ФІЗИЧНІ, ХІМІЧНІ ТА ІНШІ ЯВИЩА, НА ОСНОВІ ЯКИХ МОЖУТЬ БУТИ СТВОРЕНІ СЕНСОРИ

PHYSICAL, CHEMICAL AND OTHER PHENOMENA, AS THE BASES OF SENSORS

PACS: 42.50.-P, 72.20.JV, 72.40;
УДК 539.42: 539.184

DYNAMICS OF RADIATIVE TRANSITIONS BETWEEN STARK SUBLEVELS FOR NON-HYDROGENIC ATOMS AND DIATOMICS IN DC ELECTRIC FIELD

V. I. Mikhailenko, A. A. Kuznetsova, N. V. Mudraya, A. A. Svinarenko

Odessa National Maritime Academy, Odessa, Ukraine

DYNAMICS OF RADIATIVE TRANSITIONS BETWEEN STARK SUBLEVELS FOR NON-HYDROGENIC ATOMS AND DIATOMICS IN DC ELECTRIC FIELD

V. I. Mikhailenko, A. A. Kuznetsova, N. V. Mudraya, A. A. Svinarenko

Abstract. The quantum approach for definition of the radiation transitions between Stark sublevels for non-hydrogenic atoms and diatomics in an external electric field is underlined and based on the operator perturbation theory and model potential method. The cited radiative phenomena can be basis for construction of new types of the quantum sensor devices.

Keywords: non-hydrogenic atoms and diatomics, operator perturbation theory, external electric field

ДИНАМІКА РАДІАЦІЙНИХ ПЕРЕХОДІВ МІЖ ШТАРКІВСЬКИМИ ПІДРІВНЯМИ ДЛЯ НЕВОДНЕПОДІБНИХ АТОМІВ ТА ДВОАТОМНИХ МОЛЕКУЛ У ЗОВНІШНЬОМУ ЕЛЕКТРИЧНОМУ ПОЛІ

В. І. Михайленко, Г. О. Кузнецова, Н. В. Мудра, А. А. Свинаренко

Анотація. Сформульовано квантовий підхід до визначення ймовірностей радіаційних переходів між штарківськими підрівнями для неводнеподібних атомів та двоатомних молекул у зовнішньому електричному полі, яка базується на операторній теорії збурень і методі модельного потенціалу. Розглянуті радіаційні явища можуть бути основою для побудови нових типів квантових сенсорних приладів.

Ключові слова: неводнеподібні атоми та двоатомні молекули, операторна теорія збурень, зовнішнє електричне поле

ДИНАМИКА РАДИАЦИОННІХ ПЕРЕХОДОВ МЕЖДУ ШТАРКОВСКИМИ ПОДУРОВНЯМИ ДЛЯ НЕВОДОРОДОПОДОБНЫХ АТОМОВ И ДВУХАТОМНЫХ МОЛЕКУЛ ВО ВНЕШНЕМ ЭЛЕКТРИЧЕСКОМ ПОЛЕ

В. И. Михайленко, А. А. Кузнецова, Н. В. Мудрая, А. А. Свинаренко

Аннотация. Сформулирован квантовый подход к определению вероятностей радиационных переходов между штарковскими подуровнями для неводородоподобных атомов и двухатомных молекул во внешнем электрическом поле, который основывается на формализме операторной теории возмущений и методе модельного потенциала. Изучаемые радиационные явления могут быть основой для построения новых типов квантовых сенсорных устройств.

Ключевые слова: неводородоподобные атомы и двухатомные молекулы, операторная теория возмущений, внешнее электрическое поле

1. Introduction

The studying elementary atomic processes in plasmas, gases and other mediums in an external electric (electromagnetic) field [1-20] is related to important physical problems and attracts a great interest in the last two decades. Above a great number of different processes the most actual and complicated ones include the ionization of excited atoms by means of the photon and electron impact, radiation and unradiation (including Auger) processes [1-4]. This topics are of a great interest in direct connection with developing new sensor devices, which are based on using the quantum systems and their special properties. As the most impressive examples one could indicate on the quantum frequency measures, quantum watches, atomic Carno machines, quantum processors, quantum cryptography etc [1,2].

