POSITRON ANNIHILATION IN THE e^+ Li *SYSTEM*

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The e^+ Li atomic system is investigated by a variational method. A positron binding energy of ~ 2.13 eV and a positron lifetime against annihilation by an optical electron of Li of 3.2×10^{-10} sec are obtained. The last value agrees precisely with the one found experimentally by Bell and Jørgensen.[6]

1. INTRODUCTION

In recent years, methods using positrons have found widespread application in solid state theory, chemical kinetics, and several other fields. In this connection, a number of papers have appeared in which the interaction of positrons with atomic and molecular systems is investigated theoretically.[1-3] The most thorough study has been made of the annihilation of positrons in the system negative ion–positron,[4] where the Hartree-Fock method has proved convenient. Of the systems positron–neutral atom, only the case of hydrogen has been investigated.[1,3,5]

In the present paper we study the properties of the system Li atom–positron. The ground state energy of the system is determined by the variational method. Then the probability for annihilation of the positron with the optical electron is calculated using the variational wave functions. The calculations lead to a binding energy of the positron in Li of 2.13 eV. The lifetime of the e^+Li system against two-photon annihilation of the positron is found to be $\sim 3.2 \times 10^{-10}$ sec, which almost precisely agrees with the experimental value obtained by Bell and Jørgensen.[6]

2. THEORY

The stationary state of an atomic system consisting of n electrons and one positron is described by a Schrödinger equation with a Hamiltonian given by

$$H = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 - \sum_{i=1}^{n}\frac{Z}{r_i} + \frac{Z}{r_k} + \frac{1}{2}\sum_{i,\,j=1}^{n}{}' \frac{1}{r_{ij}} - \sum_{i=1}^{n}\frac{1}{r_{ik}}. \quad (1)$$

Here $N = n + 1$, Z is the charge of the nucleus, and the prime at the summation sign indicates that the term with $i = j$ is omitted.

For a system alkali metal + positron it is natural to divide H into the following parts:

$$H = H_0 + H_c + H_{0c}, \quad (2a)$$

where H_0 is the Hamiltonian of the core,

$$H_0 = -\frac{1}{2}\sum_{i=1}^{N-2}\nabla_i^2 - \sum_{i=1}^{N-2}\frac{Z}{r_i} + \frac{1}{2}\sum_{i,\,j=1}^{N-2}{}'\frac{1}{r_{ij}}, \quad (2b)$$

H_c is the Hamiltonian for the coupled system outer electron + positron,

$$H_c = -\frac{1}{2}\sum_{c=1}^{2}\nabla_c^2 - \frac{Z}{r_1} + \frac{Z}{r_2} - \frac{1}{r_{12}}; \quad (2c)$$

and H_{0c} is the interaction of the outer electron and positron with the electrons of the core. Here r_1, r_2 denote the distance from the outer electron and the positron to the nucleus (at the origin), and r_{12} denotes the relative distance of the two.

In the calculation of the energy of this system we shall neglect the polarization of the atomic core caused by the outer electron and the positron, and consider the motion of the outer particles in a self-consistent field formed by the nucleus and the electrons of the core. With these assumptions the wave function Ψ is given in the form

$$\Psi = \psi_{\text{core}}\psi_c, \quad (3)$$

where ψ_{core} refers to the core electrons and ψ_c to the outer electron and the positron. The functions ψ_{core} and ψ_c (and hence, Ψ) are assumed normalized. Thus the Schrödinger equation for the system under consideration can be written in the form

$$(H_0 + H_c + H_{0c})\psi_{\text{core}}\psi_c = E\psi_{\text{core}}\psi_c. \quad (4)$$

Applying the variational method to (4) and taking into account that the operator H_{0c} acts only on the function ψ_K we find

$$E = (\psi_{\text{core}}\psi_c, H_0\psi_{\text{core}}\psi_c) + (\psi_{\text{core}}\psi_c, [H_c + H_{0c}]\psi_{\text{core}}\psi_c). \quad (5)$$

Using the normalization of the functions ψ_{core} and ψ_c, we rewrite (5) in the form

$$E = (\psi_{\text{core}}, H_0\psi_{\text{core}}) + (\psi_c, [H_c + H_{0c}]\psi_c), \quad (6)$$

i.e.,

$$E = E_{\text{core}} + E_c.$$

3. BINDING ENERGY OF THE POSITRON IN THE e^+Li SYSTEM

Let us determine the energy of the ground state of the e^+Li system with the configuration $1s^2 2s(2s)$ (the symbol in parentheses refers to the state of the positron). According to (6) we can write

