

Beyond the Point Ps Approximation

Sergey V. Stepanov^{1,a}, Dmitry S. Zvezhinskiy¹, Vsevolod M. Byakov^{1,2}

¹Institute of Theoretical and Experimental Physics, B.Chermushkinskaya 25, 117218 Moscow, Russia

²D.Mendeleyev University of Chemical Technology, Miusskaya sq., 9, Moscow 125047, Russia

^astepanov@itep.ru

Keywords: pick-off annihilation, positronium bubble model, non-point Ps, contact density

Abstract. In application to positron annihilation spectroscopy, Ps atom is considered not as a point particle, but as a finite size e^+e^- pair localized in a bubble-like state in a medium. It is shown that during transition from quasifree to localized state, variation of the internal Coulombic e^+e^- attraction energy (several eV) plays an important role, which may govern Ps localization process.

Introduction

Typical lifetimes (up to annihilation) of a para-positronium atom (p-Ps; spin = 0) in condensed medium are about 130-180 ps. They are close to the p-Ps lifetime in vacuum (125 ps). The ortho-positronium lifetime in a medium is considerably shorter than that in vacuum (some ns). This is due to the so-called pick-off process -- prompt 2γ -annihilation of the e^+ , composing Ps atom, with one of the nearest e^- of surrounding molecules, whose spin is antiparallel to the e^+ spin. Just this property turns Ps into a nanoscale structural probe of matter. The theoretical task consists in establishing relation between the observable pick-off annihilation rate λ_{po} and size of the Ps trap and such properties of the medium like surface tension, viscosity, external pressure.

Originally, to explain the unexpectedly long lifetime of the ortho-Ps atom in liquid helium R.Ferrel [1] suggested that the Ps atom forms a nanobubble around itself. This is caused by a strong exchange repulsion between the o-Ps electron and electrons of the surrounding He atoms. Ferrel approximated this repulsion by a spherically symmetric potential barrier of radius R_∞ . To estimate the equilibrium radius of the Ps bubble he minimized the sum of the Ps energy in a spherically symmetric potential well, i.e. $\pi^2\hbar^2/4mR_\infty^2 = \frac{R_y}{2}(\pi a_B/R_\infty)^2$, $R_y=13.6$ eV, and the surface energy, $4\pi R_\infty^2\sigma$, where σ is the macroscopic surface tension coefficient. The following relationship is hereby obtained for the equilibrium radius of the bubble:

$$\frac{\pi^2 a_B^2}{R_\infty^2} R_y + 4\pi R_\infty^2 \sigma \leftrightarrow \min \text{ over } R_\infty \Rightarrow R_\infty = a_B \left(\frac{\pi R_y}{8\sigma a_B^2} \right)^{1/4}. \quad (1)$$

Ferrel's idea got further development in the studies of Tao [2] and Eldrup et al. [3]. They considered the Ps atom as a point particle in a liquid, i.e. in a structureless continuum. The repulsive Ps-liquid interaction was approximated by a rectangular infinitely deep spherically symmetric potential well of radius R_∞ . In such a well, the wave function of a point particle has the following standard expression:

$$\Psi(0 \leq r \leq R_\infty) = \frac{\sin(\pi r/R_\infty)}{\sqrt{2\pi R_\infty} r}, \quad \Psi(r \geq R_\infty) = 0. \quad (2)$$

Here, r is the Ps center-of-mass coordinate. Because the Ps wave function equals to zero at the bubble radius (and outside), there is no e^+ overlapping with outer electrons of a medium. So, pick-off annihilation is absent. To overcome this difficulty it was postulated that molecular electrons, which form a "wall" of the Ps bubble, may penetrate inside the potential well.

This results in the appearance of a surface layer of thickness $\delta = R_\infty - R$ having the same average electron density as in the bulk. As a result, the pick-off annihilation rate λ_{po} becomes non-zero. It is proportional to the e^+ overlapping integral with the electrons inside the bubble:

$$\lambda_{po} = \lambda_+ P_R, \quad P_R = \int_R^{R_\infty} |\Psi(r)|^2 4\pi r^2 dr = \frac{\delta}{R_\infty} - \frac{\sin(2\pi\delta/R_\infty)}{2\pi}. \quad (3)$$

