Simply atoms – atoms simply

Friedrich Herrmann[1], Michael Pohlig[1], Nelson Arias Ávila[2]
[1]*Institute for Theoretical Solid State Physics, Karlsruhe Institute of Technology,*
Wolfgang-Gaede-Strasse 1, 76131 Karlsruhe, Germany.
[2]*Faculty of Sciences and Education, Distrital University, Carrera 3 No. 26 A-40,*
Bogotá, Colombia.

E-mail: f.herrmann@kit.edu

Abstract

We introduce an atomic model that avoids some of the worst dissonances. According to this model, the electron is not point-like but extended. The square of the wave function is interpreted as the density of a fluid, the *electronium*. On the basis of the electronium model suggestive pictures and animations of the atom can be generated. We shall see and discuss pictures of the various states of a hydrogen atom as well as animations of transitions from one stationary state to another. We also shall represent the internal movement of the electronium, that is responsible of the angular momentum and the magnetic moment of the atom. From the pictures we shall directly read properties of the various states and the various transitions by only using arguments of classical physics.

Keywords: Model of the atom, electronic transition.

Resumen

Se introduce un modelo atómico con el cual se evitan algunas de las más relevantes incoherencias que se presentan al estudiar los átomos de manera tradicional. En dicho modelo el electrón no se considera puntiforme sino extendido. El cuadrado de la función de onda se interpreta como la densidad de un fluido, llamado *electronio*. Basados en el concepto de electronio se pueden generar imágenes sugestivas y animaciones representativas del átomo. Se presentan y analizan las imágenes obtenidas para varios estados del átomo de hidrógeno, así como para transiciones de un estado estacionario a otro. También se representa el movimiento interno del electronio, que es responsable del momento angular y del momento magnético del átomo. De las imágenes se podrán inferir directamente las propiedades de diversos estados y transiciones, empleando únicamente argumentos de la Física clásica.

Palabras clave: Modelo del átomo, transición electrónica.

I. PICTORIAL REPRESENTATION OF ATOMS

The appearance of an object is determined by its shape, color, transparency and surface structure. An atom does not have some of these properties. So one might conclude that the atom has no appearance. But that would mean to throw out the baby with the bath water. Indeed, in other similar situation we do not hesitate to produce pictorial representation of invisible objects. Every physics text book contains pictures of electric and magnetic fields, temperature and pressure distributions, X-ray and electron beams. So we also can generate images of the atom, and that will be done in the following.

The pictures that we will consider are graphic representations of the solutions of the Schrödinger equation. Various properties of the atom can directly be read from these pictures. One can "see" the atom's shape, its angular momentum and its magnetism. One can deduce from the pictures, why in certain states the atom radiates strongly and in others only weakly or not at all. One also sees directly if the emitted radiation is linearly or circularly polarized.

II. THE PROCEDURE

We start from the Schrödinger equation for a single-electron system:

$$i\hbar \frac{\partial}{\partial t} \psi(\boldsymbol{r},t) = \left(-\frac{\hbar^2}{2m} \Delta + V(\boldsymbol{r}) \right) \psi(\boldsymbol{r},t)$$

By means of the wave function $\psi(\boldsymbol{r}, t)$, *i.e.* a solution of the Schrödinger equation, we define two quantities ρ and $\boldsymbol{j}$:

$$\rho = \psi^* \psi \tag{1}$$

Friedrich Herrmann, Michael Pohlig, Nelson Arias Ávila

$$j = \frac{\hbar}{2m_i}\,(\psi^*\nabla\psi - \psi\,\nabla\psi^*).$$

(2)

For a single-electron system the two functions $\rho(r,t)$ and $j(r,t)$ contain the same information as the wave function.

Using the Schrödinger equation and the expressions (1) and (2) we obtain (see [1]):

$$\frac{\partial\rho}{\partial t} + \operatorname{div} j = 0$$

(3)

This equation has the form of a continuity equation. Multiplying the quantities ρ and j with the electron charge e: $\rho_e = e \cdot \rho$, $j_e = e \cdot j$, we can write Eq. (3) as:

$$\frac{\partial\rho_e}{\partial t} + \operatorname{div} j_e = 0$$

(4)

where ρ_e is the charge density and j_e the electric current density. Multiplying ρ and j with the electron mass m: $\rho_m = m \cdot \rho$, $j_m = m \cdot j$, we obtain from (3):

$$\frac{\partial\rho_m}{\partial t} + \operatorname{div} j_m = 0$$

(5)

Here ρ_m is the mass density and j_m the mass current density. Eq. (4) can be read as the continuity equation of electric charge and Eq. (5) as the continuity equation of the mass of the atomic shell.

