UDC 539.185

A. P. Fedchuk, A. V. Glushkov, Ya. I. Lepikh, A. V. Ignatenko, A. S. Kvasikova

[1]I. Mechnikov Odessa National University, 2, Dvoryanskaya str., Odessa, Ukraine
[2]Odessa National Polytechnical University, 1, Shevchenko av., Odessa, Ukraine
[3]Odessa State Environmental University, 15, Lvovskaya str., Odessa, Ukraine
e-mail: dirac13@mail.ru

ATOM OF HYDROGEN AND WANNIER-MOTT EXCITON IN CROSSED ELECTRIC AND MAGNETIC FIELDS

Spectroscopy of atoms in the crossed external electric and magnetic fields is investigated on the basis of the operator perturbation theory. The data for ground state energies of the hydrogen atom in sufficiently weak crossed external electric and magnetic fields are calculated. Generalization of the method on a case of the Wannier-Mott excitons in the bulk semiconductors in a case of the crossed fields is given.

1. This work goes on our investigations of the multi-electron atomic systems and excitons in semiconductrs in an external electric field (the Stark effect) [1-17]. The remarkable Stark effect has a long history and until recently it was believed that the Stark effect is fully understood and fundamental problems remained (look [1-16]). However, an observation of the Stark effect in a constant (DC) electric field near threshold in hydrogen and alkali atoms led to the discovery of resonances extending into the ionization continuum by Glab et al and Freeman et al (c.f.[1]). Calculation of the characteristics of these resonances as well as the Stark resonances in the strong electric field and crossed electric and magnetic fields remains very important problem of as modern atomic physics as physics of semiconductors (speech is about excitons in bulk semiconductors, quantum dots , wires etc.).

It should be noted that the same class of problems has been arisen in a physics of semiconductors (c.f.[14-17]). It is well known that the availability of excitons in semiconductors resulted experimentally in the special form of the main absorption band edge and appearance of discrete levels structure (f.e. hydrogen-like spectrum in Cu_2O). Beginning from known papers of Gross-Zaharchenya, Thomas and Hopfield et al (c.f.[13-17]), a calculation procedure of the Stark effect for exciton spectrum attracts a deep interest permanently. Very interesting physics occurs in a case of the excitons in quantum dots, wires etc, where the other geometry and energetics in comparison with the bulk semiconductor makes the field effect more intrigues. The exciton states in the quantum dots have been studied in a number of papers and have been observed by photoluminescence experiments (c.f. [14-17]). Naturally, the electronic states in quantum dots (wires) depends on either the confining potential and the interacting force between the particles. Now the electric field effect on the electron-hole states and on the confined excitonic states is often referred to the quantum confined Stark effect. In this paper we are interested by spectroscopy of atoms in the crossed external electric and magnetic fields. Method studying is based on the operator perturbation theory and analysis of the level statistics in spectra. Generalization of method on a case of the Wannier-Mott excitons in the bulk semiconductors is given.

2. As our approach to strong field DC Stark effect was presented in a series of papers (see, for example, [1-6]), here we are limited only by the

key aspects. According to [1,2], the essence of operator perturbation theory approach is the inclusion of the well known method of "distorted waves approximation" in the frame of the formally exact perturbation theory. According to [2,3], the Schrödinger equation for the electronic eigenfunction taking into account the uniform DC electric field (the field strength is F)and the field of the nucleus (Coulomb units are used: a unit is $h^2/Ze^2 m$ and a unit of $mZ^2 e^4/h^2$ for energy) looks like:

$$[-(1 - N/Z) / r + F z - 0{,}5\Delta - E\,]\,\psi = 0 \quad (1)$$

where E is the electronic energy, Z — charge of nucleus, N — the number of electrons in atomic core. Our approach allow to use more adequate forms for the core potential (c.f.[25-27]). According to standard quantum defect theory (c.f.[3]), relation between quantum defect value μ_l, electron energy E and principal quantum number n is: $\mu_l = n - z^*(-2E)^{-1/2}$. As it is known, in an electric field all the electron states can be classified due to quantum numbers: n, n_1, n_2, m (principal, parabolic, azimuthal: $n = n_1 + n_2 + m + 1$). Then the quantum defect in the parabolic co-ordinates $n(n_1 n_2 m)$ is connected with the quantum defect value of the free ($F=0$) atom by the following relation [3]:

$$\delta(n_1 n_2 m) = (1/n) \sum_{l=m}^{n-1} (2l+1)(C^{JM}_{J,M-m;lm})^2 \mu_l$$
$$J = (n-1)/2, \quad M = (n_1 - n_2 + m)/2;$$

