We prepare this understanding by elaborating and reflecting the analogy of mechanical standing waves and by interpreting the Schrödinger equation mathematically as a statement about the curvature of the ψ-functions. This view can provide a qualitative description of ψ-functions and their important features for atoms, molecules and solids without any calculation.

B. Basic physics concepts

1. *The concept of stationary state*

In quantum mechanics the concept of state is appropriate to replace the concept of orbits. Here, our discussion will be limited to stationary states. A stationary state in quantum atomic physics as well as for standing waves is defined by three important characteristics:

- A *name*: stationary states have names such as numbers, quantum numbers, ground state, higher state, etc.
- An *eigenvalue*: stationary states of electrons in atoms, molecules and solids are characterized by an energy eigenvalue, states of standing waves are characterized by an eigenfrequency.
- The *form*: an atom or a standing wave in a stationary state has a certain form. The form can be described in several different and important ways:
    - by describing the nodes (nodal points, nodal lines, or nodal surfaces), e.g. number and distances of nodes
    - by using spatial descriptions of orbitals (such as s and p orbitals),
    - by a qualitative description of the ψ-function,
    - by a graph of the ψ-function, or
    - by a formula for the ψ-function.
    (The best understanding results from using all these representations of the form of amplitude functions.)

2. *The Schrödinger equation (SEQ)*

In our course, we make the Schrödinger equation plausible by linking the de Broglie equation with the differential equation of standing waves. After that we take this equation as a given axiomatic basis and apply it to different problems, using always only one variable x or r. The Schrödinger equation in the simplest 1-dimensional case can be written as

$$\psi'' = -8\pi^2 \cdot \frac{m_e}{h^2} \cdot (E - V) \cdot \psi \tag{1}$$

where $e * \psi^2$ has the meaning of radial charge density. This equation has a very similar structure to the differential equation of standing waves. On the left side is the second derivative of a kind of amplitude function, called distribution function (ψ-function or psi-function), on the right side is the distribution function itself.

3. *Interpretation of ψ*

We briefly discuss two different kinds of interpretations of the ψ-function in stationary states.

Interpretation I: Localization probability density

In interpretation I ψ^2 is seen as probability density of finding the electron. This interpretation goes back to Born in 1926.

Fig. 1: Probability density
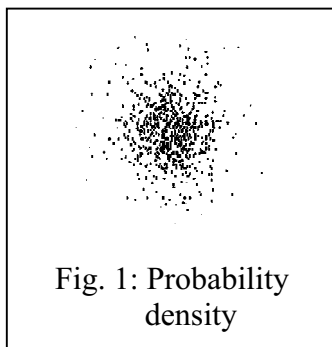
a. Fig. 1 shows the result from a few hundred localization measurements of the electron in the ground state of the H atom by displaying the localized electrons as tiny dots.

b. The probability to localize an electron in a small volume ΔV is $\psi^2 * \Delta V$.

Probability density here is visualized as density of the dots. As the density of the dots increases near the nucleus, it is more likely to find the electron close to the nucleus than further away from the nucleus. Because each dot is the result of a localization thus changing the ψ-function from one form to another, this interpretation gives not an intuitive understanding of the orbital of the ψ-function in one stationary state.

Most physics textbooks prefer this interpretation.

Interpretation II: Continuous distribution of charge density, electron cloud

In interpretation II, $e*\psi^2$ is seen as charge density, which is continuously distributed around the nucleus in stationary states of atoms.
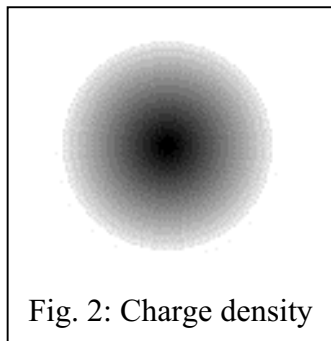

Fig. 2: Charge density

a. Fig. 2 shows the charge distribution of one electron around the nucleus in the ground state of the H atom. The charge is spread out over a large volume compared to the nucleus. [6]

b. $e*\psi^2*\Delta V$ is the part of the electron charge in the volume ΔV.

As it is important for the notion of stationary state that we abandon the notions of orbits and movement from this concept, we prefer this interpretation II with a stationary continuous distribution $e*\psi^2$ against a particle view of "probability of finding the particle" [7]. We emphasize that visualizing an electron as a particle much smaller than its orbital is confusing and not very helpful to get an intuitive picture of the electron in a stationary state. A continuum view of a distribution of density seems more adequate and can be fostered by using an (intermediate) conception of smeared charge. This view is often preferred also by chemists. This interpretation II provides a picture of the ψ-function which is easy to understand and is close to an interpretation from Schrödinger:

> *"But there is something tangibly real behind the present conception also, namely, the very real electrodynamically effective fluctuations of the electric space density."* 8

The reasons for preferring interpretation II are:

- "Finding" suggests that the particle can be found at different points, even in the unperturbed state, so it moves around. In interpretation II it is very clear that there is no motion in a stationary state. We have empirical evidence that a probability interpretation stabilizes the idea of motion between the points of measurement where the electron was localized [9].
- We found also empirical evidence of the contrary, that using the interpretation of a charge distribution helps students substantially with getting the idea of no motion in stationary states. About 80% of the students change from an electron orbit view of electrons in an atom to an electron cloud view. All students after the course abandon a description of electrons which includes the notion of motion.[10]
- This interpretation gives an intuitive notion of an atom in three dimensions in the unperturbed state, whereas in the probability picture each point results from a localization process, which destroys the original state completely. Most of our students show a consistent quantummechanical description of an atom in many different tasks after the course. [11]
- This interpretation helps students consequently to come away from the electron as a classical particle. Nearly all students develop a good notion of an electron distribution.[12]

- The idea of a charge distribution supports an intuitive understanding of many effects in atoms, molecules and solids, such as binding energies, shielding effects of inner electrons on the effective potential, size and form of atoms and molecules.
- From our qualitative empirical research, we know that this view can become especially fruitful for students to understand the effective potential in higher atoms as a result of shielding.[13].