Though, naturally, there are many theoretical and experimental papers on dynamics of the radiation transitions in multi-electron atoms, nevertheless, some important aspects are remained unclear hitherto. It is very difficult still to perform an accurate account of the inter electron correlation effects in the multi-electron atoms. These effects and other ones are not adequately described within many simplified models. Surely there is a great number more sophisticated approaches, including the SCF Dirac-Fock methods and its different multiconfiguration versions and many others [5].

Situation changes dramatically under consideration of the different radiation mechanisms under availability of the external electromagnetic fields. Even more simple case of the external static electric field effect on atomic radiation transitions is remained hitherto quantitatively undescribed especially when speech is about non-hydrogenic atomic systems. So, a great interest represent development of the consistent quantum theory of the radiation transitions dynamics for non-hydrogenic atoms in an external electric field [6-18]. Very important class of problems with availability of the external electric (electromagnetic field) in a case of the Rydberg atoms when one or several electrons of the multi-electron atom are in the highly excited (Rydberg) states (see, for example, refs.[8,3,17,19,20]). So, it is easily to understand that there is an important necessity in developing more simple and simultaneously highly-prйcised schemes to studying the radiation transitions dynamics in multi-electron atoms in a dc electric field. Naturally a studying of the atomic properties for multi-electron atoms in a strong electric field is of a great interest for many applications, including the laser physics and chemistry, quantum electronics, sensor electronics, atomic and molecular physics etc and remains very important topic of modern quantum physics [1-6,19,20]. One of the key problems is connected with definition of the intensities and probabilities of radiative transitions between Stark sublevels in a spectrum of a multi-electron atom in a DC electric filed. It is self-understood that the similar models are well developed for the hydrogen atom [6,20]. In this paper, we present the possible consistent quantum approach to definition of the radiation transitions between Stark sublevels for non-hydrogenic atoms in an external electric field, which is based on the operator perturbation theory [12,13,20] and model potential method (the Coulomb quantum defect approximation) [19,20]. The phenomena studied are of a great interest from the point of view of the construction of new types of the quantum sensor devices.

2. Theory of atomic radiation transitions and operator approach

As our main purpose is to develop and adapt consistent quantum approach for definition of the radiation transitions between Stark sublevels for non-hydrogenic atoms and diatomics in an external electric field, we should start from an accurate treating the Stark problem. Naturally the corresponding approach must be applied to any non-hydrogenic atoms without any dependence upon the electric field strength. From this point of view, the corresponding Stark problem method should be used as the starting model. Though in the last years it has been developed a set of effective non-perturbative approaches to the dc strong –field Stark effect in atomic systems (look, for example, [11-16]), for our purposes the most appropriate theoretical approach for constructing the wave functions in the Stark problem is given by the operator formalism [12,20]. It is important to note that the quantum defect version of this formalism is appropriate for treating alkali atoms and correspondingly the collisional processes with similar atoms [21]. These systems are often represented and a core and a single electron above the N-electron core.

The Schrodinger equation for atom in an uniform electric field of the nucleus (in atomic units) has a standard form and after separation of variables (1) in parabolic co-ordinates results in the system of two known equations for the functions *f, g*:

$$f'' + \frac{|m|+1}{t} f' + [0{,}5E + (\beta_1 - N/Z) / t - 0{,}25\,\varepsilon(t)\,t\,]f = 0 \qquad (1a)$$

$$g'' + \frac{|m|+1}{t} g' + [0{,}5E + \beta_2 / t + 0{,}25\,\varepsilon(t)\,t\,]g = 0 \qquad (1b)$$

coupled through the constraint on the separation constants: $\beta_1+\beta_2=1$. In equations (1) E is the eigen energy, Z — charge of nucleus, N — the number of electrons in atomic core (for example for alkali atom). Within the operator approach the uniform electric field $\varepsilon(t)=\varepsilon_0$ in Eqs. (2) is substituted by model function $\varepsilon(t)$ with parameter τ ($\tau = 1.5\ t_2$; t_2 — is the second turning point). Naturally, the final results do not depend upon the parameter τ. The two turning points for the classical motion along the η axis, t_1 and t_2, at a given energy E are the solutions of the quadratic equation ($\beta = \beta_1$, $E = E_0$). As in further we will consider first of all alkali atomic systems, one could guess suitability of using the quantum defect scheme [13,20] of the operator approach [12]. Despite the hydrogen atom, within the latter it is introduced the quantum defect [21]. Its value μ_l, is connected with the electron energy E and principal quantum number n as $\mu_l = n - z^*(-2E)^{-1/2}$ and expressed through the quantum defect value of the free ($\varepsilon = 0$) atom in the parabolic co-ordinates by standard way [21]. As usually, we use the standard classification for the electron states in a field, namely, there are used the quantum numbers: n, n_1, n_2, m (principal, parabolic, azimuthal ones). Within the operator approach [12] the two zeroth order eigen functions of the starting Hamiltonian H_0: bound state function $\Psi_{Eb}(\varepsilon, \nu, \varphi)$ and scattering state function $\Psi_{Es}(\varepsilon, \eta, \varphi)$ with the same eigen energy order are defined and used further in definition of any parameters for the quasi-stationary atomic states.