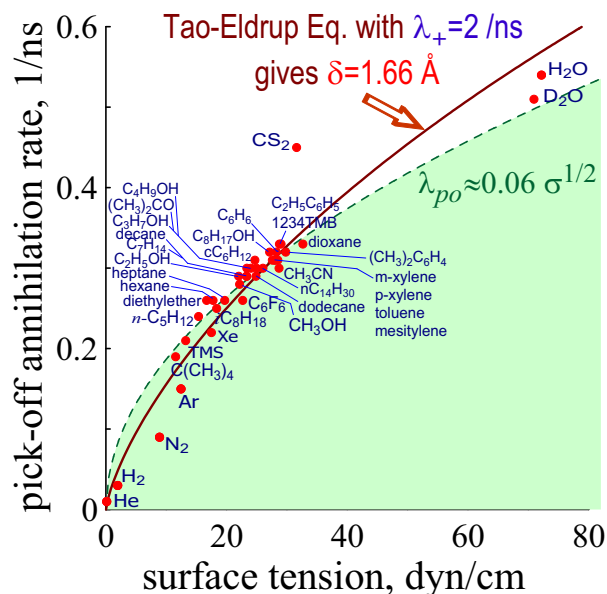


Fig. 2: Dependence of the pick-off annihilation rates [8] vs. surface tension in different liquids. Solid curve shows the correlation given by the Tao-Eldrup at $\lambda_+ = 2 \text{ ns}^{-1}$ and optimal value $\delta = 1.66 \text{ \AA}$ (obtained from fitting of these data by means of Eq. (3)). Dashed curve illustrates simplest approximation $\lambda_{po} \propto \sigma^{1/2}$. It follows from reasonable approximation $\frac{\sin x}{x} \Big|_{x < 4} \approx 1 - x/\pi$, which allows to write $\lambda_{po} \propto \delta/R_\infty - \frac{\sin(2\pi\delta/R_\infty)}{2\pi} \approx 2\delta^2/R_\infty^2 \propto \sigma^{1/2}$.

the Coulombic e^+e^- attraction energy), which is completely ignored in the "point-like" Ps models. In a vacuum or in a large bubble, the internal energy of Ps tends to $-Ry/2 = -6.8 \text{ eV}$. In a continuous liquid (no bubble) with the high-frequency dielectric permittivity $\epsilon \approx n^2$ ($n \approx 2-3$ is the refractive index) the energy of the Coulombic attraction between e^+ and e^- decreases in absolute value by a factor $\epsilon^2 \approx 4-9$. The same takes place with the total Ps binding energy, which tends to the value $-Ry/2\epsilon^2 \approx -(0.8-1.7) \text{ eV}$ (this is a simple consequence of the scaling $e^2 \rightarrow e^2/\epsilon$ of the Schrödinger equation for Ps atom). Thus, the change in the Ps internal energy during Ps formation may reach 5 eV. Obviously, this represents an important contribution to the energetics of Ps formation. The aim of the present work is to proceed with more accurate estimation of this contribution, which has not been done yet.

There is only a small number of papers where the consequences of the finite size of Ps are discussed in application to positron annihilation spectroscopy. To calculate λ_{po} , the Kolkata group [9] suggested to smear the Ps atom over the relative e^+e^- coordinate exactly in the same way as it is in a vacuum. Such an approach is valid for rather large bubbles. However, they do not discuss the variation of the internal Ps energy.

This is the well-known Tao-Eldrup formula. Here, $\lambda_+ \approx 2 \text{ ns}^{-1}$ is the e^+ annihilation rate in an unperturbed medium (it is proportional to Dirac's 2γ -annihilation cross-section and the number density of valence electrons). The thickness δ of the electron layer is an empirical parameter, which may have different values in various media. Substituting Eq. (1) for R_∞ into Eq. (3), one obtains the relationship between λ_{po} and σ with one adjustable parameter, δ . It may be easily obtained by fitting experimental pick-off annihilation rates with the relationship (3), Fig. 2. Thus we obtain $\delta \approx 1.66 \text{ \AA}$. Eq. (3) with this value of δ is widely used for recalculation of the observed pick-off annihilation rate into the free volume $4\pi R^3/3$ of the cavity, where Ps atom resides and annihilates.

Along with the development of the "infinite potential well" Ps bubble model, another approach based on the finite potential well approximation was also elaborated [4--8]. However in both approaches, the Ps atom was approximated by a point particle. This leads to a significant simplification, but it is not justified from a physical viewpoint, because:

- 1) the size of the localized state of Ps (size of the Ps bubble) does not significantly exceed the distance between e^+ and e^- in Ps;
- 2) during Ps bubble formation takes place a substantial variation of the internal energy of Ps (namely,



In [10--12] there was used path integral Monte Carlo technique to simulate two particle e^+e^- system. However, to proceed with calculations they need potentials describing e^- -atom and e^+ -atom interactions (they were taken from a variety of sources). However, the question about modification of e^+e^- interaction because of the presence of the medium remains open (in this paper we roughly take this effect into account by means of introducing high frequency dielectric permittivity).