Some textbooks are supporting this interpretation also. One example:

"Alternatively we can think of the electron as having its charge spread out, or distributed, as a kind of electron cloud " [14]

4. Meaning of ψ'' as curvature of the ψ-function

The Schrödinger equation is also used for an intuitive understanding of ψ-functions. The term ψ'' in the Schrödinger equation is interpreted as a change in slope which mainly is proportional to the curvature. By discussing the Schrödinger equation as a statement for curvature, many features of atoms (like different sizes of H, He^+, and He or spatial form of nodal distances in different states of H) can be understood in a half quantitative way without solving the differential equation. The main fact being used is

$$\psi'' \propto (E - V) \cdot \psi \qquad (2)$$

5. Relations between theory and measurement

The idea to connect theory with possible real measurements was stated above. Besides relating calculated energy eigenvalues to observed spectra, we also discuss different measurements of size in relation to the ψ-function. We focus especially on the fact that the size of an atom cannot be determined exactly because the ψ-function is approaching the zero value asymptotically. The radius of an atom can be determined either as the radius of the last maximum in our ψ-functions, or as the radius of the last turning point, or as the radius up to which something like 90% of the charge density of the electron is found inside this radius. In our manuscripts corresponding methods to determine the radius of atoms are described and measurement values from literature are documented. Other important data from measurement, which can be compared to our own theoretical calculations are: ionisation energy, binding energy of molecules, stable distance of molecules, and energy bands of solids.

6.   *The spatial conception of orbitals*

We aim at a three-dimensional spacial conception of atoms. This can be fostered by discussing three-dimensional standing sound waves in a spherical tube, and by discussing both orbitals and nodal surfaces of different states, for instance in hydrogen.[15]

7.   *The analogy of standing waves*

" In this paper I wish to consider, first, the simple case of the hydrogen atom (non-relativistic and unperturbed), and show that the customary quantum conditions can be replaced by another postulate, in which the notion of "whole numbers", merely as such, is not introduced. Rather when integralness does appear, it arises in the same natural way as it does in the case of the note-numbers of a vibrating string. The new conception is capable of generalization and it strikes, I believe, very deeply at the true nature of the new quantum rules." [16]

The fundamental equation that describes bound electrons is a differential equation, called the Schrödinger equation (1). This equation has a very similar structure to the differential equation of standing waves. On the left side is the second derivative of a kind of amplitude function, called distribution function (ψ-function, Psi-function, amplitude function), on the right side is the distribution function itself. The analogy is shown in Fig. 3.

String		Atom
Frequency f_n		Energy E_n
Amplitude $y_n(x)$	**State n**	Amplitude $\psi_n(r)$
Nodal points		Nodal surfaces
Border condition: node (y=0)		Border condition: $\psi => 0$
Mass distribution		Potential function
m' = f(x) (variable mass density)		V=V(r) (Potential well)
$y_n{''}(x) \sim - f_n^2 * m'(x) * y_n(x)$		$\psi_n{''}(r) \sim - [E_n - V(r)] * \psi_n(r)$

Fig. 3. Analogy between stationnary states on strings and in atoms

The analogy is not only mathematical, it gives a better understanding of states, spatial distribution, nodal surfaces and eigenvalues.

8. *The use of model building software*

In our courses we use modeling software like e.g. STELLA or MODELLUS to model the differential equations for standing waves and the Schrödinger equation and to find the graphical solutions for different cases such as hydrogen, helium, lithium, and hydrogen molecule ion by systematically varying the values of frequency or total energy respectively . In principle, this can be done by many different programs (like e.g. Excel or Mathematica). In Niedderer&Deylitz (1997, 1998) the model building software STELLA[17] is used for standing waves, hydrogen, helium and lithium. In Niedderer&Petri (2000) the model building software MODELLUS [18] is used for the same cases and in addition for the H2+ molecule and for simple models of solids. STELLA is a modeling software with a graphical surface, which facilitates the formulation of equations *and* helps for better understanding like a concept map.[19] The differential equation is represented by graphical objects. Each object stands for a quantity in the equation. These objects have to be connected with arrows that show how the quantities relate to each other.

 MODELLUS is equation oriented, which perhaps is easier for learners who already have a good command and understanding of mathematical equations including differential equations.

III. COURSE STRUCTURE AND STUDENT ACTIVITIES

The course was about five times taught as the fourth part of a two-year introductory course called atomic and nuclear physics. The first eight weeks of the semester were devoted to atomic physics (see Table I). Students every week had three hours of lecture, two hours of lab, and one hour working with a tutor. In addition to the lab work and the computer labs they had homework assignments with quantitative calculus based tasks every week. Textbooks which were used were mainly Orear (1982), Meyer-Kuckuck (1997), and Tipler (1991).

Table I. Course structure for second year introductory physics course

Week No.	Topic	Labwork	Computer Lab
1	Quantum view of light	Photoelectric effect	-
2	Quantum view of electrons	Electron diffraction	-
3	Standing waves: states, eigenfrequencies, amplitude function	Measuring standing waves on a string with non-homogeneous mass distribution	Modeling standing waves on a string with non-homogeneous mass distribution
4	Hydrogen atom: states and energy levels	Franck-Hertz experiment	-
5	Schrödinger equation	Hydrogen spectrum Measurement values about the size of the hydrogen atom from literature	Modeling spherically symmetric states of the hydrogen atom, determining eigenenergies and amplitude functions
6	Higher atoms: He, Li	Results about spectra and size of atoms from literature	Modeling He- and Li-atoms (ground state)
7	The H2+ molecule	Measurement values about H2+ (distance, binding energy) from literature	Modeling the H2+ molecule a. with square well potentials using "cT quantum well" software b. with Coulomb potentials
8	Solid state	Measurement values about NaCl (energy bands) from literature	Modeling a solid with 4 atoms, using square well potentials with "cT quantum well" software

IV. PREPARATION OF BASIC CONCEPTS "STATIONARY STATE", "EIGENVALUE" AND "AMPLITUDE FUNCTION" USING STANDING WAVES

A. Standing waves in 2 and 3 dimensions

The conception of standing waves in one, two and three dimensions is most helpful to develop a spatial conception of atoms with the basic concept of stationary state. Table II shows some basic structures.

