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NUMERICAL STUDIES OF e^+e^- MAGNETIC RESONANCES

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A. Dragić, A. Belić, Z. Marić

Institute of Physics P.O.B. 57, Belgrade 11001, Yugoslavia

Abstract. *Origin of coincident peaks in electron-positron energy spectra measured in heavy ion collisions is studied within the framework of Barut-Vigier model. Careful numerical analysis revealed that there are no magnetic resonances in the relevant 1-2 MeV energy interval in the most attractive L = 1, S = 1, J = 0 channel.*

1. INTORODUCTION

It is the usual practice in atomic physics to treat electromagnetic interactions other than Coulomb (spin-orbit, spin-spin etc.) as perturbations, which give only small corrections to the energy levels. Although these terms in Hamiltonian with distance behaviors $\sim r^{-3}$ and r^{-4} are indeed small compared to the Coulomb term at the atomic scale, they are comparable or even much higher than later at shorter distances. There is, in principle, a possibility that magnetic interactions at short distances give rise to the new phenomena, which can not be explained by perturbative treatment.

The first exploration of that fact, known to the authors, are made by Corben in an unpublished paper. He noticed that motion of a point charge in the field of magnetic dipole at rest is highly relativistic, and the orbits are of nuclear dimensions (see comment made by Schild [1]. The most systematic treatment of the magnetic interactions at small distances is given by Barut [2].

A two-body system where magnetic interactions play the most significant role is positronium. Both electron and positron have large magnetic moments which contribute to the second potential well in effective potential, at distances much smaller then Bohr radius. Barut and his coworkers predicted that this second potential well can support resonances [3,4].

However, these results did not attracted much attention until experiments with heavy ion collisions at GSI at Darmstadt revealed the peak structure in positron spectra [5,6] and narrow lines in coincident electron-positron spectra [7]. Similar resonances are observed in some experiments with direct $e^+ - e^-$ scattering (see for instance [8,9]). However, the

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most recent experiments by this group [10] and the others [11,12] question the statistical relevance of these lines, so that the question of their existence and origin remains open. One possible explanation, namely the process of nuclear pair conversion, dismissed at first, is now reconsidered [13]. The other is the existence of $e^+ - e^-$ resonant states. This possibility has been investigated before with mixed results.

The first theoretical prediction of a resonance was made by Wong and Becker [14]. They used the relativistic Kemmer-Fermi-Yang [15] model for positron and find a single $S = 1$, $L = 1$, $J = 0$ resonance at the total energy of 1.579 MeV. In the same model McNeil and Wallin [16] find no resonances in the energy region 1.1-2.1 MeV.

In the Blankenbecler-Sugar reduction of the Bethe-Salpeter equation Spence and Vary [17] found several narrow resonances at total energies: 1.351, 1.498, 1.659, 1.830, 2.009 and 2.195 MeV. On the other hand, Horbatsch [18] argued that with method similar to Spence and Vary, it is possible to generate spurious resonances numerically.

Dehnen and Shanin [19] reported several resonances in the approach of Barut. In the same approach, Wong and Wong [20] found no resonant solutions.

In scalar QED (Wick-Cutkosky model) Arbuzov et al. [21,22] found many resonances. Walet, Klein and Dreizler [23] did not reproduced their result by solving a similar equation.

The controversial situation regarding both experimental and theoretical results on the existence of $e^+ - e^-$ resonant states in 1-2 MeV region prompted us to undertake an investigation of this problem based on a novel self-consistent treatment of Barut-Vigier model [2].

The paper is organized as follows: model interaction used to describe positronium is given in Section 2, in Section 3 details of the calculation methods are given and in Section 4 we present the results of our analysis, focused on the region of 1-2 MeV where most of the positive results are reported.