In [13] the Ps atom is considered as a finite sized e^-e^+ pair, but the variation of the Coulombic interaction because of dielectric screening is not discussed. It was assumed that e^- is confined in an infinite potential well and e^+ is bound to it due to the Coulombic attraction. The wave function of the pair was taken as a series of orthogonal polynomials, their weights being determined from a minimization procedure of the total energy of the pair.

Hamiltonian and wave function of the e^+e^- pair in a medium. Minimization of the total energy $\langle H \rangle$. Relative contact density and pick-off annihilation rate

Let the e^+e^- pair (Ps atom) have already formed in a liquid a nanobubble (spherical cavity; Ps bubble) of radius R (the onset of coordinates is taken at the center of the bubble, Fig. 3). Together with the molecules surrounding the e^+e^- pair, one has to deal with a quite intricate many-body problem with a complex hamiltonian. We reduce it to the following form:

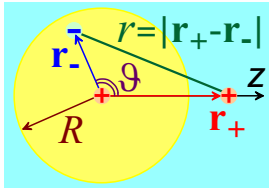


Fig. 3:

$$H \approx -\frac{\hbar^2(\Delta_+ + \Delta_-)}{2m_e} + U(\mathbf{r}_+) + U(\mathbf{r}_-) - U_c(\mathbf{r}_+, \mathbf{r}_-, R, \varepsilon). \quad (4)$$

Terms with Laplacians Δ_+ and Δ_- over \mathbf{r}_+ and \mathbf{r}_- (e^+ and e^- coordinates) stand for the kinetic energies of the particles. $U(\mathbf{r}_+)$ and $U(\mathbf{r}_-)$ describe the individual interaction of e^+ and e^- with the medium. For them we adopt the following approximation:

$$U(r_+) = \begin{cases} 0, & r_+ < R, \\ V_0^+, & r_+ > R, \end{cases} \quad U(r_-) = \begin{cases} 0, & r_- < R, \\ V_0^-, & r_- > R. \end{cases} \quad (5)$$

Here, V_0^+ and V_0^- are the e^+ and e^- work functions, respectively (V_0 is a commoner notation for the electron work function). The work function is usually introduced as the energy needed for an excess particle to enter the liquid without any rearrangement of its molecules and to stay there in a delocalized state, having no preferential location in a bulk. One may say that V_0^+ and V_0^- are the ground state energies of the quasifree e^+ and e^- , because their energies at rest after having been removed from the liquid to infinity are defined to be zero.

V_0^- consists of 1) the e^- kinetic energy, arising from its exchange repulsion from the "core" electrons of molecules (atoms), and 2) the energy due to the polarization interaction of e^- with the medium.

¹ According to the theory of the quasifree electron [14], this polarization interaction may be estimated as a sum of two parts: a) interaction of the e^- with the molecule where it resides, U_-^{int} (to calculate U_-^{int} the electron is considered as an electron cloud smeared over the molecule), and b) interaction of the e^- with all the other molecules, $U_-^{out} = (1 - 1/\varepsilon)e^2/2R_{WS}$, (this expression is similar to the well-known Born formula for the electron solvation energy).

¹ In case of e^+ the kinetic contribution to V_0^+ is due to the Coulombic repulsion from the nuclei (the exchange repulsion is absent).

Table 1: Electron work function for different liquids at room temperature [15]

Liquid	V_0^- , eV	Liquid	V_0^- , eV
helium; 4.2 K	1.3	benzene	-0.14
n-dodecane	0.2	isooctane	-0.17
n-decane	0.18	toluene	-0.22
n-heptane	0.12	neopentane	-0.38
n-hexane	0.1	MeOH, EtOH, PrOH	-0.4
nitrogen; 77.3 K	0.05	xenon; 170 K	-0.57
n-pentane, c-hexane	0.01	water	-1.2
argon; 86.4 K	0		

Experimental values for V_0^- are known for many liquids (Table 1). Because of a lack of the data for e^+ work functions, we shall admit that $V_0^+ \approx V_0^-$ and therefore $|V_0^+ + V_0^-| \lesssim 1$ eV. So $|V_0^+ + V_0^-|$ is less than the variation of the internal energy of the pair, $\approx \text{Ry}(1 - 1/\varepsilon^2)/2 \approx 5$ eV, related with the variation in the dielectric screening of the e^+e^- attraction in the bubble formation process. The case $V_0^+ > V_0^-$ will be considered later on.