$$E(e^+\text{Li}) = E(\text{Li}^+) + E_c(e^-e^+). \quad (7)$$

E_c is defined by the equation

$$(H_c + H_{0c})\psi_c = E_c\psi_c, \quad (8a)$$

where

$$H_c + H_{0c} = -\frac{1}{2}\sum_{k=1}^{2}\nabla_k^2 - \frac{Z}{r_1} + \frac{Z}{r_2} - \frac{1}{r} + V_1(r_1) - V_2(r_2).$$

$$V_m(r_m) = 2\int_0^\infty f^2(r')K_0(r_m, r')\,dr', \quad m = 1, 2,$$

$$K_0(r_m, r')\begin{cases} 1/r_m & \text{for} \quad r' < r_m \\ 1/r' & \text{for} \quad r_m < r' \end{cases} \quad (8b)$$

and $f(r)/r$ is the radial wave function of the core electrons, which is taken in the form of a hydrogen-like function. $f(r)$ satisfies the normalization condition

$$\int_0^\infty f^2(r)\,dr = 1. \quad (9)$$

Equation (8a) is an integro-differential equation of second order. It can be solved by the variational method if $f(r)$ is known and an appropriate trial function for ψ_c is chosen. In the actual calculations, $f(r)$ and ψ_c were taken of the form

$$f(r) = 2a^{3/2}re^{-ar}, \quad a = Z - {}^5/_{16}; \quad (10a)$$

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = M\Phi(\mathbf{r}_1, \mathbf{r}_2) = Mr_2^l \exp[-\xi(r_1 + r_{12})]; \quad (10b)$$

l and ξ are parameters, and M is a normalization factor defined by

$$M^{-2} = \int |\Phi(\mathbf{r}_1, \mathbf{r}_2)|^2\, dr_1^3\, dr_2^3. \quad (10c)$$

Setting $l = 2$, we obtain the energy (6) as a function of the parameter ξ after quite involved calculations. The computation of $E_{c\,\min}$ and the corresponding value of the parameter ξ was carried out on the electronic computer Minsk-2. The values obtained are

$$\xi = 0.602, \qquad E_c = -0.275415 \text{ at. un.}$$

In order to find the binding energy of the positron $\epsilon(e^+)$ we used the relation $\epsilon(e^+) = E(\text{Li}) - E(e^+\text{Li})$. Since the binding energy of the outer electron in Li is equal to 0.197 at. un. (in the Hartree-Fock method[7]), we obtain $\epsilon(e^+) = 0.0784$ at. un. or 2.13 eV. We note that Ore[1] has shown, under several assumptions, that only ions with $n > Z$ form bound systems with a positron (n is the number of electrons, Z is the number of protons). Our result leads us to assert that a bound system is also possible for $n = Z$.

It is known[5] that the system e^+H is unstable against decay into a hydrogen atom and a positron. The system e^+Li considered in this paper differs from the system e^+H only in that the outer electron and the positron move in the self-consistent field formed by the nucleus and the core electrons. This has the effect that the system is stable against decay into a neutral Li atom and a positron. On the other hand, the system e^+Li is also stable against decay into a positive Li ion and positronium. Indeed, the energy of the system Li^+ + positronium, which would result from such a decay, is

$$-6.78\text{ eV} + 5.39\text{ eV} = -1.39\text{ eV} > -2.13\text{ eV}$$

(5.39 eV is the ionization energy of Li). This does not, of course, exclude the possibility of the process

$$\text{Li} + e^+ \rightarrow \text{Li} + \text{positronium} + 1.39\text{ eV}.$$

4. ANNIHILATION OF POSITRON

The annihilation of the positron has been investigated in detail mainly in the case of free electrons and positrons[8] without account of their mutual interaction. Yuan Li[9] has considered positron annihilation in a system consisting of n electrons and one positron and obtained a formula which permits the calculation of the probability for the two-photon annihilation of the positron with one of the electrons. The probability per unit time is

$$W = \frac{k^2}{4\pi}|(\Omega_n, H'\Omega_0)|^2 \quad (11)$$

where Ω_0, Ω_n are the wave functions of the initial and final states, H' is the Hamiltonian of the interaction of the particles with the radiation field, and k is the momentum of the photon.