2. THE MODEL

The Barut-Vigier model is a simple two-body model which exhibits the main features of the resonance enigma if applied to positronium. The model essentially represents an extension of the Pauli equation to a two-body system [24] and is defined by Hamiltonian:

$$H = \frac{1}{2m_1}((\vec{P}_1 - e_1\vec{A}(\vec{r}_1))^2 + \frac{1}{2m_2}((\vec{P}_2 - e_2\vec{A}(\vec{r}_2))^2 + \frac{2}{4\pi\in_0}\frac{e_1e_2}{|\vec{r}_1 - \vec{r}_2|} + V_{dd} \tag{1}$$

where: m_i is the mass, $\vec{P}_i$ the momentum, e_i the charge, $\vec{r}_i$ the position of the particles ($i = 1,2$), $\vec{A}_i$ is electromagnetic vector potential and V_{dd} is dipole-dipole interaction term:

$$V_{dd} = -\left(\frac{\mu_0}{4\pi}\right)\vec{\mu}_1\vec{\mu}_2\delta(\vec{r}_1 - \vec{r}_2)^2 + \left(\frac{\mu_0}{4\pi}\right)\left[\frac{\vec{\mu}_1\vec{\mu}_2}{|\vec{r}_1 - \vec{r}_2|^3} - \frac{3[\vec{\mu}_1(\vec{r}_1 - \vec{r}_2)][\vec{\mu}_2(\vec{r}_1 - \vec{r}_2)]}{|\vec{r}_1 - \vec{r}_2|^5}\right]. \tag{2}$$

In the center of mass frame and with a normal magnetic moment: $\vec{\mu} = e\vec{S}/m$ Hamiltonian (1) becomes:

$$H = \frac{1}{2m}p^2 - \left(\frac{\mu_0}{4\pi}\right)\frac{e_1e_2}{4m^2}\frac{\vec{S}\vec{L}}{r^3} + \left(\frac{\mu_0}{4\pi}\right)^2\frac{e_1^2e_2^2\hbar^2}{16m^3}\frac{1}{r^4} + \frac{1}{4\pi\in_0}\frac{e_1e_2}{r} - \\ -\left(\frac{\mu_0}{4\pi}\right)\frac{4\pi e_1e_2}{4m^3}\vec{s}_1\vec{s}_2\delta(\vec{r}) + \left(\frac{\mu_0}{4\pi}\right)\frac{e_1e_2}{4m^2}\left[\frac{\vec{s}_1\vec{s}_2}{r^3} - \frac{3(\vec{s}_1\vec{r})(\vec{s}_2\vec{r})}{r^5}\right] \tag{3}$$

where r, p, $\vec{S}$, $\vec{L}$ are quantities related to the relative motion of bodies, and m is a reduced mass. The standard Pauli approximation leading to eq.(3) can be improved by keeping the energy term in the Hamiltonian. This correction is essential in the positronium problem, since the reduces mass m is of the order of resonance energies we are interested in. The new Hamiltonian depends upon energy only through the effective mass m^* given by:

$$m^* = m + \frac{E}{8c^2} \tag{4}$$

This approximation is similar in spirit to constraint dynamics approach for relativistic systems [25]. In terms of total spin and angular momenta Hamiltonian can be written as:

$$H = \frac{1}{2m^*}p^2 + \frac{1}{4\pi\in_0}\frac{e_1e_2}{r} - \left(\frac{\mu_0}{4\pi}\right)\frac{e_1e_2}{8(m^*)^2}\frac{\vec{J}^2 - \vec{L}^2 - 2\vec{S}^2}{r^3} + \left(\frac{\mu_0}{4\pi}\right)^2\frac{e_1^2e_2^2\hbar^2}{16(m^*)^3}\frac{1}{r^4} - \\ -\left(\frac{\mu_0}{4\pi}\right)\frac{4\pi e_1e_2}{8(m^*)^3}\left(\vec{S}^2 - \frac{3}{2}\hbar^2\right)\delta(\vec{r}) - \left(\frac{\mu_0}{4\pi}\right)\frac{3e_1e_2\hbar^2}{8(m^*)^2}\frac{Q}{r^3} \tag{5}$$

where operator Q is:

$$Q = \frac{1}{\hbar^2}\cdot\frac{(\vec{S}\vec{r})^2}{r^2}$$

The Hamiltonian is symmetric with respect to rotations in total Hilbert space (generated by total angular momentum $\vec{J}$, rotations in spin factor space and coordinate inversion. Therefore, good quantum numbers are: total angular momentum J, total spin S and parity π. Note that the symmetry with respect to spatial rotations is violated by the operator Q, so that L is not a good quantum number.