Usage of Eqs. (4-5) implies that polarization interactions of the e^+ and e^- with the medium remains same either e^+ and e^- are well separated (being in the quasifree states), or when e^+ and e^- form the quasifree Ps atom (qf-Ps). Since qf-Ps is nearly an electrically neutral particle, the contributions $U_-^{\text{out}} \approx U_+^{\text{out}}$, which come from a long-range polarization interaction of e^+ and e^- with the medium, should be subtracted from the sum $U(r_-) + U(r_+)$ in Eq. (4). Therefore, it is reasonable to consider at least two cases: 1) when the above mentioned polarization correction is neglected and $V_0^- + V_+ \rightarrow 0$ and 2) when the terms $U_-^{\text{out}} \approx U_+^{\text{out}} \approx -1$ eV are subtracted from the work functions and therefore $V_0^- + V_0^+ \rightarrow 2$ eV. Both cases are considered below.

In Eq. (4) U_c stands for the Coulombic interaction between e^+ and e^- in a polarizable medium. Assuming that the medium has the dielectric permittivity ε of the bulk and a spherical cavity of radius R (inside the cavity $\varepsilon = 1$), one may calculate U_c by solving the Poisson equation. Denoting the e^+ and e^- coordinates as \mathbf{r}_+ and \mathbf{r}_- , U_c may be written in the form of the following series via the Legendre polynomials $P_l(x = \cos \theta)$ [16]:

$$\begin{aligned}
\frac{U_c(r_+ < R, r_- < R)}{\text{Ry}} &= \frac{2a_B}{r} - \left(1 - \frac{1}{\varepsilon}\right) \frac{2a_B}{R} \left(1 + \sum_{l=1}^{\infty} \frac{(1+l)P_l(x)}{1+l+l/\varepsilon} \cdot \frac{r_+^l r_-^l}{R^{2l}}\right); \quad (6) \\
\frac{U_c(r_+ < R, r_- > R)}{\text{Ry}} &= \frac{2a_B}{\varepsilon r_-} \left(1 + \sum_{l=1}^{\infty} \frac{(1+2l)P_l(x)}{1+l+l/\varepsilon} \cdot \frac{r_+^l}{r_-^l}\right); \\
\frac{U_c(r_+ > R, r_- < R)}{\text{Ry}} &= \frac{2a_B}{\varepsilon r_+} \left(1 + \sum_{l=1}^{\infty} \frac{(1+2l)P_l(x)}{1+l+l/\varepsilon} \cdot \frac{r_-^l}{r_+^l}\right); \\
\frac{U_c(r_+ > R, r_- > R)}{\text{Ry}} &= \frac{2a_B}{\varepsilon r} + \left(1 - \frac{1}{\varepsilon}\right) \frac{2a_B}{R} \sum_{l=1}^{\infty} \frac{lP_l(x)}{l+\varepsilon+l\varepsilon} \cdot \left(\frac{R^2}{r_+ r_-}\right)^{l+1}.
\end{aligned}$$

Here, the argument of the Legendre polynomials is $x \equiv \cos \vartheta$, where ϑ is the angle between the z axis and the direction of \mathbf{r}_- . Note that the summation of these series is simplified considerably when using the following recurrent relationship ($P_0 = 1$, $P_1 = x$)

