

ICT-BASED TEACHING OF QUANTUM MODELING OF ATOMIC

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Abstract. The Schrodinger equation for the motion of microparticles in spherical symmetric potential field, the hydrogen atom: quantum numbers, energy spectrum, orbital impulse momentum and its spatial quantization, the selection rule for quantum transitions in simulator programs to expand the quantum mechanical imagination of students of higher education institutions. Radiation spectrum of hydrogen atoms. The width of the surfaces is modeled and the advantages of the developments and the methodology of using them are highlighted in this article.

Keywords: Schrodinger equation for the main constant state of the hydrogen atom, potential energy of the electron which is bound to the nucleus and its graph, solution of the Schrodinger equation for the hydrogen atom and energy surfaces, ionization energy, orbital, head and magnetic quantum numbers, their accepted values, determination of atomic states, explanation of the spectrum of hydrogen atom on the basis of quantum mechanics, selection rule, mechanical and magnetic moment of electron, gyromagnetic ratio, Boron magneton.

Introduction. In quantum mechanics, there is selection rule which limits transition of electron in atom from one surface to another surface. According to this rule, voluntary transitions of electrons do not take place in the central-symmetrical field of the nucleus. The transitions occur in the atom which orbital quantum numbers only change to one unit, namely $l = 1$. The formation of the spectral series of hydrogen atom is illustrated in terms of quantum mechanics in Figure 4.

The Lyman series in the spectrum of hydrogen radiation corresponds to $np \rightarrow 1S$ ($n=2,3,\dots$) transitions, and the Balmer series corresponds to $np \rightarrow 2S$, $nS \rightarrow 2p$, $nd \rightarrow 2p$ ($n=3,4,\dots$) transitions. The transition of the electron from the main state to the excited state links with increase of the energy of the atom, namely its absorption by the photon. Only the Lyman series is observed in the absorption spectrum of hydrogen, it corresponds to quantum transitions which indicate the transition of atom from the main state to the excited energy states. The energy surface of hydrogen atoms differs Z^2 times from the energy surface of hydrogen, the Balmer formula for them is expressed as follows.

$$\nu = Z^2 R \left(\frac{1}{n^2} - \frac{1}{m^2} \right)$$

In this case, Z is the sequence number of the atom in the Mendeleev periodic table. It can be seen from the above-mentioned formula, that the spectrum of hydrogen atoms shifts to shorter wavelength. For example, when $Z > 10$, the wavelength of the first spectral series is in the X-ray wavelength range. The radiant energy of heavy ions is around 100 keV. However, spectral lines which are visible from the heavy ions and correspond to the IQ field are also recorded at large values of n . The spectrum of alkali metals is similar to spectrum of hydrogen. Because they also have one electron in the outer electron shell. But the energy surface of this outer electron is so much higher than the hydrogen, it cannot pass to lower energy surfaces. Because Pauli exclusion principle do not allow it. For example, in Na ($Z = 11$) the states 1S, 2S, 2P are filled with electrons, the main state of its outer electron is the energy surface 3S. When a natrium atom is excited, this electron can pass into 3P, 3d, 4S, 4P, 4d, and others. The radiation spectrum of natrium corresponds exactly to the following formula.

$$\nu = R \left(\frac{1}{(n_1 - a_{1_1})^2} - \frac{1}{(n_2 - a_{1_2})^2} \right)$$

here $n = 3, 4, \dots$, $n_2 = n_1 + 1, n_1 + 2, \dots$ values are accepted. The a_1 correction in the formula is equal to 1,35 for case S. In other cases, it approaches to zero.

The spectrum of atoms with multiple electrons in the outer electron shell are complex and diverse. The energy of the valence electrons of such atoms is also close to the electron energy of the hydrogen atom, it depends on how far the electron is from the nucleus. The energy surfaces of the outer electrons of the various elements are around a few eV. Therefore, the radiation and absorption spectrum of complex atoms are also located in the IQ or visible field, and it is much more complicated to relate them to the sequence number of the element.

When atoms combine and form molecules and crystals, complex changes take place in their outer electron shells. Therefore, the spectrum of molecules and crystals differs from the atoms, we will consider about this in later lectures.

Although quantum mechanics rejects the notion of the electron orbit in atom, it saves the classical notion about the energy surface of the atom. Quantum mechanics also comes to the same conclusion as in Boron theory in the quantization of energy surfaces for hydrogen and ions like hydrogen. But quantum mechanics has brought certain clarity to this issue. The relationship of uncertainties in quantum mechanics not only connects the coordinates of the particle with the projection of the impulse on the coordinate axes, but also the energy of the particle and the time which it takes to be in that energy state. We discussed this in a previous lectures. The uncertainty of

the time of particle in certain state Δt , the uncertainty of is related with uncertainty of its energy ΔE as follows:

$$\Delta E \cdot \Delta t \geq \frac{h}{2}$$

Let's apply this relation to the electron in the atom. We know that the atom has main stable and excited states. Naturally, the atom can stay in its main stable state for as long as it wants. But there is a question "how long can atom be in excited state?" in this case. The time which it takes for atom to be in excited state, is very short ($10^{-8} \div 10^{-9}$ s). The time which corresponds to different energy surfaces of atoms and is in different excited states, also varies.

