BOUND STATES IN QUARKONIUM AND SUPERATOMS SYSTEMS: ENERGY LEVELS SPLITTING

A.V.Glushkov , A.V.Loboda, M.Zuda

Atomic-Molecular-Laser Spectroscopy Centre,
Odesa Hydrometeorological Institute,
a/c 108, Odesa-9, 65009, Ukraine

The problem of calculation of bound state energies for the following systems: heavy quarkonium and superatom (a spherical nucleus of some semiconductive material that is selectively doped by donors; surrounded by the intrinsic matrix from material with low band gap) is considered. *Ab initio* effective potential approach in combination with the QED and quantum mechanical perturbation theory method and polarization functional formalism is used in the calculation of the energy characteristics of the systems considered. The zeroth approximation is generated by solution of Schrödinger equation with spherically symmetric potential that includes the potential of ionized donors, the Hartree-Fock-Kohn-Sham functional. The perturbation theory second- and higher-order corrections (particle-hole interaction, mass operator iterations) are effectively taken into account. For superatomic system ($Al_{0,35}Ga_{0,65}As$ nucleus, charge Z=20; GaAs matrix) we calculate the corresponding sequence of energy levels. The energy splitting calculation for quarkonium with the use of the different forms of potential is carried out.

In the recent years great interest is attracted by the study of bound state energies for the following systems: heavy quarkonium, superatom and 1D superlattice [1–6]. 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 the above cited systems. Earlier we have developed an accurate consistent method for calculations of the atomic and molecular system properties [7–10], in particular, the quantum-electrodynamical (QED) method and 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 now is their application to the calculations of energy characteristics of quarkonium and superatom systems. The zeroth approximation is usually generated by the effective *ab initio* model functional, constructed on the basis of the gauge-invariance principle. [7–10]. The zeroth-order basis is generated by the solution of the Schrödinger equation with spherically symmetric potential that includes the potential of ionized donors, the Hartree-Fock-Kohn-Sham functional. The non-relativistic Schrödinger equation has the standard form:

$$\Psi''+2/r\Psi'+2m/h^2[E-V(r)-l(l+1)/r^2]\Psi=0 \quad (1)$$

where Ψ is the radial part of the wave function, E – the energy of the system, l –orbital quantum number, r – the distance from center of the nucleus, other designations are standard. The effective potential V for the superatom is supposed to be spherically symmetric and has the following form:

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

where r_0 is the nuclear radius, V_0 is the positive overfall of conduction band minima for the nucleus and the 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 Fig.1 The correlation corrections of the high orders can be taken into account within the Green functions method and relativistic polarization functional formalism [8-10].

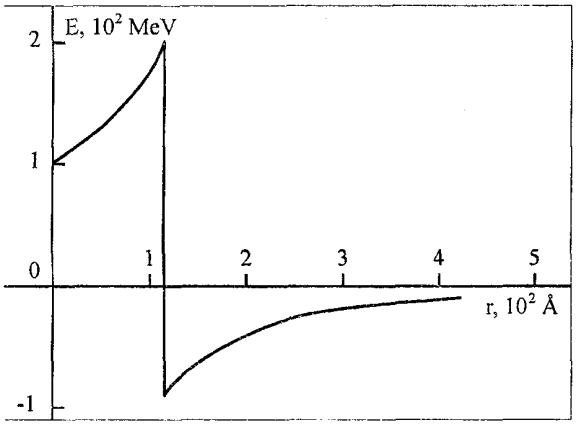

Fig.1. The potential of superatom (formula (2)).

We take into account 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. We have carried out the calculation of the superatom system ($Al_{0,35}Ga_{0,65}As$ superatomic nucleus, nuclear charge Z=20 ;: GaAs matrix) and obtained the corresponding sequence of energy levels $1s^2 2p^6 3d^{10} 2s^2$ (superatomic radius: 120 Å). Note that it is in a good agreement with the calculation results of Inoshita *et al.* [1]. With difgferent parameters (radius 160 Å and Z=20) the ground state of system is corresponding to a different configuration $1s^2 2p^6 3d^{10} 2f^2$ . . The superatomic radius is estimated as ~ 390 Å. It is clear that the properties of the superatom can be changed according to the form of the potential (2).

Such quantum-mechanical problem is known in the high-energy physics, in particular, the problem concerns the bound states of quarkonium. We have also carried out the energy splitting calculation for a quarkonium system with the use of the different forms of potential. In the zeroth limit for $E(2s)$-$E(2p)$ we have 800 MeV at $m(Q)$=45 GeV. If r→∞, the 2s-2p and 2s-1s splitting results in ~140 MeV. It is interesting to turn attention to the behavior of the value $|\Psi(0)|^2_{2\sigma} / |\Psi(0)|^2_{1s} = 0{,}5 - 0{,}6$ at $m(Q)$=45 GeV (this value is obtained in the case of the potential : $V(r)\sim 1/rLn(Ar)$ being used when $r\to 0$ and $V\sim ar$ when $r\to\infty$; A=0.1 GeV and a=0.2 GeV). In Fig. 2 we present the dependence of the value $|\Psi(0)|^2_{1\sigma}$ on the position of the θ-singularity for the potential V.

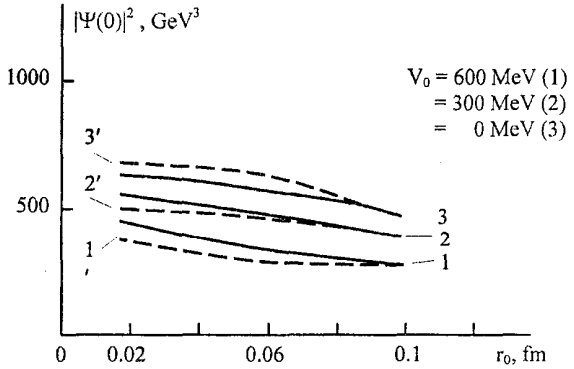

Fig. 2. The dependence of the value $|\Psi(0)|^2_{1\sigma}$ on the position of the θ-singularity for the potential V: —— data of [5]; ---- our data.

In conclusion, we pay attention to possible perspective of using superatoms in technical applications. Creation of optical logical devices on basis of superatoms for optical computers is of great interest. We consider the possibility of creation of a counter for single electrons.

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ЗВ'ЯЗАНІ СТАНИ В КВАРКОНІЇ ТА СУПЕРАТОМНИХ СИСТЕМАХ: РОЗЩЕПЛЕННЯ ЕНЕРГЕТИЧНИХ РІВНІВ

О.В.Глушков, А.В.Лобода, М.Зуда

Центр атомної, молекулярної та лазерної спектроскопії,
Одеський гідрометеорологічний інститут, а/с 108, Одеса-9, 65009

Розглянуто проблему розрахунку енергій зв'язаних станів систем: важкого кварконію та суператома (сферичне ядро напівпровідникового матеріалу, легованого донорами та оточеного бездомішковою матрицею з матеріалу з меншою шириною забороненої зони). Для розрахунку енергетичних властивостей досліджуваних систем використано метод ефективного потенціалу з перших принципів у комбінації з КЕД та квантово-механічною теорією збурень і формалізмом поляризаційного функціоналу. Сферично симетричний потенціал у рівнянні Шредінгера складається із потенціалу іонізованих донорів та функціоналу Хартрі-Фока-Кона-Шема. Для суператомної системи (ядро $Al_{0.35}Ga_{0.65}As$; заряд $Z=20$; матриця GaAs) одержано відповідну послідовність енергетичних рівнів. Виконано розрахунок енергетичного розщеплення для кварконію.