When $S = 0$ (parapositronium), orbital angular momentum L is also a good quantum number. In this case after separation of variables the radial Schrödinger equation reads:

$$\frac{d^2u}{dr^2} - \left[\frac{2m^*}{\hbar^2}\frac{1}{4\pi\in_0}\frac{e_1e_2}{r} + \frac{L(L+1)}{r^2} + \left(\frac{\mu_0}{4\pi}\right)^2\frac{e_1^2e_2^2}{8(m^*)^2}\frac{1}{r^4} + \right. \\ \left. + \left(\frac{\mu_0}{4\pi}\right)\frac{3e_1e_2}{8(m^*)^2}\frac{\delta(r)}{r^2} - \frac{2m^*E}{\hbar^2}\right]u(r) = 0 \tag{6}$$

When $S = 1$ (orthopositronium), possible values of orbital angular momentum are: $L = J - 1, J, J + 1$. Because parity is a good quantum number not all three values are allowed. There are two different cases:

a.) if $\pi = (-1)^J$ then $L = J$ and the radial Schrödinger equation is:

$$\frac{d^2u}{dr^2} - \left[\frac{2m^*}{\hbar^2}\frac{1}{4\pi\in_0}\frac{e_1e_2}{r} + \frac{L(L+1)}{r^2} + \left(\frac{\mu_0}{4\pi}\right)\frac{e_1e_2}{4(m^*)}\frac{2S(S+1)}{r^3} + \right.$$
$$\left. + \left(\frac{\mu_0}{4\pi}\right)^2 \frac{e_1^2e_2^2}{8(m^*)^2}\frac{1}{r^4} - \left(\frac{\mu_0}{4\pi}\right)\frac{e_1e_2}{8(m^*)^2}\frac{\delta(r)}{r^2} - \left(\frac{\mu_0}{4\pi}\right)\frac{3e_1e_2}{4(m^*)^2}\frac{1}{r^3} - \frac{2m^*E}{\hbar^2}\right]u(r) = 0 \tag{7}$$

b.) if $\pi = -(-1)^{-J}$ then $L = J - 1, J + 1$ and the radial Schrödinger equation takes form of two coupled second order differential equations. The only exception is the case $J = 0$, $L = 1$:

$$\frac{d^2u}{dr^2} - \left[\frac{2m^*}{\hbar^2}\frac{1}{4\pi\in_0}\frac{e_1e_2}{r} + \frac{2}{r^2} + \left(\frac{\mu_0}{4\pi}\right)\frac{e_1e_2}{4(m^*)}\frac{6}{r^3} + \right.$$
$$\left. + \left(\frac{\mu_0}{4\pi}\right)^2 \frac{e_1^2e_2^2}{8(m^*)^2}\frac{1}{r^4} - \left(\frac{\mu_0}{4\pi}\right)\frac{e_1e_2}{8(m^*)^2}\frac{\delta(r)}{r^2} - \frac{2m^*E}{\hbar^2}\right]u(r) = 0 \tag{8}$$

This case is the most important for the resonance phenomena, because the attractive spin interactions are strongest and second potential well in the effective potential is most profound. The majority of reported resonances are in the $S = 1$, $L = 1$, $J = 0$ channel. The schematic plot of the effective potential in that channel, obtained using the effective mass corresponding to the energy $E = 600$ KeV, is shown in Fig. 1.

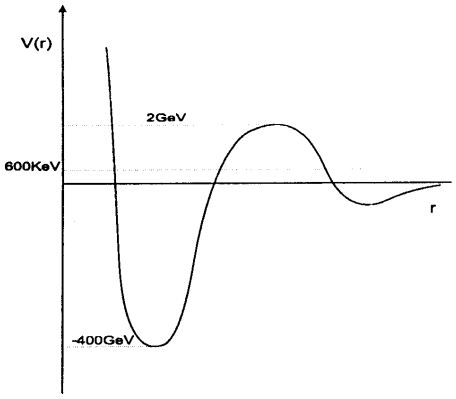

Fig. 1. Schematic plot of the effective potential for $E = 600$ KeV in $S = 1$, $L = 1$, $J = 0$ channel. Various features of the potential are drown out of scale in order to be visible.

3. THE METHOD OF CALCULATION

3.1 Bound states

Before attacking the problem of magnetic resonances, the method is first tested in the low energy limit (the usual bound states of positronium) and results are compared with perturbative QED.