$$P_l(x) = [(2l-1)xP_{l-1}(x) - (l-1)P_{l-2}(x)]/l.$$

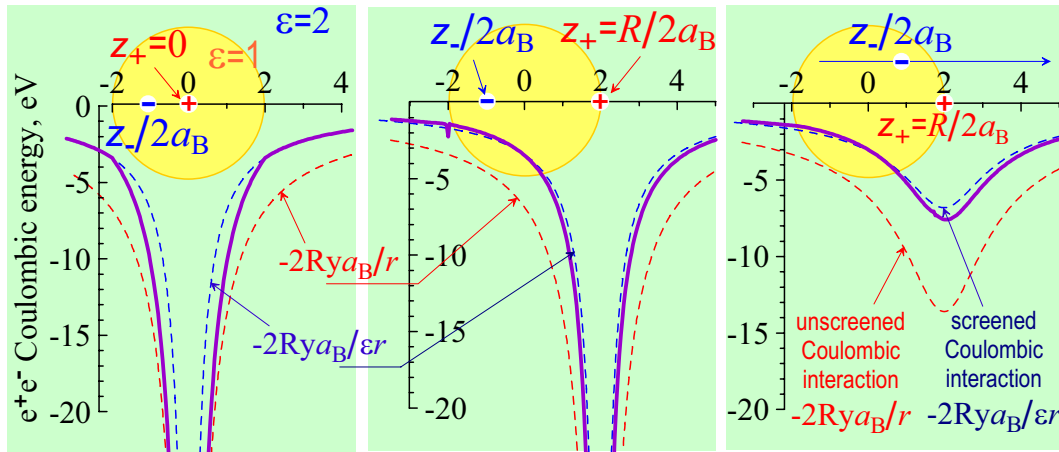


Fig. 4: Dependence of the e^+e^- Coulombic interaction energy for different locations of e^+ and e^- around the bubble (here we adopt the radius of the bubble R equal to $4a_B \approx 2 \text{ \AA}$). z_+ and z_- are the e^+ and e^- displacements from the center of the bubble along the z -axis. The dashed curves describe the unscreened (red) and completely screened (ϵ times less; blue) Coulombic energies between e^+ and e^- .

Particular dependencies of U_c for some selected arrangements of e^+ and e^- and the cavity are shown in Fig. 4. Thus, we are able to take into account the variation of the e^+e^- Coulombic energy during the formation of the Ps bubble. Similarly, the dielectric screening is used in the polaron problem and the ion-electron recombination problem (Onsager's formula) [17, 18].

Keeping in mind further use of the variational procedure, let us choose the normalized e^+e^- wave function in the following simplest form:

$$\Psi_{+-}(\mathbf{r}_+, \mathbf{r}_-) = \frac{\exp(-r/2a - r_{cm}/2b)}{8\pi\sqrt{a^3b^3}}, \quad \mathbf{r}_{cm} = \frac{\mathbf{r}_+ + \mathbf{r}_-}{2}, \quad \mathbf{r} = \mathbf{r}_+ - \mathbf{r}_-. \quad (7)$$

In both cases of a rather large bubble and a uniform dielectric continuum, Ψ_{+-} breaks into a product of two terms: the first one depends on the distance r between e^+ and e^- , and the second one depends on the center-of-mass coordinate \mathbf{r}_{cm} . Parameters a and b are the variational ones, over which we have minimized the energy of the e^+e^- pair:

$$E(a, b, R) = \langle \Psi_{+-} | H | \Psi_{+-} \rangle \rightarrow \min \Rightarrow a(R), b(R). \quad (8)$$

The simplest verification of the calculations is to recover two limiting cases. In case of large bubbles ($R \rightarrow \infty$), one should reproduce the "vacuum" state of the Ps atom: its total energy must tend to $-Ry/2 = -6.8 \text{ eV}$, the kinetic energy to $+Ry/2$ and the Coulombic energy to $-Ry$. In case of small bubbles ($R \rightarrow 0$), the delocalized qf-Ps state must be reproduced. The Schrödinger equation for qf-Ps has the same form as for the vacuum Ps, but with the substitution $e^2 \rightarrow e^2/\epsilon$. Then the total qf-Ps energy tends to $V_0^+ + V_0^- - Ry/2\epsilon^2$, its kinetic part tends to $+Ry/2\epsilon^2 = 1.7 \text{ eV}$ ($\epsilon = 2$) and the Coulombic energy tends to $-Ry/\epsilon^2 = -3.4 \text{ eV}$. Fig. 5 displays optimal values of a and b as well as different contributions to the total energy of the e^+e^- pair when $V_0^+ + V_0^- = 0$ and 2 eV .