After separation of variables, equation (1) in parabolic co-ordinates could be transformed to the system of two equations for the functions f and g:

$$f'' + \frac{|m|+1}{t} f' + [0{,}5E + (\beta_1 - N/Z) / t - 0{,}25\, F(t)\ t\,]\, f = 0 \quad (2)$$

$$g'' + \frac{|m|+1}{t} g' + [0{,}5E + \beta_2 / t + 0{,}25\, F(t)\ t\,]\, g = 0 \quad (3)$$

coupled through the constraint on the separation constants: $\beta_1 + \beta_2 = 1$.

For the uniform electric field $F(t) = F$. In ref. [11], the uniform electric field ε in (3) and (4) was substituted by model function $F(t)$ with parameter τ ($\tau = 1.5\, t_2$) . Here we use similar function, which satisfies to necessary asymptotic conditions (c.f.[11,12]) :

$$F(t) = \frac{1}{t} F\left[(t-\tau)\frac{\tau^2}{\tau^2 + t^2} + \tau\right] \quad (4)$$

Potential energy in equation (4) has the barrier. 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 ($\beta = \beta_1$, $E = E_0$). It is necessary to know two zeroth order EF of the H_0: bound state function Ψ_{Eb} (ε, ν, φ) and scattering state function Ψ_{Es} (ε, η, φ) with the same EE in order to calculate the width G of the concrete quasi-stationary state in the lowest PT order. Firstly, one would have to define the EE of the expected bound state. It is the well known problem of states quantification in the case of the penetrable barrier. We solve the (2, 3) system here with the total Hamiltonian H using the conditions [11]:

$$f(t) \to 0 \text{ at } t \Rightarrow \infty$$
$$\partial x(\beta, E) / \partial E = 0 \quad (5)$$

with

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

These two conditions quantify the bounding energy E, with separation constant β_1 . The further procedure for this two-dimensional eigenvalue problem results in solving of the system of the ordinary differential equations(2, 3) with probe pairs of E, β_1. The bound state EE, eigenvalue β_1 and EF for the zero order Hamiltonian H_0 coincide with those for the total Hamiltonian H at $\varepsilon \Rightarrow 0$, where all the states can be classified due to quantum numbers: n, n_1, l, m (principal, parabolic, azimuthal) that are connected with E, β_1, m by the well known expressions.. The scattering states' functions must be orthogonal to the above defined bound state functions and to each other. According to the OPT ideology [11,12], the following form of $g_{E's}$:is possible:

$$g_{E's}(t) = g_1(t) - z_2' g_2(t) \qquad (6)$$

with $f_{E's}$, and $g_1(t)$ satisfying the differential equations (2) and (3). The function $g_2(t)$ satisfies the non-homogeneous differential equation, which differs from (3) only by the right hand term, disappearing at $t \Rightarrow \infty$.

3. In Ref, [7] it has been presented approach, based on solution of the 2-dimensional Schrödinger equation [20,21] for an atomic system in crossed fields and operator perturbation theory [10]. For definiteness, we consider a dynamics of the complex non-coulomb atomic systems in a static magnetic and electric fields. The hamiltonian of the multi-electron atom in a static magnetic and electric fields is (in atomic units) as follows:

$$H = 1/2(p_\rho^2 + l_z^2/\rho^2) + B_z/2 + (1/8)B^2\rho^2 + \\ + (1/2)p_z^2 + F + V(r) \qquad (7)$$