We recall the physical meaning of a continuity equation: When the electric charge in a given small region decreases, there must be an outflow of charge from this region. If the charge increases, there must be an inflow of charge. The same applies for the mass. Thus, a continuity equation states the conservation of an extensive quantity that is distributed in space.

Eqs. (4) and (5) suggest to imagine the electron shell of the atom to consist of a material that is continuously distributed around the nucleus, and that is able to flow. In this model, an electron is a portion of this material with a certain mass, namely the electron mass, and a certain charge, the elementary charge. This model is as old as quantum mechanics itself. It has been proposed in 1926 by Schrödinger [2] and was shortly after worked out by Madelung [3]. The imaginary substance is sometimes called "Madelung fluid". Instead of this somewhat unwieldy name we prefer for the use at school the shorter term "electronium".

We now shall consider how ρ and j behave for the various types of the solutions of the Schrödinger equation.

The Schrödinger equation has special solutions of the form:

$$\psi_k(r,t) = u_k(r)e^{-\frac{i}{\hbar}E_k t}.$$

(6)

The corresponding states are called eigenstates (of the energy). They are numbered with the index k. To each of these solutions corresponds a particular value of the energy E_k, the energy eigenvalue. Note that in (6) the position and the time dependence are separated: The first factor $u_k(r)$ depends only on the position r, the second only on time.

Every linear combination of eigenstate solutions also solves the Schrödinger equation:

$$\psi(r,t) = \sum_k a_k u_k(r)e^{-\frac{i}{\hbar}E_k t}$$

A state that is described by such a sum is called a superposition state.

The eigenstates differ in one important feature from the superposition states. For eigenstates the density and the current density are independent of time. For superposition states ρ and j depend on time. Let us show that briefly.

For an eigenstate the electronium density is:

$$\rho_k(r,t) = u_k^*(r)e^{+\frac{i}{\hbar}E_k t} \cdot u_k(r)e^{-\frac{i}{\hbar}E_k t} = u_k^*(r)\cdot u_k(r).$$

Since the product of the exponential terms is equal to one, the time dependence vanishes. The calculation of the current density gives a similar result. Also the current density is constant in time (but not necessarily zero). Therefore the eigenstates are also called *stationary states*.

We now consider a superposition state. In the simplest case, its wave function is the sum of two eigenstate functions:

$$\psi(r,t) = c_A\psi_A(r,t) + c_B\psi_B(r,t),$$

with $\psi_A(r,t) = u_A(r)e^{-\frac{i}{\hbar}E_A t}$, and $\psi_B(r,t) = u_B(r)e^{-\frac{i}{\hbar}E_B t}$.

Since the calculation of ρ is a somewhat complicated, we give here only the result. It is an expression of the form

$$\rho(r,t) = C_0(r) + C_1(r)\cos(\omega t) + C_2(r)\sin(\omega t),$$

(7)

with $\omega = (E_A - E_B)/\hbar$.

It is seen that the density now depends on time. It consists of one term that depends only on the position and another one, that oscillates harmonically. Again, the same holds for the current density. The superposition states are therefore *non-stationary*.

The images and animated graphics, that we discuss below, correspond to the hydrogen atom. They are representations of the electronium density and current density. For stationary states the resulting images are static, for non-stationary, we have generated animations. In print, an animation can only be represented as a series of single frames that are "stroboscopically" selected. More images and animations can be found on our website [4].

Regarding our notation: An energy eigenstate is characterized by three quantum numbers n, l and m. The indication (432) means $n=4$, $l=3$ and $m=2$. The electronic spin is not visualized in our images. In the various figures, the relation between the electronium density and the color is not necessarily the same. In the 3D images the displayed surface corresponds to 10% of the maximum density.
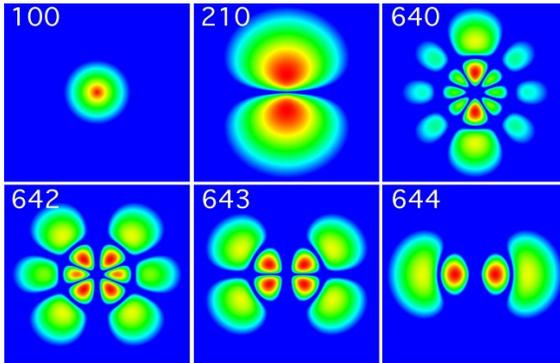
FIGURE 1. Electronium density of the hydrogen atom in various states (*nlm*). The distributions have a cylindrical symmetry with a symmetry axis through the nucleus.