Table II. Standing waves in 1, 2 and 3 dimensions

Standing wave	One-dimensional	Two-dimensional	Three-dimensional
Kind of nodes	Points	Lines	Surfaces
Nodal systems	One System	Two systems, e.g. Circles and straight lines	Three systems, e.g. spherical surfaces, planes and cones
State numbers	One, e.g. n	Two, e.g. n , m	Three, e.g. n, m, l

Especially three-dimensional standing waves, e.g. sound waves in a glass sphere, can be analyzed and modeled in full analogy to the hydrogen atom. Especially the fact that the angular functions are identical to those in hydrogen [20] proves that this is true in a very specific sense. Of course, the radial distribution is different because of the Coulomb potential. [21]

In two dimensions, we can demonstrate the concept of stationary state with a tambourin excited by appropriate frequencies by means of an ordinary loudspeaker. Some results are given in Fig. 4.
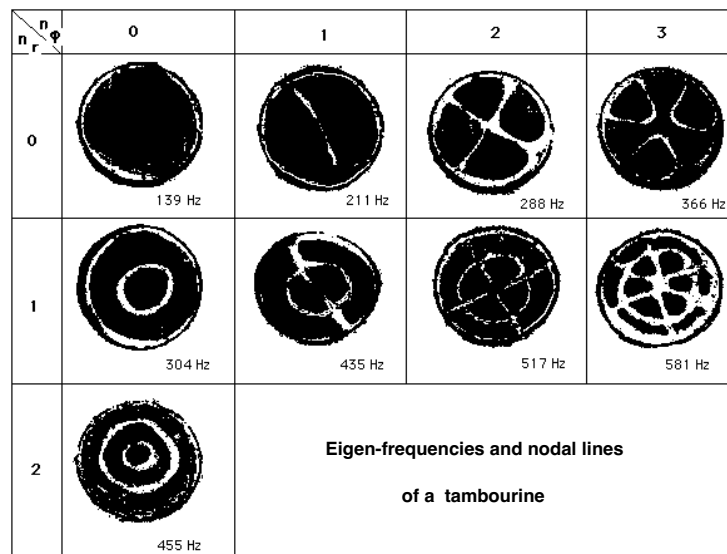

Fig. 4. Eigen-frequencies and nodal lines
of standing sound waves on a tambourine

B. Amplitude functions of standing waves on a string with non-homogeneous mass distribution

By non-homogenous mass distribution we mean that the mass density of the string is not constant over its entire length. The string is – in simple words – at some positions heavier than at others. As a result of this one could expect that the string shows different eigen-frequencies and amplitude functions for standing waves. As an example we use a string of the length of 0.53 m that has a mass density of 0.78 g/m for the first 0.38 m (only string), and 8.0 g/m for the remaining 0.15 m (string plus beads, see Fig. 5).
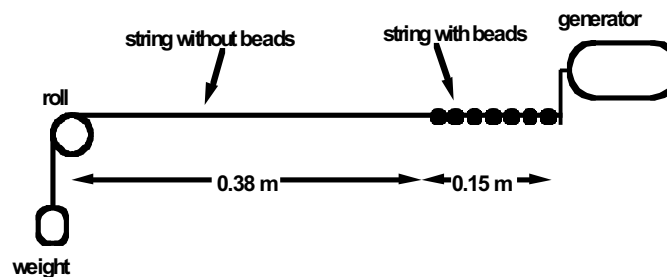

Fig.5.   Apparatus for investigating standing waves on a string
with non-homogeneous mass distribution

As a result of the weight hanging off the string at the left end we find a constant tension over the entire string. On the right side the string is connected to a generator which can move up and down with adjustable frequency to stimulate the string to oscillate. The first three states of this experiment are shown in Fig. 6.

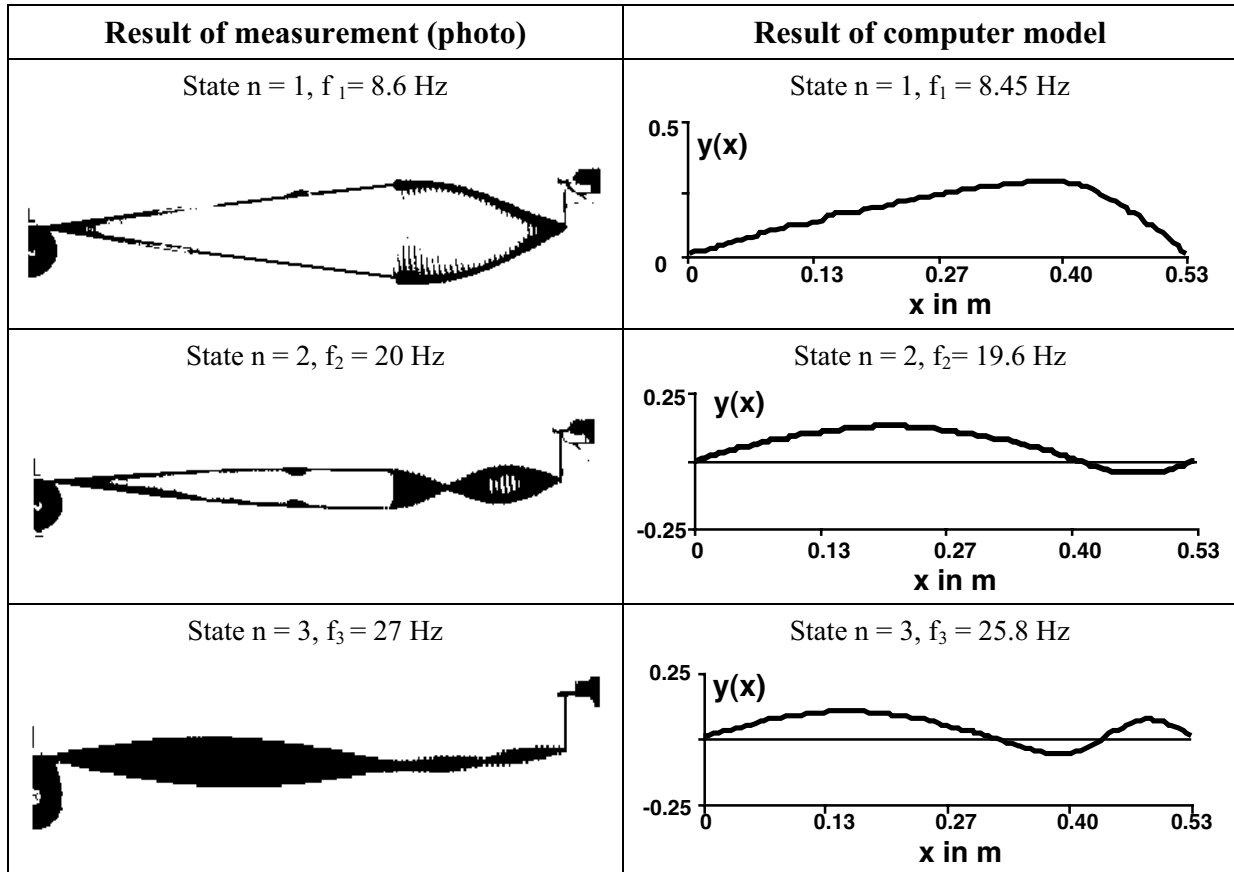| Result of measurement (photo)	Result of computer model
State n = 1, f $_1$ = 8.6 Hz	State n = 1, f_1 = 8.45 Hz
State n = 2, f_2 = 20 Hz	State n = 2, f_2 = 19.6 Hz
State n = 3, f_3 = 27 Hz	State n = 3, f_3 = 25.8 Hz

