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WANNIER-MOTT EXCITONS AND H, RB ATOMS IN A DC ELECRIC FIELD: STARK EFFECT

A numerical calculation of the DC Stark effect for H, Rb atoms and Wannier-Mott exciton in an external uniform DC electric field is carried out within the operator Glushkov-Ivanov perturbation theory method

INTRODUCTION

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. [1–5]). Calculation of the atomic characteristics in a strong electric DC field remains very important problem of modern atomic physics and physics of semiconductors too [6–30]. It is well known [28] 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. [28–30]), a calculation procedure of the Stark effect for exciton spectrum attracts a deep interest permanently. As it is well known [11], external electric field shifts and broadens the bound state atomic levels. The standard quantum-mechanical approach mutually relates complex eigen-energies (EE) $E = E_r + 0{,}5iG$ and complex eigen-functions (EF) to the resonances' shape. The calculation difficulties in the standard quantum mechanical approach are well known [3]. In refs. [10–13] a principally new consistent uniform quantum — mechanical approach to the non-stationary state problems solution had been developed including the Stark effect and also the scattering problems. The essence of the method is the inclusion of the well known method of "distorted waves approximation" in the frame of the formally exact PT [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. This method is called the operator PT (OPT) approach: Glushkov-Ivanov OPT [10–12]. It is very important to note that the hamiltonian H_0 is defined so that it coincides with the general Hamiltonian H at $\varepsilon \Rightarrow 0$. ($\varepsilon$ is the electric field strength). Let us note that perturbation in OPT does not coincide with the electric field potential though they disappear simultaneously. 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 [11, 12]. All said above regards the Wannier-Mott exciton characteristics in semiconductors as well. In ref. [13-17] the OPT approach have been used for solution of the isotopes separation problem and an account of the non-hydrogenic effects was done as well as the improvement of the convergence procedure. In ref. [18–24] the OPT approach have been successfully used for studying new laser-electron nuclear spectral effects in thermalized plasma (speech is about new cooperative laser-electron- nuclear processes), new laser-electron-nuclear effects in atoms, ions and diatomic molecules. There is very effective application of the OPT approach in conjuction with S-matrix Gell-Mann and low formalism to studying the resonance states of compound super-heavy nucleus and electron-positron pair production in heavy nucleus and ioons collisions and under availibuility of the external superintense electromagnetiv filed, when the EPPP chanell is opened [22–24].

In this paper we have used the OPT method [11, 12] for studying and exact calculation of the DC Stark effect for hydrogen, rubidium atoms and Wannier-Mott exciton in an external uniform DC electric field (excitons in the Cu_20 semiconductor, yellow series).

GLUSHKOV-IVANOV OPERATOR PERTURBATION THEORY APPROACH

As usually, the Schrödinger equation for the electronic eigen-function taking into account the uniform DC electric field 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:

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

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]) for multielectron atoms. The detailed theory of the Stark effect for multielectron systems is given in ref. [3, 14]. 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*:

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

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

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

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

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

Potential energy in equation (4) has the barrier. Two turning points for the classical motion along the 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 should be mentioned that the final results do not depend on the parameter τ. It is necessary to know two zeroth order EF of H_0: bound state function $\Psi_{Eb}(\varepsilon, \nu, \varphi)$ and scattering state function $\Psi_{Es}(\varepsilon, \eta, \varphi)$ 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]:

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

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. We preserve the n, n_1, m states-classification in the $\varepsilon \neq 0$ 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:

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

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 $t \Rightarrow \infty$. The coefficient z_2' ensures the orthogonality condition and is defined as [11]:

$$z_2' = \{\iint d\zeta d\eta\, (\zeta+\eta)\, f^2_{Eb}(\zeta) g_{Eb}(\eta) g_1(\eta)\} / \{\iint d\zeta d\eta\, (\zeta+\eta)\, f^2_{Eb}(\zeta) g_{Eb}(\eta) g_2(\eta)\}$$

The imaginary part of state energy in the lowest PT order is [11]:

$$\mathrm{Im}E = G/2 = \pi < \Psi_{Eb} |H| \Psi_{Es} >^2 \qquad (7)$$

with the general Hamiltonian H (G- resonance width). The state functions Ψ_{Eb} and Ψ_{Es} are assumed to be normalized to unity and by the $\delta(k - k')$-condition, accordingly. Note then that the whole calculation procedure at known resonance energy E and separation parameter β has been reduced to the solution of one system of the ordinary differential equations. For its solution we use our numeral atomic code ("Superatom" package [3, 10–16, 24–27]).

STARK RESONANCES ENERGIES AND WIDTHS CALCULATION RESULTS FOR ATOMS

The calculation results for Stark resonances energies and bandwidths for some states of H atom are presented in Table 1. For comparison we have indicated the data, obtained within another approach — complex eigen-values and numerical calculation (c.f. [1, 3, 11]. In fig.1 we present the dependence of critical field strength upon the effective quantum number for n for atoms of *Na, Rb:* dots –experiment; solid line 1 – theoretical estimate on the basis of classic treatment; solid line 2 – calculation within naпve hydrogen-like approximation; dashed line – our calculation. One can see that the experimental results significantly differ from theoretical estimates in classical treatment and naпve hydrogen-like approximation (solid lines 1, 2), in particular the difference is about 15–20% and strongly overcomes the experiment error. Our calculation results are in a good agreement with experiment.