III. PICTURES AND ANIMATED GRAPHICS

A. Shape of an atom

We consider the density distribution of the electronium in different stationary states, Fig. 1. Such images are largely known. They display what can be considered the shape of the atom in the various states. In some states, the atom is spherical; in others it has a lower symmetry.

B. In a stationary state the atom does not radiate

The current density is different from zero only for states with $m \neq 0$. For the state with $n = 3$, $l = 2$, $m = 1$ the left part of Fig. 2 shows the electronium density, the right part shows the absolute value of the current density in a section through the nucleus. The current density vector is perpendicular to the drawing plane. Blue corresponds to a current that is flowing into the image plane, red means it is flowing out. The streamlines are circles whose centers lie on an axis through the nucleus. Fig. 3 shows a combination of density and current density: The flow is indicated by arrows. What can we learn from these pictures?

From the fact that both the charge distribution and the current distribution are constant in time, we conclude that the atom does not emit radiation. A charge distribution that is constant in time causes a static electric field and an electric current distribution that is constant in time causes a constant magnetic field. It is well-known that according to the Bohr model of the circulating particles a contradiction to electrodynamics would result, since the particles should emit radiation. Therefore, without further ado, one declares

that electrodynamics is not valid in this case (Bohr's first "postulate"). Such a postulate is not necessary when using the electronium model. On the contrary: The electronium model predicts that in a stationary state the atom does not radiate [5].
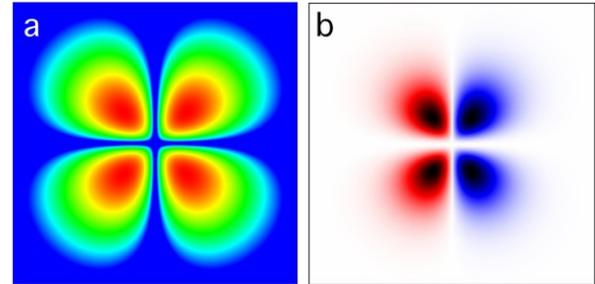
FIGURE 2. Density (a) and current density (b) in a cross section through the nucleus for the state (321). The distribution has a cylindrical symmetry.
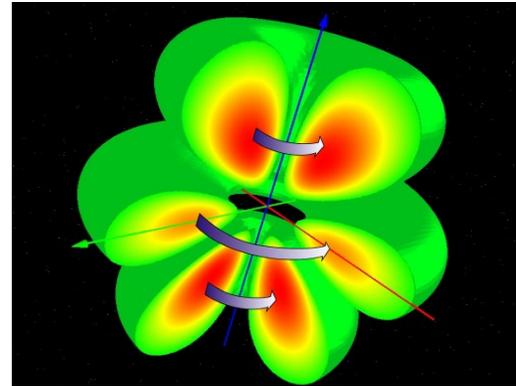
FIGURE 3. Density and current for the state (431).

C. Angular momentum and magnetic moment

We again consider the current density. In states with $m \neq 0$ we have a flow of electronium with circular streamlines. We therefore have a corresponding flow of mass and electric charge. The fact that we have a circular mass current implies that the system has angular momentum. The angular momentum can be calculated from the mass flow distribution. One finds the same value as that provided by solving the quantum mechanical eigenvalue equation. This is not surprising, since the current density distribution, from which our calculation departs, is based on the solution of the Schrödinger equation.

Apart from a mass flow in the states with $m \neq 0$ there is also a circular electric current. That means that the atom has a magnetic moment. This can be calculated from the current distribution.

Thus, the pictures allow us to read directly the orbital angular momentum and the magnetic moment of the atom.

Friedrich Herrmann, Michael Pohlig, Nelson Arias Ávila
D. Electronic transitions

We now shall discuss the non-stationary or superposition states. We restrict ourselves to the superposition of two states:

$$\psi(\boldsymbol{r},t) = c_A \psi_A(\boldsymbol{r},t) + c_B \psi_B(\boldsymbol{r},t). \qquad (8)$$

In Section II we have seen that for such states the density and the current density oscillate with the angular frequency $\omega = (E_A - E_B)/\hbar$.