Fig. 6. Results of measurement and model calculation for the first three states
of standing waves on a non-homogeneous string

Important features of this activity with experiment and computer modeling are:

- The amplitude function can be seen in the experiment also, not only theoretically
- Students are introduced to the modeling software and develop a feeling of competence by being able to directly compare their theoretical models with the obvious experimental facts.
- They observe stationary states, learn to name them, learn to find eigenvalues and amplitude functions
- Students experience the important relation between eigenvalues and boundary conditions during the process of determining the eigen frequencies by trial and error, guided by the understanding of curvature.

The amplitude functions shown on the left side of Fig. 6 are real photos, the frequencies have been measured. Because of the non-homogeneous mass distribution the frequencies do not show constant ratios and the shape of the amplitude functions has changed significantly. The curvature of the string is larger in the area of higher mass density, therefore the positions of the nodes are shifted to the area of higher mass density.

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The experiment clarifies how the curvature of the standing wave on the string depends on three parameters: the tension F_s (from the weight), the mass density m_s (mass per unit length), and on the frequency f. This – in addition to a possible theoretical derivation – gives an intuitive understanding of the differential equation:

$$y''(x) = -4\pi^2 \cdot f^2 \cdot \frac{m_s(x)}{F_s} \cdot y(x) \qquad (3)$$

The mass density m_s does not have to be constant. It can be written as $m_s(x)$, which means that the density varies with the position x, e.g. by putting beads on the string.

C. Modeling standing waves with STELLA

We give students modeling software like STELLA as a tool. With this tool, they themselves can theoretically determine the amplitude functions of standing waves with non-homogeneous mass distribution, based on the differential equation. From the model we get the amplitude-functions graphically and also the eigenfrequencies of the standing waves.

In the model (Fig. 7), all quantities from the differential equation (Equ 3) can be found. y is the amplitude function, ys its first derivative and y"=curvature its second derivative. Fs is the force of the weight attached to the string (i.e. the tension in the string), f the frequency, and ms the mass density depending on the position x.
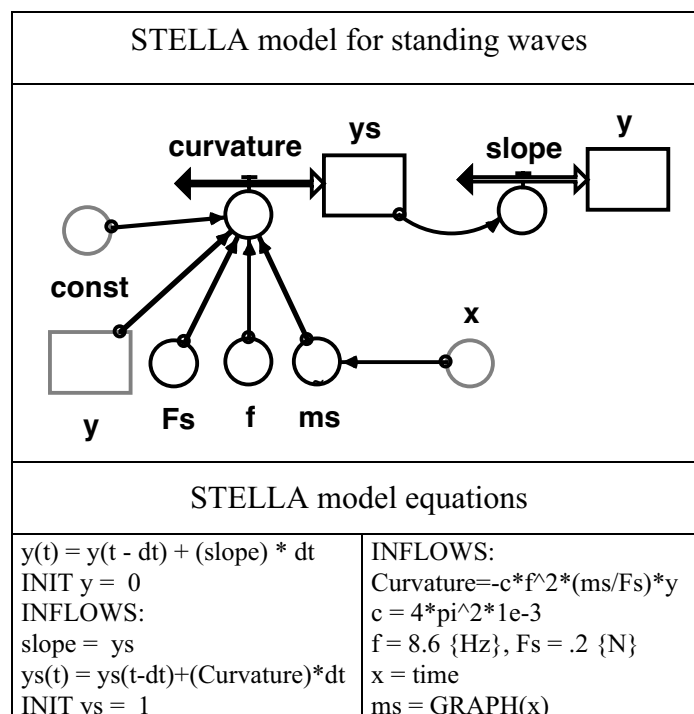

STELLA model for standing waves

STELLA model equations	
y(t) = y(t - dt) + (slope) * dt	INFLOWS:
INIT y = 0	Curvature=-c*f^2*(ms/Fs)*y
INFLOWS:	c = 4*pi^2*1e-3
slope = ys	f = 8.6 {Hz}, Fs = .2 {N}
ys(t) = ys(t-dt)+(Curvature)*dt	x = time
INIT ys = 1	ms = GRAPH(x)

Fig. 7. STELLA model and model equations
for standing waves on an inhomogeneous string

We have to enter the values for Fs, f, and ms and the initial values for y (must be zero because the amplitude function starts with a node) and ys (can be any value except zero because the amplitude function starts with a slope not equal zero). The equation for the curvature "curvature" is our differential equation. STELLA always names the x-variable TIME although in this model the x-axis is the position. Therefore we need an object for the position x with the equation x = TIME.

Results are shown in the Fig. 6 above.

V. THE HYDROGEN ATOM

A. Description of bound electrons as stationary states

Now, we describe startionary states in atoms. The basics are:

- Electrons are bound in atoms in discrete states; (stationary states, eigenstates). In atomic Physics the state numbers n, m, l are called quantum numbers.
- Each state is characterized by an eigenvalue of the binding energy of the electron. Similar to the eigenfrequencies of standing waves we find certain values of eigenenergies (discrete eigenenergies).
- According to the amplitude function of standing waves, we have the ψ–function to describe the spatial form of atoms. It is found by solving the Schrödinger equation. The Schrödinger equation in the simplest 1-dimensional case is given in equation (1).