In the framework of the developed scheme using the wave function (7) it is easy to obtain the relative contact density η_c in Ps atom:

$$\eta_c = \frac{\int \int d^3\mathbf{r}_+ d^3\mathbf{r}_- |\Psi_{+-}(\mathbf{r}_+, \mathbf{r}_-)|^2 \delta(\mathbf{r}_+ - \mathbf{r}_-)}{\int \int d^3\mathbf{r}_+ d^3\mathbf{r}_- |\Psi_{+-}^{vac}(\mathbf{r}_+, \mathbf{r}_-)|^2 \delta(\mathbf{r}_+ - \mathbf{r}_-)} = \frac{a_B^3}{a^3(R)}. \quad (9)$$

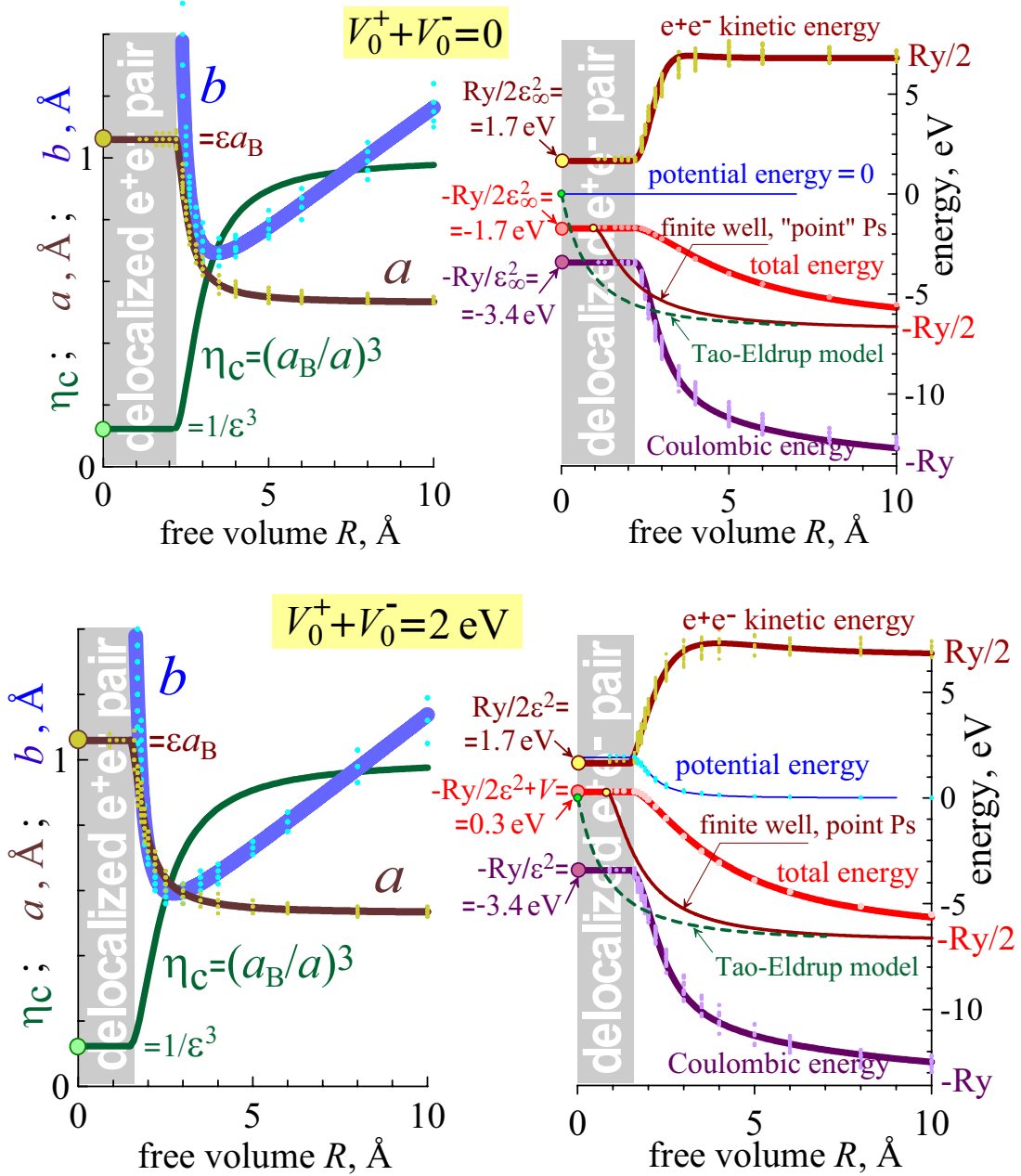


Fig. 5: Dependencies of the optimal parameters a and b vs. R , the bubble radius. They enter the e^+e^- wave function and yield the minimum of the total energy $\langle H \rangle$. The relative contact density η_c and different energy contributions to $\langle H \rangle$ (at optimal a and b) are shown as well. The upper drawings correspond to the case $V_0^+ + V_0^- = 0$ and the lower ones to $V_0^+ + V_0^- = 2$ eV. In both cases it was assumed that $\varepsilon = 2$.