We know that an oscillating charge and current distribution generally leads to the emission of an electromagnetic wave. Thereby, the atom loses energy, which means that it can not remain in the state, which we adopted as initial state. Instead it gradually goes into that of the two states which has lower energy. The part $\psi_A(\boldsymbol{r},t)$, that corresponds to the higher energy decreases, that of $\psi_B(\boldsymbol{r},t)$ increases. Therefore, for a non-stationary state the weight factors in Eq. (8) are time-dependent:

$$\psi(\boldsymbol{r},t) = c_A(t)\psi_A(\boldsymbol{r},t) + c_B(t)\psi_B(\boldsymbol{r},t).$$

As a result, in the density of Eq. (7) also those terms are now time-dependent, which previously have not been:

$$\rho(\boldsymbol{r},t) = C_0(\boldsymbol{r},t) + C_1(\boldsymbol{r},t)\cos(\omega t) + C_2(\boldsymbol{r},t)\sin(\omega t). \qquad (9)$$

However, the temporal change of the coefficients C_0, C_1 and C_2 is slow, and it is not periodical. For a transition $(210) \rightarrow (100)$, for example, they describe how the "p-state lobes" steadily and smoothly transform into the "s-state sphere". This slow deformation is modulated by a fast oscillation, which ensures that an electromagnetic wave is emitted. Thereby the atom loses energy.
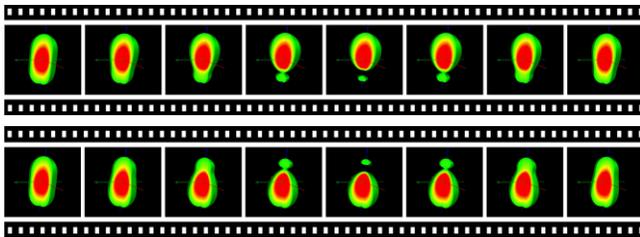
FIGURE 4. Superposition of states 210 and 100 with a percentage of 50% each. The charge density moves as in a dipole antenna.

We now assume that at the beginning the atom is in an excited stationary state, *i.e.* $c_A = 1$ and $c_B = 0$. The transition to state B cannot begin without help. However, a weak perturbation is sufficient to initiate the transition. This perturbation can be due to collisions with other atoms, or to the fluctuations of the electromagnetic field in its ground state. This description of an electronic transition in which the electron is treated quantum-mechanically, whereas the

radiation is treated classically, is called "semi-classical".

The energy loss per oscillation period due to radiation is extremely low. The transition $(210) \rightarrow (100)$ takes about 10^{-8}s, whereas the oscillation period is about 10^{-15}s. Thus the transition of the electronium lasts for about 10^7 oscillation periods. During this interval of time, the percentage of $\psi_A(\boldsymbol{r},t)$ decreases from 100% to 0% whereas that of $\psi_B(\boldsymbol{r},t)$ increases from 0% to 100%.

Fig. 4 shows a sequence of frames from a video of a superposition state, that is composed of the states (210) and (100), 50% each. The pictures cover one oscillation period.

The entire 10^7 oscillation periods can not be represented as an animation. If in the animation we stretch the oscillation period to one second, then the whole transition would need about half a year.

To make the whole transition visible in a reasonable time, we have applied a "stroboscopic" method: The animation consists of snapshots of the transition that are made in large and regular time intervals. The instants of the snapshots are chosen in such a way that the oscillation phase of two consecutive frames increases only little. In this way the impression of a slow oscillation results. Fig. 5 shows a few frames of the transition $(210) \rightarrow (100)$.
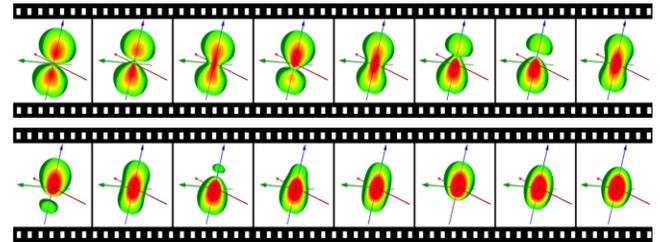
FIGURE 5. Transition from 210 to 100.

