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CONSISTENT QUANTUM APPROACH TO QUARKONY ENERGY SPECTRUM AND SEMICONDUCTOR SUPERATOM AND IN EXTERNAL ELECTRIC FIELD

The problems of calculation of the bound states energies for semiconductor superatom (spherical nucleus of some semiconductor material that is selectively doped by donors; it is surrounded by the intrinsic matrix from material with low band gap) and heavy quarkony in external strong electric field are considered. Ab initio effective potential approach in combination with the operator perturbation theory method is used in calculation.

In last years studying behaviour of the mesosystems such as superatom and 1D super-lattice attracts, exciton, bi-exciton complexes, elementary atomic systems etc. in external electric and magnetic field attracts a great interest (c.f. [1–5]). Superatom represents the spherical nucleus of some semiconductive material, that is selectively doped by donors and surrounded by the intrinsic matrix of material with low band gap. All these systems can be calculated on the basis of the same unified quantum mechanical method. In this paper we consider the corresponding method (energy approach) in order to carry out the accurate calculations of the energy characteristics for systems above cited. Earlier we have developed the accurate consistent methods for calculation of properties of such systems (c.f. [5, 6]), in particular, relativistic perturbation theory with effective potential of the zeroth order (energy approach), ab initio quasi-particle density functional formalism (Dirac-Kohn-Sham-Ivanov schemes). The main purpose of this work is to make more exact the data regarding the energy characteristics of the quarkony and semiconductor superatom systems. We will use these approches, namely, ab initio effective potential approach in combination with the operator Glushkov-Ivanov perturbation theory method [7] as basis for formulation of the corresponding theory cited systems in an external strong electric and magnetic field. Let us note that earlier we gave the preliminary estimates for cited characteristics [12].

2. Let us start from considering superatom [3–5]. In the zeroth approximation we use usually the effective ab initio model functional, constructed on the basis of the gauge invariance principle [6]. The zeroth order basis is generated by the solution of the Dirac equation with spherically symmetric potential that includes the potential of ionized donors, the Dirac-Fock-Kohn-Sham functional. The relativistic Dirac equation can be written in the central field in a two-component form as follows (reltivistic units are used):

$$\frac{\partial F}{\partial r}+(1+\chi)\frac{F}{r}-(\varepsilon+m-V)G=0$$

$$\frac{\partial G}{\partial r}+(1-\chi)\frac{G}{r}+(\varepsilon-m-V)F=0. \qquad (1)$$

Here we put the fine structure constant $\alpha = 1$. The moment number

$$\chi=\begin{cases}-(1+1), & j>1\\ 1, & j<1\end{cases},$$

where F and G are the big and small components of the Dirac wave function, ε — energy, r – distance from center of nucleus, other designations are standard. Effective potential $V(r)$ for super atom is supposed to be by the spherically symmetric and has the following form:

$$V(r)=V_0\theta(r_0-r)+V_N(r)+V_H+V_{XC}(r), \qquad (2)$$

where r_o is the nuclear radius, V_0 is the positive overfall of minimums of conductivity zones for nucleus and matrix; $\theta(x)=0$, $x<0$ and $=1$ if $x>0$; V_N is a potential of the ionized donors; V_H, V_{XC} are the Hartree and exchange-correlation potentials. The shape of potential (2) is presented in the fig. 1.

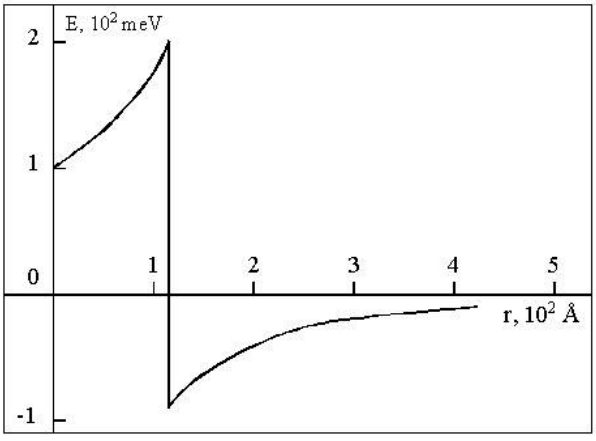

Fig. 1. The shape of potential (2) (see text)

The next sep is an account the external electric filed potential. As it is well known, external electric field shifts and broadens the bound state atomic levels. The standard quantum-mechanical approach relates complex eigen- energies (EE) $E=E_r+0,5iG$ and complex eigen-functions (EF) to the shape resonances [6]. The calculation difficulties in the standard quantum mechanical approach are well known. In Glushkov-

Ivanov paper [6,7] it has been developed a consistent uniform quantum — mechanical approach to the non-stationary state problems solution including the Stark effect and also 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 perturbation theory. 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 has been shown that G/$E \leq 1/n$ even in the vicinity of the "new continuum" boundary (n is the principal quantum number). This method is called as the operator PT (OPT) [6,7]. It is very important to note that the hamiltonian H_0 is defined so that it coincides with the total Hamiltonian H at $\varepsilon \Rightarrow 0$ (ε is the electric field strength; potential is -zε).

