ON THE BOUND STATE OF e^++Yb SYSTEM

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A phenomenological optical potential is used to investigate the bound states of $e^{\pm}$+Yb system near the threshold of the elastic scattering channel. It was determined that bound s–state e^++Yb system exists at energies below –100 meV.

It has been predicted in [1] that the bound e^+Yb-state exists at negative energies. The energy of this s-state, -205 meV, was found by using the polarization potential obtained within the assumption of the existence of stable Yb^- ion in the $^2P_{1/2}$-state with the –54 meV energy [2]. As regards the $^2P_{3/2}$-state, the last was shown in [2] as quasi-bound (i.e. resonance) state with the 10 meV energy. Later on, in the experimental work [3] the fact of the existance of the stable Yb^- was called in question, while the theoretical paper [4] stated that both $^2P_{1/2}$ and $^2P_{3/2}$ states were the shape resonances in the low energy e^-+Yb-scattering at 20 and 80 meV, respectively. Therefore, it appeared to be interesting to repeat the studies on the bound state of the e^++Yb-system, but with the inclusion of results [4].

Below, similarly to [1], for the case of the positron scattering we shall use the polarization potential obtained for the electron scattering.

For the case of e^-+Yb system the optical potential

$$V(r,E) = V_s(r) + V_{so}(r) + V_e(r,E) + V_p(r) \qquad (1)$$

is used. Here E is the impact energy (we used atomic units, $h=e=m_e=1$).

The electrostatic potential is:

$$V_s(r) = -\frac{Z}{r}\sum_{i=1}^{3} A_i \exp(-b_i r) \qquad (2)$$

and the electron density of the target atom is:

$$\rho(r) = \frac{Z}{4\pi r}\sum_{i=1}^{3} A_i b_i^2 \exp(-b_i r) \qquad (3)$$

where parameters A_1=0.1267, A_2=0.7734, A_3=0.0999, b_1=31.681, b_2=3.9727 and b_3=0.9288 are obtained in the Dirac-Hartree-Fock-Slater approximation [5].

We have included the spin-orbit interaction by potential [6]

$$V_{so}(r) = \xi(j,\ell)\frac{1}{r}\left(\frac{dV_s(r)}{dr}\right)\frac{\alpha^2}{[2+\alpha^2(E-V_s)]} \qquad (4)$$

where α=1/137 is the fine-structure constant, $\xi(j,\ell) = \ell/2$ for $j = \ell+1/2$ and $\xi(j,\ell) = -(\ell+1)/2$ for $j = \ell - 1/2$, ℓ is the orbital momentum and j is the total angular momentum of one electron.

$V_e(r,E)$ is the local exchange potential in the free electron gas approximation (see, e.g., [7] and references therein).

The polarization potential is:

$$V_p(r) = -\alpha_d\left\{1-\exp\left[-(r/d)^6\right]\right\}/2r^4 \qquad (5)$$

where α_d is a dipole polarizability and d is an adjustable parameter.

The dipole polarizability α_d =167.84 a_0^3 and the ionization potential I = 6.354 eV for the Yb atom were obtained from the density functional theory [7,8].

Similarly to [7], the variable phase method [9,10] is used to find the partial phaseshifts $\delta_\ell(E)$ and to study the bound states.

1. Quasibound $^2P_{1/2}$-state. Having taken d=5.08a_0 for V_p and solved the phase equation [9] for ℓ=1 and j=1/2 at E=1 meV we have obtained four leaps by π and the phase shift δ_1=12.57 rad ≅ 4π in the phase function $\delta_1(r)$ behaviour. The calculation of the energy dependence $\delta_1(E)$ showed that $\delta_1 \to 4\pi$ at $E \to 0$. Since the Yb atom has four filled p-subshells (2p, 3p, 4p and 5p) and the additional electron, according to the Pauli's principle, can be bound with the atom only in the unfilled subshell, one may conclude that no bound p-state exists in the $V_1 \equiv V(d=5.08a_0)$ potential (1). The calculation of the energy dependence $\delta_1(E)$ for j=1/2 with the use of V_1 gave a rapid increase of the phaseshift δ_1 from 4π to 5π within the E=5÷43 meV energy range and at 21 meV δ_1=14.08 rad ≅ 4π+π/2. Hence, for V_1 we deal with the $^2P_{1/2}$-shape resonance at 21 meV. The calculation of $\delta_1(E)$ for j=3/2 resulted in the $^2P_{3/2}$-shape resonance at 69 meV.

