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STARK EFFECT AND RESONANCES IN THE IONIZATION CONTINUUM FOR EXCITONS IN QUANTUM DOTS AND ATOMS IN AN ELECRIC FIELD

The Stark effect for non- hydrogenic atom of the rubidium and excitons in semiconductor in an external uniform electric field is theoretically studied within the operator perturbation theory method (J.Phys.B26, L379 (1993)). The Stark resonance energies in the rubidium atom and te excitons in the Cu_20 semiconductor and in the GaAs quantum dots in the external uniform electric field are listed.

1. Introduction

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. 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 remains very important problem of modern atomic physics.

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.[14-17]), 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. Now it is represented an interest to study an influence of quantum well concentration profile and width on Stark shifts in case of such a system as system GaAs-AlGaAs etc. In this paper we study the Stark effect for non-H atom of rubidium and for excitons in an external uniform electric field within the operator perturbation theory method. The Stark resonance energies in rubidium and the Stark shift for the n=2 state of the Wannier-Mott excitons in the Cu_20 semiconductor and excitons in the parabolic quantum dot (GaAs) in the electric field are listed.

2. Stark effect for atomic systems: Operator perturbation theory

Regarding the operator perturbation theory approach, let us note that this method, originally proposed Ref. [2], is in details presented in [1] and used in many papers. So, 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 [11]. The zeroth order Hamiltonian H_0 of this PT possesses only stationary bound and scattering states. In order to overcome the formal difficulties, the zeroth order Hamiltonian was defined using the set of the orthogonal EF and EE without specifying the explicit form of the corresponding zeroth order potential. In the case of the optimal zeroth order spectrum , the PT smallness parameter is of the order of G/*E*, where G and *E* are the field width and bound energy of the state level. It is true that G/*E* £ 1/n even in the vicinity of the "new continuum" boundary (where n is the principal quantum number). An influence of the corresponding electric potential model function choice on the values of the Stark resonances energies and bandwidths does not significantly change the final results for the resonances shifts and widths [1].

According to [3], the Schrödinger equation for the electronic eigen-function 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^2e^4/h^2 for energy) looks like:

$$[-(1 - N/Z) / r + F z - 0{,}5D - E] y = 0 \qquad (1)$$

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]), including the most consistent quantum electrodynamics procedure for construction of the optimized one-quasi-electron representation and *ab initio* core potential , providing a needed spectroscopic accuracy. For multielectron atom one may introduce the ion core charge z^*. According to standard quantum defect theory (c.f.[3]), relation between quantum defect value m_l, electron energy *E* and principal quantum number *n* is: $m_l=n-z^*(-2E)^{-1/2}$. 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 $d(n_1n_2m)$ is connected with the quantum defect value of the free ($F=0$) atom by the following relation [3]:

$$d(n_1n_2m)=(1/n)\sum_{l=m}^{n-1}(2l+1\ \ C^{JM}_{J,M-m;lm})^2\mu_l$$

$$J=(n-1)/2,\ \ M=(n_1-n_2+m)/2;$$

Naturally, it is possible to use more complicated forms for the ion core potential (c.f.[1]). 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*:

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

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

coupled through the constraint on the separation constants:

$$b_1 + b_2 = 1.$$

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

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

Potential energy in equation (4) has the barrier. Two turning points for the classical motion along the *h* axis, t_1 and t_2 , at a given energy *E* are the solutions of the quadratic equation ($b = b_1, E = E_0$). It should be mentioned that the final results do not depend on the parameter t . It is necessary to know two zeroth order EF of the H_0: bound state function Y_{Eb} (e, n, j) and scattering state function Y_{Es} (e, h, j) 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]:

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

with

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

These two conditions quantify the bounding energy E, with separation constant b_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, b_1. The bound state EE, eigenvalue b_1 and EF for the zero order Hamiltonian H_0 coincide with those for the total Hamiltonian H at e Þ 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, b_1, m by the well known expressions. We preserve the n, n_1 ,m states-classification in the e¹0 case . 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:

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

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 $t \to \infty$.