The Dirac equation for the electron function with taking into account the uniform electric field and the field of the nucleus:

$$[\alpha\, cp - \beta mc^2 - V(r) + \varepsilon\, z - E]\, \psi = 0. \qquad (3)$$

Here E is the electron energy. The key moment of the further considering is to establish coupling between basis of functions of the zeroth approximetion (eq. (1)) in the spherical coorrdinates and corresponding basis in parabolic co-ordinates. According to standard quantum defect theory for multielectron systems with the separated closed shells core and external quasiparticles, relation between quantum defect value μ_l, electron energy E and principal quantum number n is: $\mu_l = n\text{-}z^*(-2E)^{-1/2}$. 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 $\delta(n_1 n_2 m)$ is connected with the quantum defect value of the free (ε=0) atomic system by the following relation [7]:

$$\delta(n_1 n_2 m) = (1/n)\sum_{l=m}^{n-1}(2l+1)(C^{JM}_{J,M-m;lm})^2 \mu_l,$$
$$J = (n-1)/2,\ M = (n_1 - n_2 + m)/2. \qquad (4)$$

Naturally, it is possible to use more complicated forms for the ion core potential. Equation 95) gives the recept of coupling between basis of functions of the zeroth approximation (eq. (1)) in the spherical coordinates and corresponding basis in parabolic co-ordinates.

3. The next key moment is connected with account of the correlation corrections to energy. It can be done by means relativistic density functional formalism and QED perturbation theory (c.f. [6, 8, 12]). This approach allows accounting all correlation corrections of the perturbation theory second order and also a contribution of the high orders diagrams (particle-hole interaction, mass operator iterations etc.). It is very important to note that the nuclear diameter in the superatom is compared with the general size of system and a singularity in the coordinates center is absent in contradistinction of the heavy atom. That is why, the levels with large angular moment become more energetically profitable. In ref. [5, 12, 13] it has been carried out a calcualtion, which has shown for superatom (nucleus: $Al_{0,35}Ga_{0,65}As$; nuclei charge Z=20; nucleus radius: 175A; matrice: GaAs) that the configuration $1s^2 2p^6 3d^{10} 2f^2$ is corresponding to the ground state of system. The calculation of the superatom system (superatomic nucleus $Al_{0,35}Ga_{0,65}As$; nuclear charge Z=20; matrix: GaAs; radius of the nucleus: 125A) was carried out and obtained the corresponding sequence of energy levels $1s^2 2p^6 3d^{10} 2s^2$. With other parameters (radius of the nucleus 170A and Z=20) the ground state of system is corresponding to another configuration $1s^2 2p^6 3d^{10} 2f^2$. The superatomic radius is estimated 351A. It is clear that the properties of the superatom can be changed according to the shape of potential (2). It is obvvious that these properties can be essentially changed in a presence of external field. The preliminary estimate shows that the Stark shift for the considered super atom in DC external electric field (strength 0,001 atomic units) is 0,15 meV.

4. For heavy quarkony the corresponding theory has the same form, excepting only the numerical parameters of corresponding effective potential. Earlier in ref. [5] we presented the results of calculating the energy splitting for quarkony with the use of the different forms of potential [9–11]. We have also carried out the energy splitting calculation for quarkony system with the use of the different forms of potential. In the zeroth limit for E(2s)-E(2p) the more exacted value is 830 MeV under m(Q)=45 GeV. If $r \to \infty$, the 2s-2p and 2s-1s splitting results in ~145 MeV. Especial interest attracts behavior of the value:

$$|\Psi(0)|^2_{2\sigma} / |\Psi(0)|^2_{1s} = 0{,}5 - 0{,}6 \qquad (5)$$

under m(Q)=45 GeV (this value is obtained in a case of the use of the potential : $\mathbf{V}(r) \sim 1/r\mathrm{Ln}(\mathrm{Ar})$ when $r \to 0$ and $\mathbf{V} \sim ar$ when $r \to oo$; A=0,1 GeV and a=0,2 GeV). These properties can be essentially changed in a presence of the strong external electric or magnetic field.

5. So, we present here a consistent quantum approach to calculation of the bound states energies for following systems: superatom (spherical nucleus of some semiconductor material that is selectively doped by donors; it is surrounded by the intrinsic matrix from material with low band gap) in weak external electric field and more exacted data for heavy quarkony. As it has been indicated earlier a consideration together such different physical systems as semiconductor superatom and heavy quarkony is connected with a fact that the mathematical structure of the master equations is practically the same, excepting surely the energy parameters of the corresponding effective potentials.

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ПОСЛЕДОВАТЕЛЬНЫЙ КВАНТОВЫЙ ПОДХОД В ТЕОРИИ КВАРКОНИЯ И ПОЛУПРОВОДНИКОВОГО СУПЕРАТОМА ВО ВНЕШНЕМ ЭЛЕКТРИЧЕСКОМ ПОЛЕ

Рассмотрена проблема расчета энергий связанных состояний систем: тяжелого кваркония и полупроводникового суператома (сферическое ядро полупроводникового материала, легированного донорами и окруженного беспримесной матрицей из материала с меньшей шириной запрещенной зоны) во внешнем сильном электрическом поле. Метод ab initio эффективного потенциала в комбинации с операторной теорией возмущений использован для расчетов.

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ПОСЛІДОВНИЙ КВАНТОВИЙ ПІДХІД У ТЕОРІЇ КВАРКОНІЮ ТА НАПІВПРОВІДНИКОВОГО СУПЕРАТОМУ У ЗОВНІШНЬОМУ ЕЛЕКТРИЧНОМУ ПОЛІ

Розглянуто проблему розрахунку енергій зв'язаних станів систем: важкого кварконія та суператому (сферічне ядро півпроводникового матеріалу, легірованого донорами та оточеного бездомішковою матрицею з матеріалу з меньшею шириною забороненої зони) у зовнішньому сильному електричному полі. Метод ab initio ефективного потенціалу у комбінації з операторною теорією збурень використано для розрахунків.