In our case we consider only the two-photon annihilation of the positron with the outer electron and neglect the effect of the annihilation of the pair on the core wave function, so that the wave functions have the form

$$\Omega_0 = \Psi_{\delta_3\delta_4\delta_1\gamma_2}(\mathbf{r}_3, \mathbf{r}_4, \mathbf{r}_1, \mathbf{r}_2) = \psi_{\text{core}}\psi S(\delta_3\delta_4\delta_1\gamma_2), \quad (12a)$$

$$\Omega_n = \Psi_{\delta_3\delta_4}(\mathbf{r}_3, \mathbf{r}_4) = \psi_{\text{core}} S(\delta_3\delta_4). \quad (12b)$$

Here δ_3, δ_4, and δ_1 denote the spin states of the core and outer electrons, and γ_2 labels the spin of the positron. According to the formula of Yuan Li, we have

$$(\Omega_n, H'\Omega_0) = -\frac{\pi e^2\sqrt{2}}{km}\sqrt{n}\int \psi^*_{\text{core}}S^*(\delta_3\delta_4)\exp[-i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{r}_2]$$
$$\times (K_{\gamma_2\delta_1} - K_{\delta_1\gamma_2})\psi_{\text{core}}\,\psi(\mathbf{r}_2, \mathbf{r}_2) S(\delta_3\delta_4\delta_1\gamma_2)\, dr_3^3 dr_4^3 dr_2^3. \quad (13)$$

The integral sign in (13) implies integration over the space coordinates as well as summation over the spins.

Separating out the spin part in (13), we have

$$(\Omega_n, H'\Omega_0) = -\frac{\pi e^2\sqrt{2}}{km}\sqrt{n}\,\rho\int \exp[-i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{r}_2]$$
$$\times\ \psi^*_{\text{core}}\psi_{\text{core}}\psi(\mathbf{r}_2, \mathbf{r}_2)\, dr_3^3 dr_4^3 dr_2^3,$$

$$\rho = S^*(\delta_3\delta_4)(K_{\gamma_2\delta_1} - K_{\delta_1\gamma_2})S(\delta_3\delta_4\delta_1\gamma_2). \quad (14)$$

Here $S(\delta_3\delta_4)$ is a function of a system of two particles with spin $\frac{1}{2}$; in the para-state it has the form of a matrix

$$S(\delta_3\delta_4) = \begin{pmatrix} 0 & 2^{-1/2} \\ -2^{-1/2} & 0 \end{pmatrix}. \quad (15)$$

$S(\delta_3\delta_4\delta_1\delta_2)$ is a function of a system of four particles with spin $\frac{1}{2}$. According to the theory of the coupling of angular momenta,[10] we have, taking account of the fact that the Clebsch-Gordan coefficient is equal to unity for the para-state,

$$S(\delta_3\delta_4\delta_1\gamma_2) = \begin{pmatrix} 0 & 2^{-1/2} \\ -2^{-1/2} & 0 \end{pmatrix}\begin{pmatrix} 0 & 2^{-1/2} \\ -2^{-1/2} & 0 \end{pmatrix}. \quad (16)$$

After some computation we obtain for ρ the expression

$$\rho = -im^{-1}\mathbf{k}(\mathbf{e}_1\mathbf{e}_2). \quad (17)$$

Taking out the matrix element for free positronium we obtain from (14) and (17)

$$(\Omega_n, H'\Omega_0) = -(\Omega_n, H'\Omega_0)_{\text{pos}}\sqrt{n}$$
$$\times\frac{\sqrt{8\pi}}{2}\int \exp[-i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{r}_2]\psi^*_{\text{core}}\psi_{\text{core}}\psi(\mathbf{r}_2, \mathbf{r}_2)\, dr_3^3 dr_4^3 dr_2^3. \quad (18)$$

It is known that the probability for the two-photon annihilation is largest for $|\mathbf{k}_1+\mathbf{k}_2| = 0$. Using (11) and (18), summing over the photon polarizations, and taking account of the normalization of ψ_{core}, we obtain with the help of (10b)

$$W = W_{\text{pos}}\cdot 2\pi n M^2\int|\Phi(\mathbf{r}_2, \mathbf{r}_2)|^2 dr_2^3. \quad (19)$$

Finally, for $l = 2$, $\xi = 0.602$ we have after some computation

$$W / W_{\text{pos}} = {}^9/_5\xi^3 \approx 0.392. \quad (20)$$

The lifetime of positronium against annihilation is well known. If the positron is bound in an atomic system, one must sum over the annihilation probabilities of the positron with the electrons in different states, and the reciprocal of this sum gives the lifetime of the positron in the system. Since the annihilation probability of the positron with the electrons of the core is much smaller than the annihilation probability with the optical electron, the lifetime τ is equal to

$$\tau = W^{-1} = \tau_{\text{pos}}/0.392. \quad (21)$$

Using $\tau_{\text{pos}} = 1.25 \times 10^{-10}$ sec, we find $\tau = 3.18 \times 10^{-10}$ sec. This value for the lifetime agrees with the experimental value of Bell and Jørgensen:[6] $\tau \approx (2.9 \pm 0.2) \times 10^{-10}$ sec. We note that our value of τ for e^+Li is somewhat larger than the lifetime of the positron against annihilation in the system e^+H, as calculated in [3]. This is in agreement with the experimentally observed[6] increase of τ with Z.

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