where the electric field F and magnetic field B are taken along the z-axis in a cylindrical system; In atomic units: 1 a.u.B=2.35×10^{5}T, 1a.u.F=5,144×10^6 kV/cm. If one consider only the m=0 state, thus l_z=0; $V(r)$ is a one-electron model potential, which can be in principle choosed in the standard form for multielectron atom; naturally, it results in the usual Coulomb potential for hydrogen one. For solution of the Schrödinger equation with hamiltonian equations (7) we constructed the finite differences scheme which is in some aspects similar to method [7]. An infinite region is exchanged by a rectangular region: $0<\rho< L_\rho$, $0<z< L_Z$. It has sufficiently large size; inside it a rectangular uniform grid with steps h_ρ, h_Z was constructed. The external boundary condition, as usually, is: $(\partial\Psi/\partial n)_r = 0$. The knowledge of the asymptotic behaviour of wave function in the infinity allows to get numeral estimates for L_ρ, L_Z. A wave function has an asymptotic of the kind as: $exp[-(-2E)^{1/2}r]$, where $(-E)$ is the ionization energy from stationary state to lowest Landau level. Then L can be estimated as $L\sim9(-2E)^{-1/2}$. The more exact estimate is found empirically. The difference scheme is constructed as follows. The three-point symmetric differences scheme is used for second derivative on z. The derivatives on ρ are approximated by (2m+1)-point symmetric differences scheme with the use of the Lagrange interpolation formula differentiation. The eigenvalues of hamiltonian are calculated by means of the inverse iterations method. The corresponding system of inhomogeneous equations is solved by the Thomas method. To calculate the values of the width G for resonances in spectra of atomic system in crossed electric and magnetic field one can use the modified operator perturbation theory method (see details in ref.[10,20]). Note that the imaginary part of the state energy in the lowest PT order is defined as follows:

$$\mathrm{Im}E = G/2 = \pi < \Psi_{Eb} \mid H \mid \Psi_{Es} >^2 \qquad (10)$$

with the total Hamiltonian of system in an electric and magnetic field. The state functions Ψ_{Eb} and Ψ_{Es} are assumed to be normalized to unity and by the δ(k -k')-condition, accordingly. Other calculation details can be found in ref. [7].

The above presented method can be naturally generalized for description of the Stark effect for the Wannier-Mott excitons in the bulk semiconductors [4]. Really, the Schrödinger equation for the Wannier-Mott exciton looks as follows:

$$[-\hbar^2\nabla_e^2/2m_e^* - \hbar^2\nabla_h^2/2m_h^* - e^2/\varepsilon r_{eh} + \\ + eFr_e - eFr_h]\Psi = E\Psi \qquad (11)$$

where m^*_e (m^*_h) are the effective-mass for the electron (hole), ε is the background dielectric constant. Introducing the relative coordinates: $r = r_e - r_h$ and the momentum p with reduced mass p= $m^*_e m^*_h/M$ (the momenta P with the total-mass M= m^*_e + m^*_h ,) and center-of-mass coordinate $\rho = (m_e^* r_e + m_h^* r_h)(m_e^* + m_h^*)$, one could rewrite (15) as:

$$[-\hbar^2\nabla^2/2\mu - e^2/\varepsilon r - \hbar/2\cdot(1/m_h^* - 1/m_e^*)K\cdot p - \\ - eFr]\Psi F = [E - \hbar^2K^2/8\mu]\Psi \qquad (12)$$

This equation then could be solved by the method, described above. The other details can be found in Refs. [1,4]. A problem of the combined Stark and

Zeemane effects for quantum dots requires more detailed consideration.

4. As an illustration,, we make computing the energy of the ground state of the hydrogen atom in crossed fields and compare results with data obtained within analytical perturbation theory by TurbinerV (see. [8]) for the case of sufficiently weak fields. According TurbinerV, the expansion for the energy of the hydrogen atom in crossed fields is as follows:

$$E = E_{SZ} + E^{(\|,\perp)} \qquad (13)$$

where E_{SZ} - the total energy of the fields F and B separately:

$$E_{SZ} = -1 - \frac{9}{2}F^2 + \frac{B^2}{2} - \frac{3555}{32}F^4 - \frac{53}{96}B^4 + \ldots \qquad (14)$$

a $E^{\|,\perp}$ contains a previously unknown cross members for mutually parallel ($E^{\|}$) and perpendicular ($E^{\perp}$) directions of fields F и B:

$$E^{\|} = \frac{159}{16}F^2B^2 - \frac{1742009}{26880}F^2B^4 + \ldots \qquad (15a)$$

$$E^{\perp} = \frac{93}{4}F^2B^2 - \frac{22770991}{107520}F^2B^4 + \ldots \qquad (15b)$$