This quantity determines the observable Ps annihilation rate constant (including the case with applied permanent magnetic field). The resulting dependencies of η_c are shown in Fig. 5 (on the left). Because, for qf-Ps, parameter a is equal to εa_B , for qf-Ps the value of η_c should be $1/\varepsilon^3 = 1/8$, which is well recovered in numerical calculations. When R increases, η_c approaches unity, because a tends to its vacuum value a_B . Knowing the expression for the wave function (7), one may calculate the positron overlapping P_R with molecular electrons, surrounding the Ps atom, and therefore find out the pick-off annihilation rate constant:

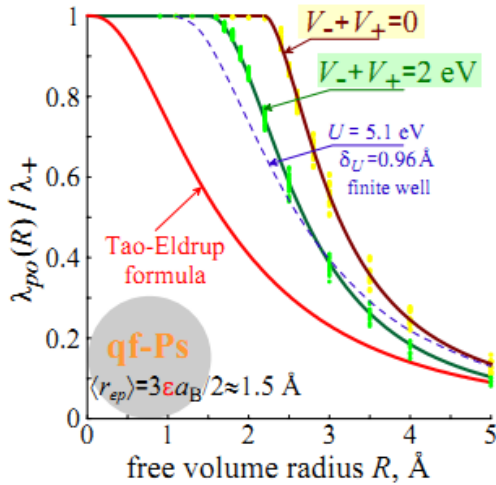


Fig. 6: Pick-off annihilation rate constant of Ps, localized in a bubble of R when $V_+ + V_- = 0$ (green curve) and $V_+ + V_- = 2$ eV (brown curve). For small R ($\lesssim 2$ Å) the calculated values of λ_{po} are equal to λ_+ . The red line shows pick-off annihilation rate constant, calculated according to the Tao-Eldrup formula. The dashed line is the calculation according to the finite potential well model (for comparison we adopted that the depth of the well is $(1 - 1/\epsilon^2)\text{Ry}/2 \approx 5.1$ eV and its radius is R . The minimal radius of the well when there appears an energy level is $\delta_U = 0.96$ Å).

$$\lambda_{po}(R) \approx \lambda_+ P_R, \quad P_R \approx \int_{r_+ > R} d^3 \mathbf{r}_+ \int d^3 \mathbf{r}_- |\Psi_{+-}(\mathbf{r}_+, \mathbf{r}_-)|^2. \quad (10)$$

Here, $\lambda_+ \approx 2 \text{ ns}^{-1}$ is the annihilation rate constant of "free" positrons. Results of calculations of $\lambda_{po}(R)$ for optimal a and b values, which correspond to the minimal Ps energy at a given R , are shown in Fig. 6.

Results and Conclusions

1) It is usually considered that Ps is a solvophobic particle, i.e., it forms a bubble when entering a liquid because of exchange repulsion between e^- in Ps and the surrounding molecular electrons. If the work functions of e^+ and e^- are negative ($V_0^+ \approx V_0^- < 0$), each particle considers a cavity as a potential barrier. So they are pulled to the bulk by polarization interaction with the medium. Nevertheless, even in this case the Ps bubble may be formed due to an enhancement of the Coulombic e^+e^- attraction inside the cavity (no dielectric screening inside). This feature cannot be taken into account when Ps is simulated as a point particle.

2) It is seen that the behavior of the total energy of the pair (red curves in Fig. 5) strongly differs from the Tao-Eldrup prediction (green dashed curves; the first term in Eq. (1), where R_∞ is replaced by R), as well as from the expectation based on the finite potential well model (brown curves in Fig. 5; the Coulombic potential cannot be approximated well by a rectangular spherically symmetric potential). The same is true for the pick-off annihilation rate, Fig. 6.

3) Calculations demonstrate one common feature: up to $R \lesssim 1.5 - 2.2$ Å all dependencies remain the same as in a medium without any cavity, but at larger R there are significant deviations. This is related to the known quantum mechanical phenomenon -- absence of a bound state of a particle in a small finite 3d-potential well. In such cavities, Ps cannot be bound, it does not exert any repulsive pressure on their walls and does not stimulate their transformation towards the equilibrium Ps bubble. The possibility of finding a suitable preexisting cavity, sufficient at least for preliminary localization of qf-Ps, may be a limiting factor for the formation of the Ps bubble state.