Definition of the corresponding eigen energies and functions results in the solution of the well known problem of the states quantification in the case of the penetrable barrier. According to ref. [12,13], the system (2) is solved with the total Hamiltonian H using the conditions, which quantify the bounding energy E, with separation constant β_1:

$$f(t) \to 0 \text{ at } t \Rightarrow \infty\,,\ \partial x(\beta, E) / \partial E = 0, \qquad (2)$$

with

$$x(\beta, E) = \lim_{t \Rightarrow \infty} [\, g^2(t) + \{g'(t) / k\}^2 \,]\, t^{|m|+1}. \qquad (3)$$

The further procedure for the 2D eigen value problem results in solving of the system (5) with probe pairs of E, β_1. It is very important that the bound state energy, eigenvalue β_1 and eigen function for the zero order Hamiltonian H_0 coincide with those for the total Hamiltonian H when the field strength at $\varepsilon \to 0$. The scattering states' functions $g_{E's}$ are defined according to the operator formalism special algorithm [12].

Further one can introduce the definition of intensity of the Stark components through the matrix elements of the r coordinate of an atomic electron:

$$I\left(nn_1n_2m \to n'n_1'n_2'm'\right) = \frac{4e^4\varpi_0^4}{3c^3}\left|\left\langle nn_1n_2m\middle|r\middle|nn_1n_2m\right\rangle\right|^2, \qquad (4)$$

where ω_0 is non-perturbed frequency of transition $n \to n_1$. Usually the Stark components are divided on the π and σ-components in dependence upon polarization (linear $\Delta m = 0$, or cycle $\Delta m = \pm 1$). Intensities of the π- components are defined by the

matrix elements of z-component $\boldsymbol{r}$, and intensities of the σ-компонент — by x (or y)-components $\boldsymbol{r}$.

In the literature there are the known general formulas for matrix elements, derived by Gordon and expressed in the hyper geometric function (see, for example, [6]). One should note that these formulas are very cumbersome and can be used only in particular cases. Naturally the similar formula are absent for the multi-electron atoms in an electric field.

As usually, a probability of transition *B (nkm, n')* from parabolic state $|\, nkm >$ into all states, belonging to the level *n'*, is as follows:

$$B(nkm,n') = \omega(n,n') \sum_{k',m'} \left| \langle nkm | r | n'k'm' \rangle \right|^2, \quad (5)$$

where

$$\varpi(n,n') = \frac{4e^2 a_0^2}{3\hbar c^3} \left(\frac{1}{n^2} - \frac{1}{n'^2} \right)^3.$$

So, in order to define the probabilities (intensities) of the radiation transitions in an electric field one could estimate the matrix elements (5). In a new scheme of calculation we propose to use system of the quantum defect approximation wave functions, which are the solutions of the system (1). In fact such an approach is corresponding to using the sturmian functions basises, which have he following form in the spherical coordinates:

$$\left\langle r,\theta,\phi \,|\, S^{\alpha}_{n,l,m} \right\rangle = D(n,l) \exp\left(\frac{-r}{\alpha} \right) \left(\frac{2r}{\alpha} \right)^l \times$$

$$\times L^{(2l+1)}_{n-l-1}\left(\frac{2r}{\alpha} \right) Y_{l,m}(\theta,\phi), \quad (6)$$

where

$$D(n,l) = \sqrt{\frac{(n-l-1)!}{(n+l)!}}, \; |m| \le l < n.$$

L is the Lagerre polynomial, Y — spherical harmonics, α- parameter, which defines a scale of oscillations of the sturmian functions. This parameter can be estimated within the quantum defect method as $E_n = -1/(2n^2\alpha)$.