Table 1 shows the values of the energy of the ground state of the hydrogen atom (the following designations: $E+E^{\|}$ - energy for the case of the electric and magnetic fields are parallel;$E+E^{\perp}$corresponds to the case of the electric and magnetic fields are perpendicular). Since the examined fields are sufficiently weak, between the results of both calculations there is a very good agreement. At the same time it is clear that the perturbation theory in the version by Turbiner V is correct only for weak fields, while for strong fields it can lead to substantially inaccurate data. Numerical finite-difference method can be used to calculate the characteristics of the atom in crossed electric and magnetic fields of arbitrary strength.

Table 1

Energy values (Ry) of the H ground state in electric F (1au=5.14·10^9 V/cm) and magnetic B (1 au.B=2.35·10^5 T) fields

F,B 10^{-2}	$E+E^{\|}$ Turbiner theory [8]	$E+E^{\perp}$ Turbiner heory [8]	$E+E^{\|}$ This work	$E+E^{\perp}$ This work
0,0	-1,000000	1,000000	-1,000000	-1,000000
0,1	-1,000004	1,000004	-1,000004	-1,000004
0,5	-1,000099	1,000099	-1,000099	-1,000099
1,0	-1,000402	1,000401	-1,000401	-1,000401
1,5	-1,000906	1,000905	-1,000905	-1,000904
2,0	-1,001617	1,001615	-1,001616	-1,001614
2,5	-1,002542	1,002537	-1,002540	-1,002535
3,0	-1,003685	1,003674	-1,003682	-1,003671
3,5	-1,005054	1,005037	-1,005053	-1,005033
4,0	-1,0066619	1,006628	-1,006659	-1,006626
4,5	-1,008520	1,008465	-1,008517	-1,008463
5,0	-1,010642	1,010558	-1,010636	-1,010553

References

1. Glushkov A.V., Atom in electromagnetic field.-Kiev: KNT, 2005.-400P.
2. 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.
3. Glushkov A.V., Ambrosov S.V., Ignatenko A.V., Korchevsky D.A., DC Strong Field Stark effect for non-hydrogenic atoms: consistent quantum mechanical approach // Int.Journ.Quant. Chem.-2004.-Vol.99,N5.-P.936-949.
4. Glushkov A.V.,Lepikh Ya.I.,Khetselius O.Yu.,Fedchuk A.P., Ambrosov S.V , Ignatenko A.V.,Wannier-mott excitons and atoms in a DC elecric field: photoionization, Stark effect, resonances in the ionization continuum// Sensor Electr. and Microsyst. Techn.-2008.-N4.-P.5-11.
5. Ambrosov S.V., Khetselius O.Yu., Ignatenko A.V., Wannier-mott exciton and H, Rb atom in a dc elecric field: Stark effect// Photoelectronics.-2008.-N17.-P.82-85.