To solve the three-dimensional Schrödinger equation for spherically symmetric cases (l=0, s-states), the three-dimensional Schrödinger equation can be reduced to the following form

$$u''(r) = -8\pi^2 \cdot \frac{m_e}{h^2} \cdot (E - V(r)) \cdot u(r) \tag{4}$$

with $\psi(r) = \frac{u(r)}{r}$, and $e*u^2$ having the meaning of radial charge density. So the students solve the one-dimensional problem with the modeling software and get u(r). From that they can easily calculate the three dimensional state functions of spherical symmetric eigenstates as displayed in almost every textbook as $\psi(r) = \frac{u(r)}{r}$.

The potential V(r) is the Coulomb potential of the nucleus. The equation shows the Coulomb potential of the hydrogen atom.

$$V(r) = -\frac{1}{4 \cdot \pi \cdot \varepsilon_0} \cdot \frac{e^2}{r} \tag{5}$$

If we use nm as unit for r and eV as unit for V, we get V(r)=-1.44/r.

We want to summarize how to calculate the charge distribution (see diagrams below):

- put in the potential V(r) of the nucleus into the Schrödinger equation
- solving the equation gives the eigenenergy E and the radial distribution function u(r)
- dividing the radial distribution function u(r) by r gives the distribution function ψ (r)
- $e*\psi (r)^2$ gives the charge density of the cloud around the nucleus
- now we can draw $e*\psi (r)^2$ in two dimensions to get the picture of the charge cloud.

B. Modeling the Hydrogen atom with STELLA

We can solve the Schrödinger equation analytically (a second order differential equation) for hydrogen, and we do it with our second year teacher students. But more important cases for higher atoms, molecules and solids can only be solved iteratively with help of the computer. So we let STELLA do the work for us. For this purpose we need a STELLA model, which is very similar to the model of standing waves.

STELLA model for hydrogen

STELLA model equations

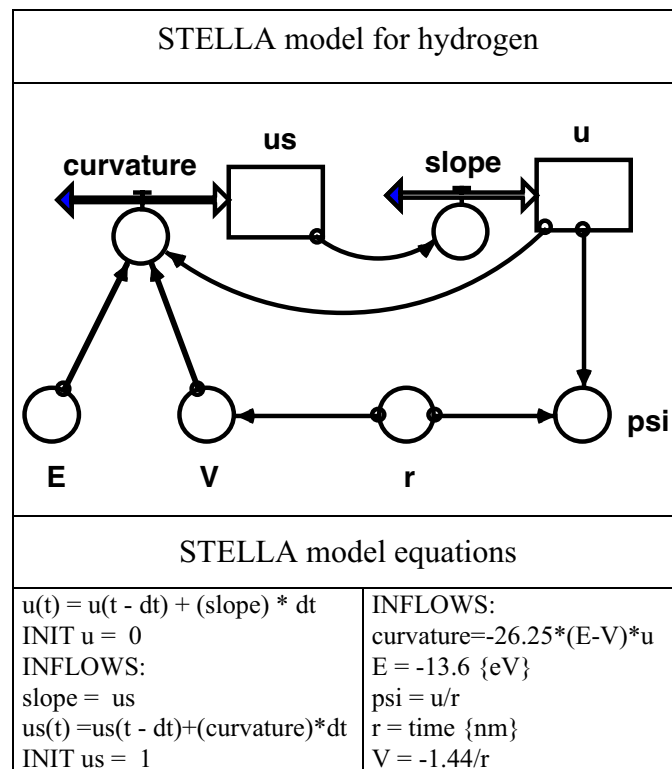|	
u(t) = u(t - dt) + (slope) * dt	INFLOWS:
INIT u = 0	curvature=-26.25*(E-V)*u
INFLOWS:	E = -13.6 {eV}
slope = us	psi = u/r
us(t) =us(t - dt)+(curvature)*dt	r = time {nm}
INIT us = 1	V = -1.44/r

Fig. 8. STELLA model and model equations
for calculating s-states in hydrogen atom

The model (Fig. 8) contains all quantities of the equation (4): energy E, potential V, radial distribution function u(r) and its second derivative curvature (=u''(r)). Two objects have been added. r = TIME (the radius) and Psi = u/r (definition of the Psi-function). Here, we use

$8\pi^2 \cdot \dfrac{m_e}{h^2} = 26.25$ for units nm and eV. This is the input for the STELLA model. The starting

value for radial distribution functions u(r) is zero, the slope can be any value except zero (e.g. 1). Now the eigenstates with there energy and u(r) are determined by trial and error, using

tentatively different values of E. An eigenstate is found, if the u(r)-function approaches zero when r becomes large. Only in these cases we find the electron *inside* the atom!