4) One may find an equilibrium Ps bubble radius by minimizing the sum of the total e^+e^- energy $\langle H \rangle$ and the surface energy of the bubble. For water it turns out to be 5-5.2 Å which is about 2 Å larger than predicted by the Tao-Eldrup model. For such a large bubble, the relative contact density is $\eta_c \approx 0.9$, Fig. 5. It is somewhat higher than the experimental values (0.65-0.75 [19]). This discrepancy may indicate that e^+ and e^- really interact with a medium in a different way, for example, $V_0^+ > V_0^-$. It means that the Ps positron may be trapped by a cavity, and e^- will be bound to this trapped e^- by the

Coulombic attraction. This scenario may be also considered in the framework of the present approach, but the expression for the trial wave function of the new pair must be written in an "asymmetric" (towards e^+ and e^-) form:

$$\Psi_{+-}(\mathbf{r}_+, \mathbf{r}_-) \approx \frac{\exp(-|\mathbf{r}_+ - \mathbf{r}_-|/2a - r_+/2b)}{8\pi\sqrt{a^3b^3}}. \quad (11)$$

5) Any Ps bubble model reduces the original many-body (multi-particle) problem to a simpler one, that of one or two particles in an external field, which simulates the interaction with the medium. To calculate this field one usually relies on some macroscopic approaches. However, their validity always remains uncertain (for example, how to relate the actual arrangement of molecules around the Ps bubble with the jump of dielectric permittivity outside the bubble and so on).

This work is supported by the Russian Foundation of Basic Research (grant 11-03-01066).

References

- [1] R.A. Ferrel: Rev. Mod. Phys. **28(3)** (1956), p. 308; Phys. Rev. **108** (1957), p. 167
- [2] S.J. Tao: J. Chem. Phys. **56** (1972), p. 5499
- [3] M. Eldrup, D. Lightbody and J.N. Sherwood: Chem. Phys. **63** (1981), p. 51
- [4] A.T.Stewart, C.V.Briscoe, in: Positron Annihilation, Proceedings of the Conference. Wayne State University. Eds. A.T. Stewart and L.O. Roellig, Academic Press, New York (1959), p.383
- [5] A.P. Buchikhin, V.I. Gol'danskii, A.O. Tatur and V.P. Shantarovich: Zh. Eksp. Teor. Fiz. **60(3)**, p. 1136
- [6] L.O.Roellig, in: Proc. Wayne State University Conf. on Positron Annihilation. Eds. A.T.Stewart and L.O.Roellig, Academic Press, New York (1967), p.127
- [7] C. Dauwe, N. Balcaen, S. Van Petegem and D. Segers: Radiat. Phys. Chem. **58** (2000), p. 681
- [8] S.V. Stepanov, V.M. Byakov: J. Structural Chemistry, **43(6)** (2002), p.949
- [9] D. Dutta, B. Ganguly, D. Gangopadhyay et al.: Phys. Rev. B, **65** (2002), 094114
- [10] B.N. Miller, T. Reese: Nucl. Instr. Methods in Phys. Research B **192** (2002), p.176
- [11] L.Larrimore, R.N.McFarland, P.A.Sterne, A.L.R. Bug: J. Chem. Phys., **113(23)** (2000), p.10642
- [12] A.L.R.Bug, M.Mulneh, J.Waldman, P.A.Sterne: Mater. Sci. Forum Vols. **445-446** (2004), p.375
- [13] T. Fülöp, Z. Farkas, A. Seeger, J. Major: arXiv:cond-mat/0304442v1 (2003)
- [14] B.E. Springett, J. Jortner and M.N. Cohen: J. Chem. Phys., **48(6)** (1968), p.2720
- [15] *Handbook of Radiation Chemistry*, edited by Y. Tabata, Y. Ito, S. Tagawa (CRC Press, Boca Raton, 1991)
- [16] V.V. Batygin, I.N. Toptygin: "Problems on electrodynamics", Moscow, NIC RKhD, 2002 (Problems No. 157, 158); in Russian
- [17] S.I. Pekar: "Investigations on electronic theory of crystals", (GITTL, Moscow, Leningrad, 1951. In Russian)
- [18] R.S. Knox: "Theory of excitons", (Rochester, New York. Academic Press, 1963)
- [19] S.V. Stepanov, D.S. Zvezhinski, G. Duplatre et al.: Mater. Sci. Forum Vol. 666 (2011), p. 109

Positron and Positronium Chemistry X

10.4028/www.scientific.net/MSF.733

Beyond the Point Ps Approximation

10.4028/www.scientific.net/MSF.733.7