The Schrödinger equation is numerically integrated with implementation of the "shooting method" [26]. In order to achieve accurate results, two separate integrations are performed: outward integration from the origin to the matching point and inward integration from some large r to the matching point. Energy eigenvalues are determined by an iterative procedure. The approximate energy at each step was obtained by equating the wave functions and their first derivatives at the matching point, which was placed at the inner classical turning point. This energy was put back in the effective mass (eq. 4) and the procedure was repeated until convergence was achieved. Integrator was based on the Numerov algorithm [26]. Outward inte-

gration is initiated near the origin using a solution of approximate radial Schrödinger equation, valid in all *S* and *J* channels:

$$\frac{d^2u_0}{dr^2} - \frac{b}{r^4}u_0 = 0\,, \tag{9}$$

which is:

$$u_0 = r\exp\{\sqrt{b}/r\}\,, \quad b = \left(\frac{\mu_0}{4\pi}\right)^2 \frac{e^4}{8(m^*)^2}\,. \tag{10}$$

Inward integration is initiated at a point right of the Coulomb potential well where approximate radial Schrödinger equation:

$$\frac{d^2u_\infty}{dr^2} + k^2u_\infty = 0 \tag{11}$$

has physically meaningful exponentially decaying solution:

$$u_\infty = e^{-kr}\,, \quad k^2 = -\frac{2m^*E}{\hbar^2}\,. \tag{12}$$

3.2. Resonances

We adopt a definition of the resonant state as a solution of the radial Schrödinger equation which satisfies "the outgoing wave only" boundary condition at large distances [27]. At the origin solution must be regular. As a consequence of a complex boundary condition, the energy is treated as complex quantity. The usual convention is:

$$\in = E - \frac{i}{2}\Gamma \tag{13}$$

The real part *E* is resonance energy, while imaginary part Γ is resonance width and could be related, via uncertainty relations, with the mean life of the resonance.

3.2.1. Complex coordinate rotation technique

In practice, direct integration of the Schrödinger equation with the above boundary condition does not produce accurate results. The reason could be seen from large *r* asymptotic. Approximate Schrödinger equation in this region:

$$\frac{d^2u}{dr^2} + k^2u = 0 \tag{14}$$

with $k^2 = \frac{2m}{\hbar^2}\left(E - \frac{i}{2}\Gamma\right)$ and $k = k_r - ik_i\,(k_r\,, k_i > 0)$, has solution:

$$u(r) \approx C_1e^{ikr} + C_2e^{-ikr} = C_1e^{ik_rr}\cdot e^{k_ir} + C_2e^{-ik_rr}\cdot e^{-k_ir}$$

The second term with incoming wave behavior exponentially decays at large distances. For this reason it is difficult to notice its presence in total solution and to implement

outgoing wave boundary condition, necessary for definition of a resonance. The problem is solved by placing r into the complex plane [28]. If potential $V(r)$, from which the centrifugal term is explicitly removed, is analytic function of r, one can perform coordinate rotation: $r = x \cdot e^{i\theta}$ to obtain the rotated radial Schrödinger equation:

$$\frac{d^2u}{dx^2} + \left\{ k^2 e^{2i\theta} - \frac{2m}{\hbar^2}\left[e^{2i\theta} V(xe^{i\theta}) - \frac{\hbar^2 L(L+1)}{2mx^2} \right] \right\} u = 0 \,. \tag{15}$$

In the asymptotic solution of this equation:

$$u(x \to \infty) \approx e^{i(k_r \cos\theta + k_i \sin\theta)} \cdot e^{-x(k_r \sin\theta - k_i \cos\theta)}$$

the first factor is oscillatory and the second decays as x increases, if the condition:

$$tg\theta > k_i / k_r \,. \tag{16}$$

is satisfied. Hence, with the proper choice of θ, the wave function will tend to zero both at the origin and for large distances. With these boundary conditions bound-state-like procedure of integrating Schrödinger equation can be applied. The shooting method to a suitably chosen mid-point starting from the asymptotic forms of the radial wave function similar to these of section 3.1 can be used again to obtain the resonance energies and widths. The difference is that matching of logarithmic derivatives of inward and outward wave functions now amounts to a two-dimensional problem which is treated by Newton-Raphson method. The other difference concerns the iterative procedure, since both the resonance energies and widths must be self-consistently determined. However, it should be noted that only the real part E of a complex energy enters the effective mass m^*. To start the iterative procedure the semiclassical formula for resonance energies and widths is usually used [28]. Unfortunately, the energy thus obtained lies outside the region in which our self-consisted procedure is expected to converge. More details on this problem will be given in the next section. To circumvent this problem, we have adopted an alternative strategy. The lattice of initial guesses of energies and widths is formed, covering energy range of interest and iterative procedure is started at each of this points.