3. Generalization of the operator-quantum defect approach for diatomic molecules

The generalization of the underlined scheme for diatomic molecules can be directly carried out with accounting for the symmetry of the corresponding diatomic problem. To define the wave functions and electron states energies in external electric field, one needs to carry out the diagonalization of the energy matrice, calculated between states with the same main quantum number. In ref. [20,22] there are underlined the corresponding schemes for calculating the Stark resonances parameters in the diatomic molecules on example of the hydrogen molecule. The generalization of theses schemes can be performed by implementation of the model potential (the Coulomb quantum defect) approximation and finite differences numeral scheme. In particular, it is easily to write the Hamiltonian in the cylindrical coordinates (ρ,z) (the atomic units are used):

$$H\psi(\rho,z) = E\psi(\rho,z) \quad (7)$$

$$H = -1/2(\partial^2/\partial\rho^2 + 1/\rho\partial/\partial\rho + \partial^2/\partial z^2 - 1/[(z+R/2)^2 + \rho^2]^{1/2} - 1/[(z-R/2)^2 + \rho^2]^{1/2} - \varepsilon_0 z + V(\rho,z). \quad (8)$$

Here ε_0 denotes an electric field; V_c is effective potential for an account of field of the molecular electron shells. This potential can be chosen in the quantum defect approximation [19]. To solve the equation (7) one should use one of the versions of the finite differences method. Under the differences solution (7), an infinite region is exchanged by a grid (ρ, $L_{z^-} < z < L_{z^+}$). For $z<0$ it should be used a condition of the smallness of wave function on the boundary. For z>0 the boundary condition has the form of plane divergent wave. The differences scheme is constructed in the same way as the known Ivanov model [22]. The eigen values of hamiltonian can be calculated by means of the inverse iterations method. The corresponding system of inhomogeneous equations is usually solved by the Thomas method. To define the resonances energy and width and the radiation transitions probabilities one should use the expressions, which are similar to above presented ones.

4. Estimates and conclusion

So, in this paper we underlined the possible consistent quantum approach to definition of the radiation transitions probabilities (intensities) between Stark sublevels for non-hydrogenic atoms and diatomic molecules in an external electric field, which generalizes the operator perturbation theory for H atom [12,13] and bases on the model potential method (the Coulomb quantum defect approximation) [19,20]. The last moments differ the presented theory from the other approaches

(see refs. [5,7,13,22]). The numerical realization of the approach for alkali atoms is now in a progress. However, for illustration we present below the known data on the radiation transition probabilities B(i) (eq.5) for hydrogen atom (from level n=10), which are obtained from analytic approximate formulas within the usual perturbation theory (column A) [6], operator perturbation theory (column C) [23], and the exact results (column B) by means the Gordone's formulas [6,23]. The agreement between exact data and operator approach results is quite acceptable.

Table 1
The radiation transition probabilities (eq.5) for H atom (from level n=10)

i	A	B	C
2	0,5472	0,5523	0,5521
3	0,3623	0,3658	0,3656
4	0,2703	0,2722	0,2721
5	0,2155	0,2163	0,2162
7	0,1532	0.1532	0.1532
9	0,1186	0,1188	0,1188

Obviously, one could wait for the same situation in a case of the non-H atomic systems. From physical point of view, availability of external electric field can lead to significant changing of the radiation transitions probabilities in dependence upon the field strength. The key moment is connected with definition of the transition matrix elements within the Coulomb quantum defect scheme as for non-H atoms as non-H diatomic molecules. It is obvious that the described approach is especially useful in treating the radiation transitions probabilities between the Stark sublevels for the Rydberg systems in an electric field, where the known sophisticated methods are dealing with the significant numerical difficulties [1-3]. The alternative quasiclassical models [6] are working only on a case of the weal external electric field and fail in an opposite case (strong-field Stark effect). In conclusion we also note that the approach can be used for studying not only the radiation transitions (decay) dynamics of multi-electron atoms (molecules) in an external electric field, but for defining probabilities of other non-radiation processes, including the Auger transitions etc too.