It can be seen that the charge oscillates similarly as that of a macroscopic dipole antenna. An oscillation has such a dipole character only if $\Delta l = \pm 1$. Such transitions are called dipole transitions. For a dipole transition, the atom radiates strongly, and that means that the transition proceeds rapidly. Dipole transitions are said to be allowed.

E. Slow transitions

How fast a transition is, *i.e.* how quickly the coefficients c_A and c_B change, depends on how strongly electromagnetic radiation is emitted. The intensity of emission depends on the spatial distribution and temporal variation of the charge density and the current density. With a little practice one can judge from an animation whether the transition proceeds quickly, slowly or not at all. (It is understood that the duration of the animation is not a measure for the duration of the transition, since we have chosen the stroboscopic sampling rate arbitrarily).

If Δl is equal to ± 2, the oscillation has quadrupole character, and that can also be seen in the animation. The atom radiates only weakly - just as a macroscopic

quadrupole antenna (*i.e.,* two adjacent dipole antennas oscillating in phase opposition) would do. Quadrupole transitions are said to be forbidden.
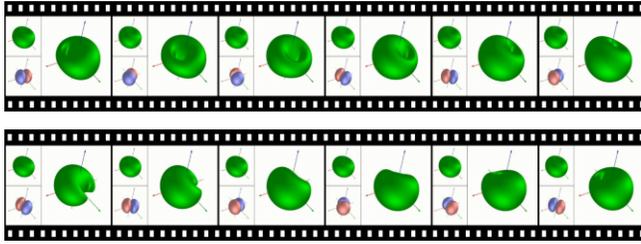
FIGURE 6. Quadrupole transition from 520 to 400.

An interesting superposition state is one, in which for both contributing states we have *l* = 0. The charge distribution oscillates, but it always retains its spherical symmetry. Therefore, it can not emit at all. A transition can not take place.

F. Polarization of the radiation

If the quantum number *m* is the same in the initial and final state (and $\Delta l = \pm 1$), the electronium executes a reciprocating movement. It radiates like a dipole antenna, and therefore emits linearly polarized light. This is the case for the dipole transitions that we have considered previously.

If the quantum number *m* of the participating states differs by one, *i.e.* if $\Delta m = \pm 1$, the charge distribution makes a kind of circular motion. As a consequence, the atom emits a circularly polarized wave. Fig. 6 shows some frames of such a transition. The two small sub-images on the left side of each image show the non-periodic and the periodic component of the density, see Eq. (9). In the periodic component red means positive charge (*i.e.,* a positive deviation from the overall negative charge) and blue negative charge. It is seen that the rapid, harmonic movement is similar to that of a rotating dipole.

IV. CONCLUSIONS

With the help of the wave function of a single electron system two variables ρ and j can be defined. They are related by an equation that can be read as a continuity equation. This suggests to interpret these quantities as a density and the current density of the electric charge and the mass of a substance that is distributed in space. From the distribution of this "electronium" and from the change in time, several properties of the atom can be predicted correctly by only applying well-known laws of classical physics.

1. Since the charge density and the electric current density are stationary, an atom does not radiate when in an energy eigenstate. Bohr's first postulate is not needed.

2. From the mass current and charge current distribution follow the correct values of the orbital angular momentum and the magnetic moment.

3. From the way a charge distribution of a superposition state is oscillating, one can deduce whether the atom emits strongly or weakly or not at all (whether a transition is allowed or forbidden).

4. From the oscillation of the charge distribution the polarization of the radiation can be inferred.

REFERENCES

[1] Schiff, L. I., *Quantum mechanics,* (McGraw-Hill, New York, 1968), p. 26.
[2] Schrödinger, E., *Quantisierung als Eigenwertproblem*, Erste Mitteilung, Ann. Phys. **79**, 361-376 (1926).
[3] Madelung, E., *Quantentheorie in hydrodynamischer Form*, Zeitschrift für Physik **40**, 322-326 (1927).
[4] http://www.physikdidaktik.uni-karlsruhe.de/software/hydrogenlab/elektronium/index.html *and* http://www.physikdidaktik.uni-karlsruhe.de/software/hydrogenlab/index.shtml.
[5] Döring, W., *Atomphysik und Quantenmechanik*, II. Die allgemeinen Gesetze, (Walter de Gruyter, Berlin, 1976), p. 20.