The atom in the excited state can spontaneously move to lower energy state. The time which is taken for the number of atoms in the excited state to decrease e times is called the time which is taken for the atom to live in the excited state. But there can be such metastable states in atom, in this case its lifetime can be much longer, is equal in share of tenths of a second. In quantum mechanics is said about the average lifetime of atom. Quantum mechanics cannot tell how long a certain atom will be in excited state. The transition of atom from its excited state to its normal state occurs by chance. Hence, Δt uncertainty always exists in the time which the atom is in the excited state. The uncertainty of this time is related to the uncertainty of the energy, namely

$$\Delta E \approx \frac{h}{\Delta t}$$

If we take into account that the average lifetime of atom in the excited state $\Delta t = 10^{-8}$ s, we obtain the following result for the uncertainty of energy:

$$\Delta E \approx \frac{h}{10^{-8}} \approx 10^{-7} \text{ eV}$$

This value of ΔE is very small relative to the difference in energy surfaces.

Each energy surface (line) of atom can vary randomly in the range of $\Delta E 10^{-7}$ eV. This causes the energy surface to be wider. As the excitation energy of the atom increases, its average lifetime decreases. As a result, the width of the high energy surfaces increases ΔE (Figure 5.) $\Delta E \approx 10^{-7}$ eV value is considered the natural width of the energy surface.

The expansion of the energy surface also causes the atomic spectral line to expand to certain extent. Namely:

$$\Delta \nu = \frac{\Delta E}{h} = 10^8 \text{ Gs}$$

It is derived that the radiation emitted by the atom is not strictly monochromatic, as Boron theory. The spectral line has a certain width and occupies a

certain area in the spectrum. The obtained value $\Delta\nu$ is taken as the natural width of the spectral line. In spectroscopy, the value $\Delta\nu=10^8$ Gs is considered very small.

If we take in account that the frequency of visible light is around $\nu\approx 10^{14}$ Gs, the following (Fig. 3) is derived.

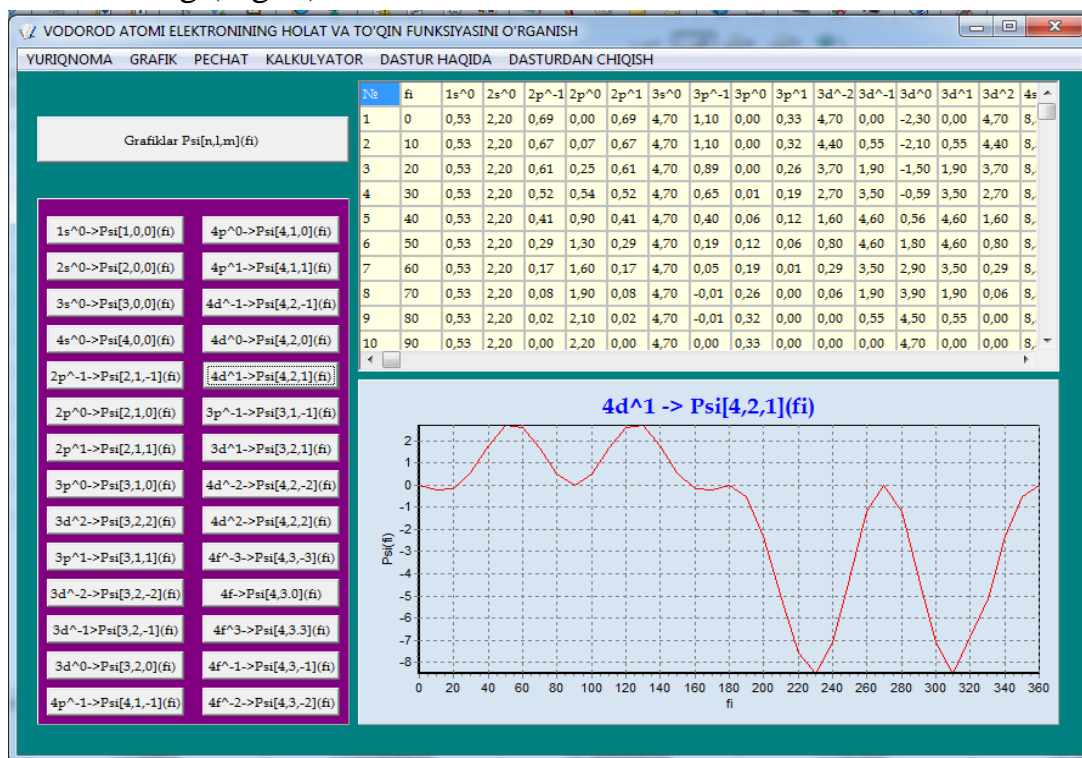


Figure 3.

There are other reasons for the expansion of spectral lines. We can take as an example of this is the Doppler expansion of the spectral line. Doppler expansion is related to the heat rate of the radiating atoms. As the radiating atom approaches the spectrometer, its frequency increases (according to the Doppler effect); if it moves away from the spectrometer, its frequency decreases. As a result, the spectral line which is recorded by the spectrometer, expands in two directions. In general, the radiation frequency of moving atom differs from stationary atom. The expansion of the spectral line because of the Doppler effect is much larger than the natural expansion which we mentioned above. Thus, quantum mechanics concludes that atoms generate non-monochromatic radiation spectrum.

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