3. Stark effect for exciton

The above analogous method can be formulated 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:

$$[-\hbar^2\nabla_e^2 / 2m_e^* - \hbar^2\nabla_h^2 / 2m_h^* - e^2 / \varepsilon r_{eh} + \\ + eFr_e - eFr_h]\Psi = E\Psi \tag{7}$$

where m^*_e(m^*_h) are the effective-mass for the electron (hole), e is the background dielectric constant. Introducing the relative coordinates: $r = r_e - r_h$ and the corresponding momenta 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 (7) as:

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

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 Stark effect for quantum dots requires more detailed consideration. For definiteness, below we study the Stark effect in the parabolic quantum dot. Within the effective-mass approximation and neglecting the band-structure effects , the Hamiltonian of an exciton in a parabolic quantum dot with the same quantization energy $\hbar\Omega$ (for the electron and hole), nd subjected to an external electric field , can be expressed as :

$$H = -\hbar^2\nabla_e^2 / 2m_e^* + (1/2)(\, m_e^*)\Omega^2 r_e^2 - \hbar^2\nabla_h^2 / \\ / 2m_h^* + (1/2)(\, m_h^*)\Omega^2 r_h^2 - e^2 / \varepsilon r_{eh} + eFr_e - eFr_h \tag{9}$$

where all notations are defined above. Further, as above, using the relative coordinate, the momenta with reduced mass and center-of-mass coordinate and the momenta with the total-mass M, the Hamiltonian H (7) can be represented as :

$$H = P^2 / 2M + (1/2)M\Omega^2\rho^2 + p^2 / 2\mu + \\ + (1/2)\mu\Omega^2 r^2 - e^2 / \varepsilon r + eFz \,. \tag{10}$$

Further let us note that the part which depends only on the center-of-mass coordinate in Eq.(10) is corresponding to the Hamiltonian of a well-known 3D harmonic oscillator and the exciton properties is essentially determined by the relative Hamiltonian H_r.

The field term added to the z-direction confinement describes a displaced harmonic oscillator centred in $z_0 = eF/mW^2$ with the frequency W_r inferior to W. Besides, as usually [17], in order to solve the Hamiltonian H_r , one should introduce an interaction potential which obeys to the known Hooke's force with the parameter l by adding and substracting the potential:

$$V(r) = \lambda[(1/2)\mu\Omega^2 r^2 - \hbar\Omega] \,.$$

Surely then the Hamiltonian H is splitted into two terms with the one term being exactly solvable while the other can be treated as a perturbation. Such a scheme is corresponding to method by Jaziri-Bastard-Bennaceur [17]. Our approach is in he direct numerical solving the problem. Let us remind that the introduced potential is similar to the interaction potential between electron-electron used by Johnson-Payne and it can hardly

be considered as the correct potential for the all electron-hole separation. Nevertheless, here one could adjust the interaction parameter *l* so in order to provide the best fit of the true interaction which is the Coulomb interaction, and for the dominant range of separation *r* [17]. The attraction potential *V*(*r*) will have negative value with positive *l* , and it yields a physically reasonable fit to the exact interaction for electron-hole separation $r<(2)^{1/2}R_0$ (here R_0 is the quantum dot radius defined as $\sqrt{\hbar/\mu\Omega}$. As usually, the total energy corresponding to exciton ground state is obtained as :

$$E_T = (3/2)\hbar\Omega + (3/2)\hbar\Omega_r - \lambda\hbar\Omega - (e^2F^2)(2\mu\Omega^2)$$

where $\Omega_r = \Omega\sqrt{1+\lambda}$. The field-induced energy shifts can be expressed as: $DE = E_T(F=O)-E_T(F)$, where E(*F*=0)is the corresponding energy in the free (i.e. zero-field) state. The main aim is to determine the exciton binding energy defined by $E_B = E_e+E_h-E_T$, where E_e,E_h are the energies corresponding to the one-particle Hamiltonian.

4. Results and conclusions

The calculation results for Stark resonances energies in the rubidium atom for the electric field strength *e*=2.189 kV/cm are presented in Table 1. For comparison we have also presented the experimental data [13], the results of calculation within the *1/n*-expansion method by Popov etal [12]. For the most long-living Stark resonances with quantum numbers $n_2 = 0$, m = 0, a width of energy level is significantly less than a distance between them. These states are mostly effectively populated by p-polarized light under transitions from states with (n_1-n_2) = max, m = 0. As a result, the sharp isolated resonances (their positions under E>0 are determined by energies of quasi-stationary states with $n_2=0$, m=0) are appeared under photo ionization from these states in a case of p-polarization

In ref. [4] there are listed the preliminary estimates of the Stark shifts of the n=2 state of excitons in the Cu_20 semiconductor (yellow series) at the electric field strength 600 V/cm results and indicated on the physically reasonable agreement with the known results by Thomas and Hopfield (TH) [14].