4. Results and Discussion

4.1. Bound states

Bound state energies are calculated for several states using the method of Sec. 3. Integration is performed for different step size. After extrapolation to zero step size results are compared with known energy levels of positronium, calculated up to order of α^5 [29, 30, 31].

As shown in Table 1 the eigenenergies are reproduced with theaccuracy of five digits.

Table 1. The comparison of the energies (in eV) of the low-laying states calculated using our self-consistent procedure (column 2) with perturbative QED $O(\alpha^5)$ ones (column 3).

State	this method	QED
2^1P_1	−1.697881(15)	−1.6978771
2^3P_1	−1.697882(13)	−1.6978796
2^3P_0	−1.697896(9)	−1.6978897
1^1S_0	−6.79125(16)	−6.791924
2^1S_0	−1.69798(5)	−1.6979358

4.2 Resonances

In the semiclassical treatment linear connection formula can be used for the energies far from both the top of the potential barrier and the bottom of the potential well. Also, the Langer correction for spherically symmetric potentials: $L(L+1) \to (L+1/2)^2$ should be used. Semiclassical quantization formula for resonances, with complex turning points is given in ref. [28]. Alternatively, with the usual approximation for sharp resonances, one can avoid to calculate complex turning points and the resonance energies and widths are determined separately from the formulas:

$$\frac{1}{\hbar}\int_a^b \sqrt{2m(E_n - V)}dx = \pi\left(n + \frac{1}{2}\right) \tag{17}$$

and

$$\Gamma_n \cdot \frac{2m}{\hbar}\int_a^b \frac{dx}{\sqrt{2m(E_n - V)}} = \exp\left\{-\frac{2}{\hbar}\int_b^c \sqrt{2m(E_n - V)}dx\right\}. \tag{18}$$

Here, a, b and c ($a < b < c$) are turning points. We have investigated resonances in the $J = 0$, $L = 1$, $S = 1$ channel in the range of 1-2 MeV total energy. More precisely, we have studied the semi-classical formulas (17), (18), for a range of values of initial energies $E = 1,\ 1.1,\ 1.2,...,2$ MeV. Each of these values defines a different potential well as explained in Sec. 2, and each of these wells is found to have only one bound state solution corresponding to $n = 0$. For example, for $E = 1.65$ MeV that level lies at $E' = -14.8$ GeV. However, it is easy to see that iteration procedure started with such E and E' fails to converge. Thus, in our semiclassical calculation we did not find any resonance within the convergence of the self-consistent method.

To alleviate this problem quantum calculations with two-dimensional lattice of initial guesses is performed, also with negative result. We started the iterative procedure from a grid of energy values spanning the region of 1-2 MeV in increments of 10 KeV. For each value of the energy E, several starting widths $\Gamma = 0$, 10^{-7} E, 10^{-5} E, 10^{-3} E and 10^{-1} E were considered. In each of these cases, the iteration energy has quickly left the region of interest, typicaly after only ~ 1−5 steps.

To conclude, we have performed both semiclassical and quantum calculation of magnetic resonances in $e^+ - e^-$ system using novel self-consistent treatment of Barut-Vigier model, and found that there are no resonances within 1-2 MeV region, in agreement with most recent experimental and theoretical predictions.

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NUMERIČKO ISPITIVANJE e^+e^- MAGNETNIH REZONANCI

A. Dragić, A. Belić, Z. Marić

Problem porekla koincidentnih pikova u energetskim spektrima elektrona i pozitrona dobijenih u sudarima teških jona je analiziran u okviru Barut-Vigier-ovog modela. Pažljivo numeričko pretraživanje relevantnog energetskog intervala 1-2 *MeV je pokazalo da u njemu nema magnetnih rezonanci u najprivlačnijem kanalu* $L = 1$, $S = 1$, $J = 0$.