References

1. Matter in superintense laser field. Eds.Batani D., oachain C.;- N-Y:AIP, 2007-560p.
2. Ullrich C., Erhard S., Gross E.K.U., Superintense Laser Atoms Physics. — N. — Y: Acad. Press., 2007. — 580p.
3. Letokhov V.S. Nonlinear selective photoprocesses in atoms and molecules. — M.: Nauka, 1983. — 408P.
4. Ivanov L.N., Letokhov V.S. Spectroscopy of autoionization resonances in heavy elements atoms// Com. Mod.Phys.D.:At.Mol.Phys. — 1985. — Vol.4. — P.169-184.
5. Wilson W. Handbook on Molecular Physics and Quantum Chemistry/ Wilson W. — Chichester: Wiley, 2003. — 680P.
6. Lisitsa V.S., New in effects of Stark and Zeeman// Usp.Phys.Nauk. — 1987. — Vol.153. — P.379-422.
7. Harmin D., Theory of non hydrogenic Stark effect// Phys.Rev.Lett. — 1982. — V.49. — P.128-131.
8. Zimmerman M.L., Littman M., Kash M., Kleppner D. Stark structure of Rydberg states of alkali-metal atoms//Phys.Rev.A. — 1979-V.20. — P.2251-2275.
9. Rosmej F.B., Hoffman D.H., Geissel M. et al, Advanced X-ray diagnostics based on an observation of high-energy Rydberg transitions from autoionizing levels in dense laser-produced plasmas// Phys. Rev. A. — 2001-Vol.63. — P.063409-063418.
10. Silverstone H., Adams B., Cizek J., Otto P., Stark effect in hydrogen: Dispersion relations, asymptotic formulas and calculation of the ionization rate via high-order perturbation theory//Phys.Rev. Lett. — 1979. — Vol.43,N20. — P.1498-1501.
11. Harmin D.A. Theory of the Non hydrogenic Stark Effect// Phys.Rev.Lett. — 1982. — Vol.49,N2. — P.128-131.
12. Glushkov A.V.,Ivanov L.N., DC Strong-Field Stark-Effect: consistent quantum-mechanical approach// J.Phys.B: At. Mol. Opt. Phys. — 1993. — Vol.26,N16. — P.L379-L386.
13. Glushkov A.V., Lepikh Ya.I., Fedchuk A.P., Ignatenko A.V., Khetselius O.Yu., Ambrosov S.V , Wannier-Mott excitons and atoms in a DC electric field: photoionization, Stark effect, resonances in the ionization continuum// Sensor Electr. and Microsyst. Techn. — 2008. — N4. — P.5-11.
14. Filho O, Fonseca A.,Nazareno H.,Guimaraes P.,Different approaches to Stark effect: Application to H ground state//Phys.Rev.A-1990. — Vol.42. — P.4008-4014.
15. Stambulchik E., Maron I., Stark effect of high-*n* hydrogen-like transitions: quasi-continuous approximation//J.Phys.B:At.Mol.Opt.Phys. — 2008-Vol.41-P.095703.
16. Rao J., Delande D.,Taylor K., Quantum manifestations of scattering orbits in scaled spectrum of non-hydrogenic atom in crossed fields// J.Phys.B:At.Mol. Opt.Phys. — 2002. — V.35. — P.L1-10.
17. Buchleitner A., Delande D., Secular motion of the three-dimenssional Rydberg states in a microwave field//Phys.Rev.A. — 1997. — Vol.55. — P.1585-1598.

18. Bayfield J.E.,, Casati G., Guarneri I., Sokol D.W.,Localization of chaotic diffusion for hydrogen atom in microwave fields//Phys.Rev.Lett. — 1989. — Vol.63. — P.364-368.
19. Moores D.L., Saraph E., Theory of quantum defect and its applications// In: Atoms in astrophysics. Atoms in astrophysics, Eds. Burke P.G., Eissner W.B., Hummer D.G., Persival L.C. — N. — Y., Plenum Press. — 1984. — P.174-212.
20. Glushkov A.V., Atom in an electromagnetic field. — Kied:KNT. — 2005. — 450P.
21. Mikhailenko V.I., Kuznetsova A.A., Penning and stochastic collisional ionization of atoms in external electric field// Sensor Electr. and Microsyst. Techn. — 2009. — N4. — P.11-16.
22. Ivanov V, Grid calculation of energies and widths for ground state of hydrogen molecule in a strong electric field// Opt.Spectr. — 1994. — Vol.78. — P.711-713.
23. Ignatenko A.V., Probabilities of radiative transitions between stark sublevels in spectrum of atom in dc electric field: New approach//Photoelectronics. — 2007. — N16. — P.71-74.