Table 1

The energies E_r (at. units) and widths G (at.units)of Stark resonances of the hydrogen atom ina DC electric field with strength: $\varepsilon = 6{,}5\ kV/cm$.

(n n_1 n_2 m)	*E*, Ref. [5]	G , Ref. [5]	*E* , Present paper	G , Present paper
24,23,0,0	0,1192	0,2752	0,1194	0,2754
25,23,1,0	0,2748	1,0868	0,2749	1,0871
25,23,0,1	0,8298	0,7484	0,8301	0,7487
25,24,0,0	1,4329	0,4175	1,4331	0,4177

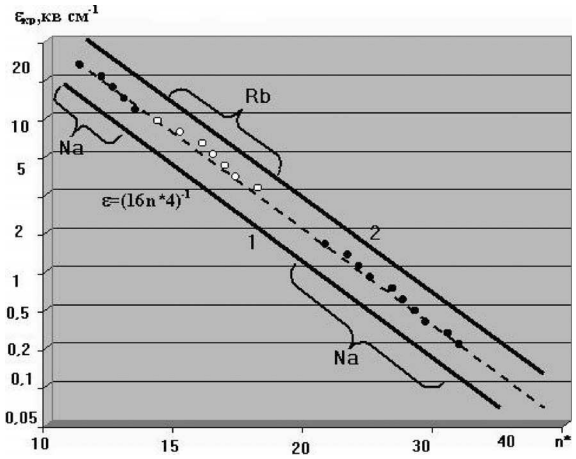

Fig. 1. Dependence of critical field strength upon the effective quantum number for n^* for atoms of *Na, Rb*: dots –experiment; solid line 1 – theoretical estimate on the basis of classic treatment; solid line 2 – calculation within naпve hydrogen-like approximation; dashed line – our calculation

WANNIER-MOTT EXCITONS IN A DC ELECTRIC FIELD

The analogous method can is formulated for description of the Stark effect in the Wannier-Mott exciton in semiconductors (CdS, Cu2O). The Schrodinger equation for the Wannier-Mott exciton has a standard form:

$$[-\hbar^2\nabla_e^2/2m_e^* - \hbar^2\nabla_h^2/2m_h^* - e^2/\varepsilon r_{eh} - -eEr_e - eEr_h]\Psi = E\Psi. \quad (8)$$

Here all notations are standard. A vector potential is as follows: *A(r)=1/2 [Hr].* Under transition to system of exciton masses centre by means of introducing the relative coordinates: $r = r_e - r_h$

$$\rho = (m_e^* r_e + m_h^* r_h)/(m_e^* + m_h^*)',$$

one could rewrite (9) as:

$$[-\hbar^2\nabla^2/2\mu - e^2/\varepsilon r - \hbar/2\cdot(1/m_h^* - 1/m_e^*)K\cdot \cdot p - eEr]F = [E - \hbar^2K^2/8\mu]F. \quad (9)$$

This equation then could be solved by the method, described above. Preliminary estimates show that this approach, in a case of electric DC field, gives the results for Stark states in a reasonable agreement with known results of Thomas and Hopfield (TH) [28–30]. According to our advanced calculation, the Stark shift for the n=2 state of excitons in the Cu_20 semiconductor (yellow series) at the electric field strength 600 V/cm results in $-3{,}1\cdot10^{-4}$ eV. This value agrees well with experimental data of Gross et al. [28]. Ionization of the exciton in an electric DC field occurs if a change of potential on a small enough distance (the orbits diameter) is comparable with a bonding energy of particle on this orbit. According to data of Gross et al., the corresponding electric field is ~9 10^3 V/cm. Our calculation agrees with this value.

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A numerical calculation of the DC Stark effect for H, Rb atoms and Wannier-Mott exciton in an external uniform DC electric field is carried out within the operator Glushkov-Ivanov perturbation theory method.

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ЕКСІТОН ВАН'Є-МОТТА І АТОМИ H, RB У ПОСТІЙНОМУ ЕЛЕКТРИЧНОМУ ПОЛІ: ШТАРК ЕФЕКТ

На підставі методу операторної теорії збурень Глушкова-Иванова виконано розрахунок Штарк-ефекту для атомів **H, Rb** та ексітонів Ван'є-Мотта (напівпровідник Cu_2O) у однорідному електричному полі.

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ЭКСИТОН ВАНЬЕ-МОТТА И АТОМЫ H, RB В ПОСТОЯННОМ ЭЛЕКТРИЧЕСКОМ ПОЛЕ: ШТАРК ЭФФЕКТ

На основе метода операторной теории возмущений Глушкова-Иванова выполнен расчет Штарк-эффекта для атомов H, Rb и экситона Ванье-Мотта (полупроводник Cu_2O) в однородном электрическом поле.