C. Results from STELLA calculations of the Hydrogen atom
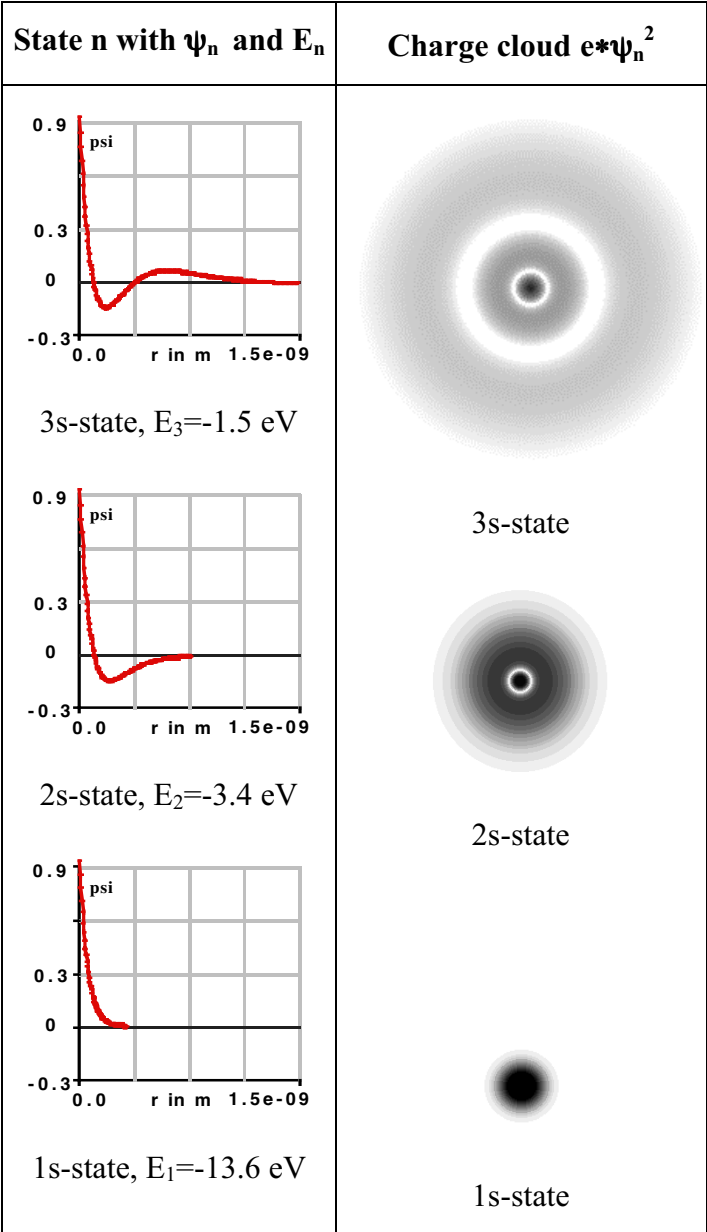
(first three states)

State n with ψ_n and E_n	Charge cloud $e*\psi_n^2$
3s-state, E_3=-1.5 eV	3s-state
2s-state, E_2=-3.4 eV	2s-state
1s-state, E_1=-13.6 eV	1s-state

Fig. 9. Results from STELLA calculations
with the first three states of the hydrogen atom

The charge density pictures were produced form our own STELLA data with a special software[22].

VI. FURTHER CALCULATIONS ON HIGHER ATOMS

A. He atom

For calculating shielding effects in atoms with more than one electron e.g. He, Li and Be - we use the following basic ideas for simplification:

- The potential for small values of r in the neighbourhood of the nucleus is proportional to $V = -z*1.44/r$, where z is the number of protons in the nucleus.
- The potential for an electron being far outside is the same as the hydrogen potential $V = -1,44/r$, because the positive charge is $z*e$ and the negative charge is $(z-1)*e$ coming from the other electrons.
- So we assume that the potential for one electron is determined by a potential running in between $V = -2*1.44/r$ and $V = -1,44/r$.
- The shielding effect of one electron on the potential at a distance r can be estimated by the "part of the electron (el-part)" being found in distances smaller than r:

$$\text{shielding charge (r)} = e \cdot \int_0^r u^2 \cdot dr \quad \text{or} \quad el - part(r) = \int_0^r u^2 \cdot dr \tag{6}$$

- With this equation, the effective potential for electron 1 with a shielding effect from electron 2 can be written for helium in the following way:

$$V\_1 = -(2 - el-part2)*1.44/r \tag{7}$$
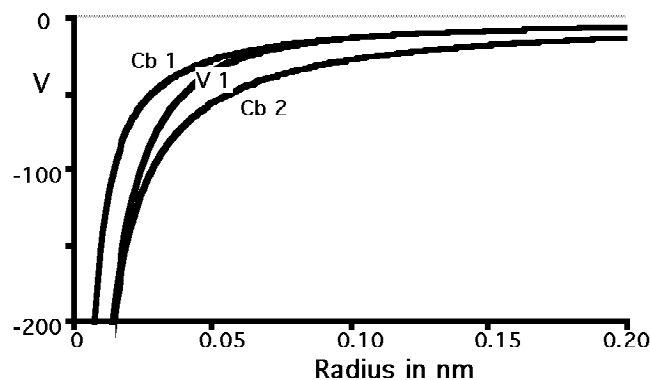
This potential is shown in Fig. 10.

Fig. 10. The effective potential V1 for electron 1, calculated with STELLA,
compared to the H-potential Cb1 and He-potential Cb2

This means a slightly different potential than the one usually used in the Hartree approach.[23]

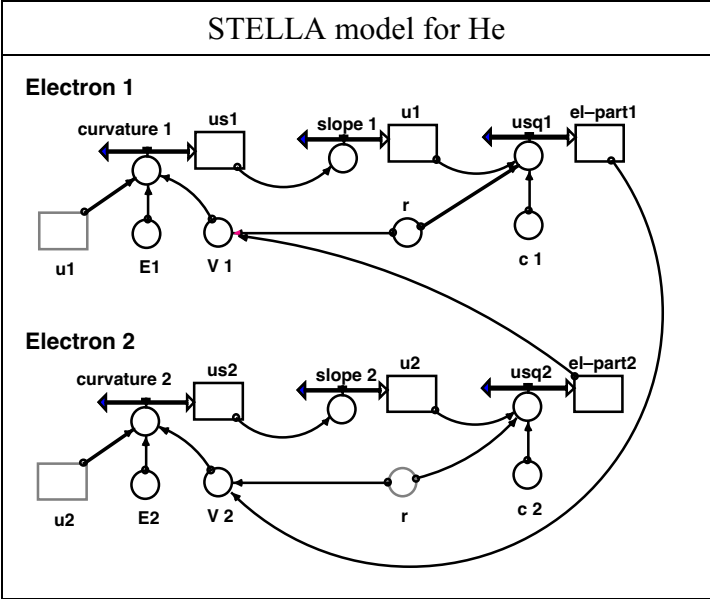Thus, for the helium atom, we get the model shown in Fig. 11 and results shown in Fig. 12 and 13.