Table 1. The energies (cm^{-1})of the Stark resonances for the Rb atom (ε = *3,59 kV/cm)*:
A-experimental data ; B- Popov et al; C- OPT approach.

n_1n_2m	*d*	A	B		C
23,0,0	0,656	133,1	132,8	132,9	133,0
22,0,0	0,681	157,0	157,1	157,2	157,1
21,1,0	0,517	161,1	159,5	160,6	160,9
20,2,0	0,400	163,9	163,2	163,7	163,9
21,0,0	0,708	185,2	184,2	184,8	185,1
20,1,0	0,531	186,3	185,4	185,8	186,2
20,0,0	0,737	217,2	214,6	214,9	216,9
18,1,0	0,561	248,4	247,2	247,3	248,2
16,2,0	0,428	-	-	-	285,5
18,0,0	0,802	-	-		289,3

Our final value for the Stark shift of the n=2 state excitons in the Cu_20 semiconductor (yellow series) at the electric field strength 600 V/cm results in – 0,308 meV in a good agreement with experimental data of Gross et al.[28]. Under increasing the electric field strength changing a potential on a small enough distance (the orbits diameter) will become comparable with the bond energy of particle on this orbit. According to our data and data by Gross et al., the corresponding electric field is ~ 9×10^3 V/cm. we have tried to discover the chaotic behavior of the exciton dynamics in an electric field, however near ionization boundary exciton does not demonstrate behaviour of quantum chaotic system, which is similar to hydrogen or on-H atom dynamics in a strong field and manifested as unusual features in a photoionization spectra (alkali atoms) [5,14]. Further we list some data on the Stark shifts excitons in a GaAs semiconductor quantum dot (table 2).

Table 2. The Stark shifts (meV) for exciton in the GaAS quantum dot: A- Jaziri-Bastard-Bennaceur method; B- OPT approach

F (kV/cm)	*R* (A)	A	B
50	50	3.9	4.0
50	80	14	14.1
50	120	45	45.2
100	50	13	13.1
100	80	56	56.6
100	120	158	159.8

Comparison of the presented preliminary data shows that the different results are in the physically reasonable agreement. The corresponding accuracy is of the order of 1%, however, is should be noted [17] that though the method [17] is much simpler in comparison with the direct variational approach, but it cannot enviseaged for any strength electric field and/nor any quantum dot size. The important feature of the operator perturbation theory formalism is that it can be applied for any strength electric field.

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STARK EFFECT, RESONANCES IN THE IONIZATION CONTINUUM FOR EXCITONS INQUANTUM DOTS AND ATOMS IN AN ELECRIC FIELD

Abstract

The Stark effect for non-H atom of rubidium and exciton in semiconductor in an external uniform electric field is studied within the operator perturbation theory method. The Stark resonance energies in rubidium and excitons in the Cu_20 semiconductor and in the GaAs quantum dots in the electric field are listed.

Key words: atom, exciton, Stark effect

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ШТАРК ЕФЕКТ ТА РЕЗОНАНСИ У ІОНІЗАЦІЙНОМУ КОНТИНУУМІ ДЛЯ ЕКСІТОНІВ І АТОМІВ У ЕЛЕКТРИЧНОМУ ПОЛІ

Резюме

На підставі методу операторної теорії збурень виконано дослідження Штарк-ефекту для атому рубідію та ексітонів в напівпровідниках у зовнішньому однорідному електричному полі. Надані дані щодо енергій штарківських резонансів для атому рубідію та ексітонів у Cu_20 та GaAs напівпровідників в електричному полі.

Ключові слова: атом, ексітон, Штарк-ефект

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ШТАРК ЭФФЕКТ И РЕЗОНАНСЫ В ИОНИЗАЦИОННОМ КОНТИНУУМЕ ДЛЯ ЭКСИТОНОВ И АТОМОВ В ЭЛЕКТРИЧЕСКОМ ПОЛЕ

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Резюме

На основе метода операторной теории возмущений выполнено исследование Штарк-эффекта для атома рубидия и экситонов в полупроводниках во внешнем однородном электрическом поле. Получены данные по энергиям штарковских резонансов для атома рубидия и экситонов в полупроводниках Cu_20 и GaAs в электрическом поле.

Ключевые слова: атом, экситон, Штарк-эффект