6. Ambrosov S.V., Ignatenko V.M., Korchevsky D.A., Kozlovskaya V.P., Sensing stochasticity of atomic systems in crossed electric and magnetic fields by analysis of level statistics for continuous energy spectra//Sensor Electronics and Microsystems Technologies-2005.-N2.-P.19-23.;
7. Superintense Laser Atoms Physics.Eds. C.A Ullrich., S Erhard., E.K.Gross.-N-Y: Kluwer,2005.
8. Lisitsa V.S. New in Stark and Zeemane effects for Hydrogen Atom// Usp.Fiz. Nauk.- 1997.-Vol.153,N3.- P.379-422.
9. Harmin D.A. Theory of the Non hydrogenic Stark Effect// Phys.Rev. Lett.-1992.-Vol.49,N2.-P.128-131.
10. Krajewska K, Kaminski J.Z., Potvliege R.M., Stabilization of Resonance States in Crossed Magnetic and Laser Fields in a Parabolic Quantum Well// Laser Physics.-2005.-Vol.15,N2.-P.238-244.
11. Glushkov A.V.,Malinovskaya S.V., Chernyakova Yu.G., Svinarenko A.A., Cooperative Laser-Electron-Nuclear Processes: QED Calculation of Electron Satellites Spectra for Multi-Charged Ion in Laser Field// Int.Journ.Quant.Chem.-2004.-Vol.99, №5.-P.889-894.
12. Popov V.S., Mur V.D., Sergeev A.V., Weinberg V.M., Strong field Stark effect: perturbation theory and 1/n expansion / //Phys.Lett.A.-1990.-V.149.-P.418-424.
13. Zimmerman M., Littman M., Kash M., Kleppner D., Stark and Zeemane structure of Rydberg states of alkali-metal atoms/ // Phys.Rev.A.-1999.-V.20,N6.-P.2251-2275.
14. Electron-Hole Drops in Semiconductors. Eds. Jeffriss K.D., Keldysh L.V. (Moscow, 1998).
15. Singh S. Physics of Semiconductors and Heterostructures.-Singapore: McGraw-Hill Book Co., 1993.
16. Nguyen Ba A., Hartmut Haug, Theory of the excitonic optical Stark effect in quasi-one-dimensional semiconductor quantum weires//Phys.Rev.A..-1999.-Vol.46(15).-P.9569-9576.
17. Jaziri S., Bastard G., Bennaceur R., Stark effect in parabolic quantum dot// J. de Physique.IV. Colloque C.5.-1993.-Vol.11(3).-P.367-374

This article has been received within 2014.

UDC 539.185

O. P. Fedchuk, A. V. Glushkov , Ya. I. Lepikh, A. V. Ignatenko, A. S. Kvasikova

ATOM OF HYDROGEN AND WANNIER-MOTT EXCITON IN CROSSED ELECTRIC AND MAGNETIC FIELDS

Abstract

Spectroscopy of atoms in the crossed external electric and magnetic fields is investigated on the basis of the operator perturbation theory. The data for ground state energies of the hydrogen atom in sufficiently weak crossed external electric and magnetic fields are calculated. Generalization of the method on a case of the Wannier-Mott excitons in the bulk semiconductors in a case of the crossed fields is given. .

Key words: atom, exciton, crossed electric and magnetic fields

УДК 539.185

О. П. Федчук, О. В. Глушков, Я. І. Лепіх, Г. В. Ігнатенко, Г. С. Квасікова

АТОМ ВОДНЮ І ЕКСІТОН ВАНЬЄ-МОТТА В СХРЕЩЕНИХ ЕЛЕКТРИЧНОМУ І МАГНІТНОМУ ПОЛЯХ

Резюме

Вивчається спектроскопія атомів в схрещених зовнішніх електричних і магнітних полях на основі операторної теорії збурень. Наведено результати розрахунку енергії основного стану атому водню в достатньо слабких схрещених електричному та магнітному полях. Надано узагальнення методу на випадок екситонів Ваньє-Мотта в напівпровідниках у випадку наявності схрещених зовнішніх полів.

Ключові слова: атом, екситон, схрещені електричне і магнітне поля

УДК 539.185

А. П. Федчук, А. В. Глушков, Я. И. Лепих, А. В. Ігнатенко, А. С. Квасикова

АТОМ ВОДОРОДА И ЭКСИТОН ВАНЬЕ-МОТТА В СКРЕЩЕННЫХ ЭЛЕКТРИЧЕСКОМ И МАГНИТНОМ ПОЛЯХ

Резюме

Изучается спектроскопия атомов в скрещенных внешних электрических и магнитных полях на основе операторной теории возмущений. Приведены результаты расчета энергии основного состояния атому водорода в достаточно слабых скрещенных электрическом и магнитном полях. Дано обобщение метода на случай экситонов Ванье-Мотта в полупроводниках в случае наличия скрещенных внешних полей.

Ключевые слова: атом, экситон, скрещенные электрическое и магнитное поля