Fig. 11. STELLA model for the He-atom

For the ground state of helium, we assume both electrons being in a 1 s state. The values for energy and normalization constant are found by systematical trial and error.
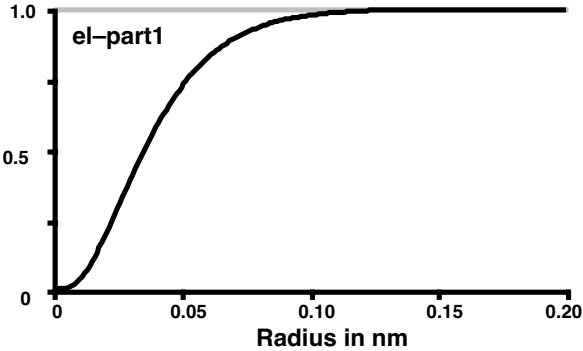

Fig. 12. The part of electron one (el-part1)
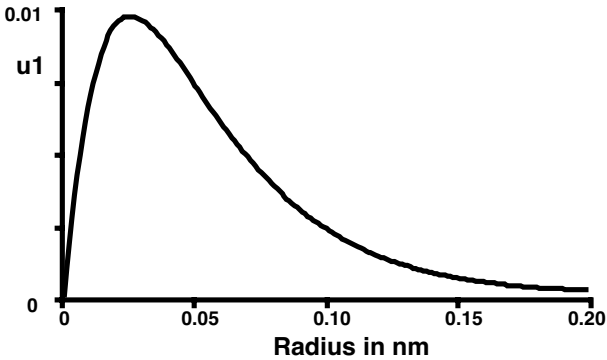being inside r (normalized)

Fig. 13. Resulting u-function for the two 1s-electrons in He,
calculated with STELLA

From the energy eigenvalues of the two electrons we get a total energy for the ground state of 73 eV. For comparison: the measured value for the total ionisation energy is 79 eV. From the u^2-curve we see that the helium atom is smaller than the hydrogen atom. Its radius is about 0.025 nm, compared to 0.05 nm for H. The measured and calculated radii are given in Table III below.

B. Li atom

For the lithium atom we can get a STELLA model working in the same way. For each of the three electrons we have one part of the model (see Fig. 14). The effective potential for one electron then is influenced by the shielding effects from the two other. So we get for instance the effective potential for electron one in the following equation:
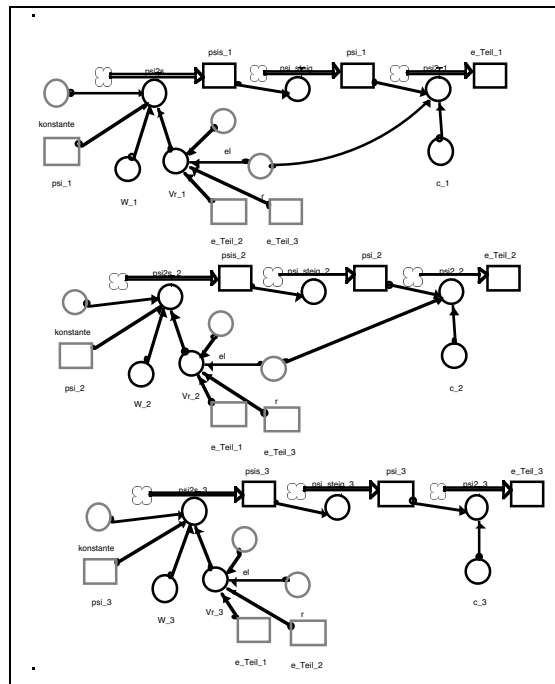
$$V\_1 = -(3 - \text{el-part2} - \text{el-part3})*1.44/r$$

Fig. 14. STELLA model of the Li-atom

Our results for energies are E1 = E2 = -95.3 eV, e3 = - 5.72 eV. This means the total energy in the ground state becomes - 196.3 eV. From literature we know the value is 203.5 eV.

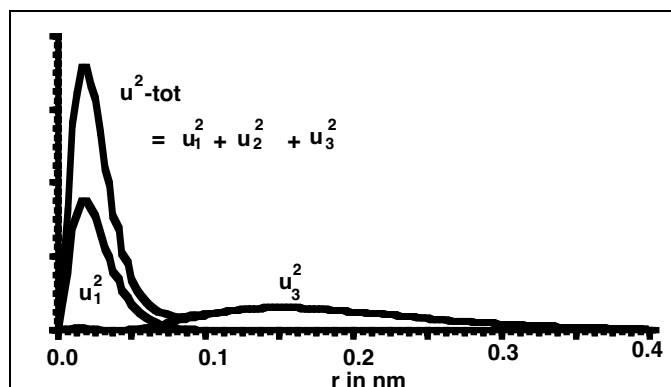With this STELLA model, we come to the following u^2-graphs:

Fig. 15. Resulting u^2-functions for the Li-atom
(calculated with STELLA)

From this graph, we can estimate the radius of the lithium atom with about 0.2 nm for the outer turning point, from literature we get the value 0.23 nm (see Table III).

Excited states can be calculated in similar ways (see our manuscripts).

For molecules and solids we have done some similar calculations for the H2+ molecule and for a model solid with four atoms.[24]

VII. COMPARISON WITH MEASUREMENTS

A. Balmer spectrum for H, spectral lines for He and Li

Using the hydrogen Balmer spectral lamp, students can make measurements of spectral lines themselves and compare them with the differences between there own results of energy eigenvalues, which gives the well known equal results. For He and Li, students get selected spectral lines from literature for comparison with their STELLA calculations.

B. Size of different atoms

From their own calculations with STELLA, students get estimates of the size of different atoms. These are compared to different given measurement values from literature. Table III below shows measured radii with different methods from literature[25] and our own calculated atomic radii of Hydrogen, Helium, Lithium and the Lithium+-ion.

Table III. Measured and calculated values for radii of atoms

	Measured radii from literature		
Element	Covalent bond	Van der Waals	Ion bond
H	0.030 nm	0.14 nm	-
He	-	0.14 nm	-
Li	0.23 nm	-	-
Li +	-	-	0.068 nm
	Calculated radii from STELLA models		
element	Last maximum of u	70% of charge	90% of charge
H	0.053 nm	0.093 nm	0.14 nm
He	0.025 nm	0.045 nm	0.070 nm
Li	0.14 nm	0.22 nm	0.30 nm
Li +	-	0.030 nm	0.050 nm

These comparisons show to students that they themselves were able to calculate basic features of some atoms in a satisfactory way.

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1 The development of this approach was influenced by similar ideas in the Nuffield A Level Physics approach "Waves, particles, and atoms" (1971) and in J. Ogborn, "Introducing quantum physics", Physics Education **9**, 436-443 (1974).