2. Bound $^2P_{1/2}$-state. The numerical solution of the phase equation with $V_2 \equiv V(d=4.8a_0)$ for ℓ=1 and j=1/2 at low energy gives 5 leaps by π in the phase function $\delta_1(r)$, whereas the calculation of the energy dependence $\delta_1(E)$ shows that $\delta_1 \to 5\pi$ at $E \to 0$. Hence, five p-bound states are possible in the V_2 potential, only fifth of wich (6p) being the "true" bound state. Thus, the reduction of the parameter d from 5.08a_0 to 4.8a_0 gives us more effective potential enabling the quasibound $^2P_{1/2}$-state to be "drawn" into the bound state, i.e. to the discrete spectrum.

In the phase function method for the states with negative energies the so-called pole equation has been obtained [10]:

$$\frac{d}{dr}\gamma_\ell(r,\chi) = -\frac{2V(r)}{\chi}\left\{i_\ell(\chi r)\cos\gamma_\ell(r,\chi) + \frac{2}{\pi}[k_\ell(\chi r)\sin\gamma_\ell(r,\chi)]\right\}^2 \qquad (6)$$

where $\gamma_\ell(r,\chi)$ is the pole function, $\chi^2=-2\varepsilon$, ε is the energy of the bound state in the potential V, i_ℓ and k_ℓ are Riccati-Bessel functions of imaginary argument. Equation (6) is solved subject to the boundary condition $\gamma_\ell(0,\chi)=0$.

If $\varepsilon_1,\ldots,\varepsilon_5$, $\varepsilon_1>\varepsilon_2>\ldots>\varepsilon_5$, are the energies of the above mentioned bound states in V_2, then the function γ_ℓ satisfies the conditions:

$$\gamma_\ell(\infty,\chi_n) = \frac{1}{2}(2n+1)\pi\ , \qquad \chi_n^2 = -2\varepsilon_n\ . \ (7)$$

We adjust the parameter d=4.8a_0 to have the additional bound 6p-state with j=1/2 and with the energy ε_5 =–54 meV in the potential V_2. In other words we adjust d so that equation (6) has the solution $\gamma_1(r,\chi)$ at $\chi=\chi_5$ that satisfies the condition

$$\gamma_1(\infty,\chi_5) = \frac{11}{2}\pi\ ,\ \ \frac{1}{2}\chi_5^2 = -\varepsilon_5\ . \quad (8)$$

Similarly to [2] we have obtained the $^2P_{3/2}$ state to be quasibound, namely a resonance one at 7 meV.

The potential $V^+=V_s^+ + V_p$, where $V_s^+ = -V_s$, is used to investigate the bound states of e^++Yb system.

The obtained energy dependences of the partial phaseshifts for elastic positron scattering by the Yb atoms , show that at $E \to 0$ the s-wave phaseshift tends to π, unlike the p-wave and d-wave phaseshifts. Hence, the e^++Yb system has at least one bound state, namely s-bound state. Since the ionization potential I=6.354 eV for Yb atom is less than the energy of the positronium formation (6.8 eV), we conclude (similarly to the case of the positron-alkali system [11]), that bound e^+Yb-state exists at negative energies below the Yb^+-positronium continuum. We have found that the condition $\gamma_0(\infty,\chi_1) = 3\pi/2$ for V^+ with $d = 4.8a_0$ is satisfied at the $\varepsilon_1 = -\chi_1^2/2 = -205$ meV energy and for V^+ with $d = 5.08a_0$ it is satisfied at the $\varepsilon_1 = -130$ meV energy (see Table 1).

Table 1. The pole function $\gamma_0(\infty,\chi_1)$.

γ_0 (rad)	$-\varepsilon_1$ (meV)	
	d=5.08a_o	d=4.8a_o
1.571	132	207
1.571	131	206
4.712	130	205
4.712	129	204

Hence, investigation of the bound states of $e^{\pm}$+Yb system within the both above mentioned assumptions of $^2P_{1/2}$-state of Yb atom confirms the existence of the bound s-state of e^++Yb-system at energies less than –100 meV.

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ПРО ЗВ'ЯЗАНИЙ СТАН СИСТЕМИ e^++Yb

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Із застосуванням феноменологічного оптичного потенціалу досліджені зв'язані стани $e^{\pm}$+Yb системи в околі порога каналу пружнього розсіювання. Встановлено, що зв'язаний s-стан e^++Yb системи існує при енергіях менших за –100 меВ.