[2] H. Niedderer and H. Deylitz, S., "Atome, Moleküle und Festkörper - Verständnis ihrer Eigenschaften auf der Basis der Schrödingergleichung unter Zuhilfenahme des Computers." Basistext für Schüler. Institut für Didaktik der Physik, Universität Bremen (1997), 129 Seiten;   H. Niedderer and J. Petri, "Mit der Schrödinger-Gleichung vom H-Atom zum Festkörper - ein Unterrichtsvorschlag für Physik Leistungskurse", Institut für Didaktik der Physik, Universität Bremen (2000) 168 Seiten http://didaktik.physik.uni-bremen.de/niedderer/projects/quanten/;

[3] An English short version was written for a trial at the university of Perth in Australia: H. Niedderer and S. Deylitz, "Introduction to Atomic Physics - A concept based on the Schrödinger equation. Textbook for students." Printed Perth/Bremen (1998), 30 pages http://didaktik.physik.uni-bremen.de/niedderer/projects/quanten/ see also H. Niedderer, T. Bethge, H. Cassens, "A Simplified Quantum Model - a Teaching Approach and Evaluation of Understanding", *Relating Macroscopic Phenomena to Microscopic Particles - A Central Problem in Secundary Science Education* edited by P.L. Lijnse, P. Licht, W. De Vos, & A.J. Waarlo (Utrecht : CD-ß Press, 1990), pp. 67-80.

[4] T. Bethge, "Aspekte des Schülervorverständnisses zu grundlegenden Begriffen der Atomphysik (Aspects of student's matrices of understanding related to basic concepts of atomic physics)". Ph.D. dissertation, University of Bremen, 1988 (unpublished); J. Petri, *"Der Lernpfad eines Schuelers in der Atomphysik - Eine Fallstudie in der Sekundarstufe II* - (The learning pathway of one student in atomic physics - A case study in upper secondary school)". Ph.D. dissertation, University of Bremen (Aachen: Mainz 1996), 365 pages; S. Deylitz, *"Lernergebnisse in der Quantenphysik - Evaluation des Bremer Unterrichtskonzepts* (Learning results in quantum atomic physics – evaluation of the Bremen approach))". Ph.D. dissertation, University of Bremen, (Berlin: Logos 1999)

[5] A new name "electronium" for this form of the electron has been suggested by F. Herrmann, "A critical analysis of the language of modern physics", *Thinking Physics for Teaching*, edited by C. Bernardini, C. Tarsitani, & M. Vicentini, (New York: Plenum Press, 1995) pp. 287-293.

[6] This is expressed in a more radical way by Herrmann: "We propose a model of the atom which avoids the above mentioned incongruities. In particular, it makes definite statements about the shape of the parts of the atom and about their movement, and it does not contain the concept of "the probability of finding a particle at a

location". According to this model the atom consists of a small heavy nucleus and a big light shell. The shell in turn consists of a continuously distributed substance, the electronium.", see Ref. 5, p. 291

[7] M. Alonso & E. J. Finn, *Physics* (Workingham: Eddison-Wesley 1992), p. 973

[8] E. Schrödinger, "Quantisation as a problem of proper values (part IV)" Annalen der Physik **81**, (4) (1926), in E. Schrödinger, *Collected papers on wave mechanics* (Chelsea Publi. Comp New York, 1978), p. 120

[9] Students in interviews were shown similar density plots as in Fig. 1. A typical statement was: "Well, actually I completely put aside the concept of trajectory in the area of atomic physics. ... (With respect to the density plot:) 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.", see Bethge in Ref. 4, 113-119

[10] S. Deylitz and H. Niedderer, "Evaluation of a New Approach in Quantum Atomic Physics in high school", in D. Zollman (ed.) Research on teaching and Learning quantum mechanics, Papers presented at the annual meeting National Association for Research in Science Teaching March, 1999, 23 – 27 (http://www.phys.ksu.edu/perg/papers/narst/)

[11] See Deylitz in Ref.4 and Ref.10

[12] See Ref. 10 and J. Petri and H. Niedderer, "A learning pathway in high-school level quantum atomic physics". Int. J. Sci. Educ., **20** (9), 1084 (1998)

[13] See Petri in Ref. 4

[14] R.P. Olenick, T.M. Apostol, and D.L. Goodstein, *Beyond the mechanical universe - from electricity to modern physics* (Cambridge: Cambridge University Press 1986), p. 500

[15] See Ref. 2 Niedderer&Deylitz, pp. 72 and 73.

[16] E. Schrödinger, "Quantisation as a problem of proper values (part I)", Annalen der Physik **79**, (4) (1926), in E. Schrödinger, *Collected papers on wave mechanics* (Chelsea Publi. Comp New York, 1978), p.1

[17] STELLA High Performance: http://www.hps-inc.com/Education/new_Stella.htm

[18] MODELLUS: http://phoenix.sce.fct.unl.pt/modellus/

[19] H. Schecker, *Physik – Modellieren - Grafikorientierte Modellbildungssysteme im Physikunterricht*" (Stuttgart: Klett 1998) (English translation being prepared); H. Schecker, "Integration of Experimenting and Modeling by Educational Technology: Examples from Nuclear Physics", *International Handbook of Science Education* edited by Fraser, B.J. & Tobin, K. (Dordrecht: Kluwer 1998), Part I, 383-398

[20] R. Courant and D. Hilbert, *Methoden der mathematischen Physik*, (Berlin: Springer 1968), p. 270

[21] We have developed a special experimental device to demonstrate the nodal surfaces in a real experiment by a glowing wire. Coming to a stable state, the wire glows only at those points, where the air is without movement, that means at the intersection between wire and nodal surface. We have also produced a video-tape, which shows the whole experiment with standing sound waves from 2 kHz to 10 kHz with the upcoming structure of the bright points on the glowing wire according to the states 1s, 2s, 3s, and others.

[22] Called "eWolke", written by H. Lüdicke

[23] The integral should not go from 0 to r, but from 0 to ∞, see T. Mayer-Kuckuck, *Atomphysik* (Stuttgart: Teubner, 1997), p. 165.

[24] See Ref. 2, H. Niedderer and J. Petri, part II; H. Niedderer, H. Cassens, J. Petri, "Anwendungsorientierte Atomphysik in der S II - Zustände und Orbitale von Atomen, Molekülen, Festkörpern. (Atomic Physics Towards Applications - States and Orbitals of Atoms, Molecules and Solids)", Physik in der Schule **32**, Part I. Heft 7/8, 266 – 270, Part II. Heft 10, 339-340

[25] J. d'Ans and Lax, *Taschenbuch für Chemiker und Physiker*, Band III: Elemente, anorganische Verbindungen und Materialien, Minerale; (Berlin: Springer, 1998), pp. 254-258