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# VACUUM POLARIZATION EFFECTS IN LOW-ENERGY MUONIC ATOM COLLISIONS

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A way for studying relativistic aspects of the Coulomb three-body problem by analyzing the bound states of muonic molecules ( two hydrogen nuclei bound by a negative muon ) has been suggested in [1] and considerable progress has been achieved in this approach since that time [2]. The first perturbative calculations of the relativistic corrections to the energy levels used the non-relativistic three-body wave functionctions obtained in the adiabatic representation ( also refered to as the "method of Perturbed Stationary States ( PSS )" [3]. ); later the more refined variational wave functions were used instead [4],[5]. At present, thanks to significant progress in the non-relativistic calculations all the leading relativistic, QED and nuclear electromagnetic structure corrections $\Delta\varepsilon_{J\vartheta}^{rel}$ to the bound states of muonic molecules have been evaluated. The relativistic description has been tested in muon catalyzed fusion experiments by the measurement of the binding energies $\varepsilon_{J\vartheta} + \Delta\varepsilon_{J\vartheta}^{rel}$ of the weakly bound states $J = \vartheta = 1$ of the $dd\mu$ and $dt\mu$ molecules with an accuracy of the order of $0.1meV$ for $dd\mu$ and $1meV$ for $dt\mu$ respectively [6]. Theoretical evaluations give the following values: $\varepsilon_{11} + \Delta\varepsilon_{11}^{rel}(dd\mu) = -1974.8 + 9.6meV$ and $\varepsilon_{11} + \Delta\varepsilon_{11}^{rel}(dt\mu) = -660.2 + 28.4meV$ [6].

Analysis of the continuous spectrum of the muonic three-body system $a\mu - b$ ( muonic atom - nucleus ) is not as well advanced as for the bound states $ab\mu$, although some results have recently been obtained by applying the multilevel PSS approach to the problem of slow collisions in the system of three Coulomb particles $a\mu - b$ [7]. Using this approach, an Atlas of the cross sections for muonic atom scattering in mixtures of hydrogen isotopes has been calculated with controlled accuracy [8]. This has permitted an application of Monte Carlo analysis to the experiments for muonic hydrogen diffusion[9] with the cross sections calculated by solving the non-relativistic Schrödinger equation for the scattering states $a\mu - a$. Corrections due to the molecular and screening effects are important at low energies, and have also been taken into account [10]. Since the analysis has shown quite strong sensitivity of the experimental data to the scattering cross sections, the question has arisen of possible corrections due to relativistic aspects of the problem. In this paper we estimate for the first time the manifestation in the low-energy muonic atom scattering of the VP correction to the Coulomb interaction in the three-body system $a\mu - b$ with comparable masses $M_a, M_b$ and $m_\mu$. Muonic systems are much more sensitive than normal electronic ones to the VP alteration of the Coulomb interaction at short distances, because the Bohr radius of the muonic atom $a_\mu = \hbar^2/m_\mu e^2 \simeq 2.5\cdot 10^{-11} cm$ is close to the Compton electron wavelength $\lambda_e = \hbar/m_e c \simeq 3.9\cdot 10^{-11} cm$. Moreover, it has been found that VP corrections to the energy levels of the muonic molecules are dominant among relativistic and other short-range corrections [2],[4],[5].

We first turn to the analysis of the bound states already performed to obtain a rough estimate of the magnitude of the VP-effect in scattering, and the peculiarities in the Coulomb three-body amplitude which may amplify the VP-effect. The relative VP-shifts $\Delta\varepsilon^{VP}/\varepsilon$ to the non-relativistic binding energies $\varepsilon_{J\vartheta}$ of the muonic molecules are presented in Table 1. The shifts $\Delta\varepsilon^{VP}_{J\vartheta}$ have been evaluated in the frameworks of the two-level PSS [1] and variational [5] approaches with a perturbation VP-potential

$$\Delta V^{VP} = \sum_{i\neq j} z_i z_j V(r_{ij}) \qquad (1)$$

was the sum of binary Uehling potentials [11]

$$V(r_{ij}) = \alpha\cdot\frac{2}{3\pi r_{ij}}\cdot\int_1^\infty \frac{\sqrt{x^2-1}}{x^2}\cdot(1+\frac{1}{2x^2})\cdot e^{-2(r_{ij}/\lambda_e)x}\cdot dx,$$

describing an effective interaction between Coulomb charges $z_i$ and $z_j$ due to the virtual production and annihilation of a single $e^+e^-$ pair, $\alpha = e^2/\hbar c \simeq \frac{1}{137}$. Table 1. demonstrates the rather surprising fact that the simple two-level PSS evaluation already gives a quite close approximation of $\Delta\varepsilon^{VP}$ to results obtained by advanced varialtional calculations using a large number ( 400 – 1200 ) of trial functions. The only exceptions are the P-states of the strongly asymmetric molecules $pd\mu$ and $pt\mu$ ( $M_a \neq M_b$), and a loosely bound state $J = \vartheta = 1$ in the $dt\mu$-molecule.

For the analysis of the VP effects in muonic atom S-wave scattering, we use here the "improved" two-level PSS approximation [12], which provides correct thresholds and momenta in the scattering channels $a\mu + b$ and $b\mu + a$, and as a result more accurate scattering amplitudes for both symmetric and asymmetric collisions then the standard two-level PSS [7],[8]. In this approach the three-body wave function is expressed as an

Table 1: The relative VP-shifts $\Delta\varepsilon^{VP}/\varepsilon \times 100$ (in percent) to the non-relativistic binding energies $\varepsilon_{J\vartheta}$ of the muonic molecules.

| | $J\vartheta$ | 00 | 01 | 10 | 11 | 20 | 30 | |
|---|---|---|---|---|---|---|---|---|
| symmetric systems | $pp\mu$ | 0.117 | | 0.062 | | | | Ref.[1] |
| | | 0.1125 | | 0.0472 | | | | Ref.[5] |
| | $dd\mu$ | 0.122 | 0.087 | 0.100 | -0.41 | 0.019 | | Ref.[1] |
| | | 0.1268 | 0.109 | 0.09979 | -0.44 | | | Ref.[5] |
| | $tt\mu$ | 0.132 | 0.123 | 0.116 | 0.082 | 0.0770 | 0.088 | Ref.[1] |
| | | 0.1323 | 0.119 | 0.1148 | 0.0754 | | | Ref.[5] |
| asymmetric systems | $pd\mu$ | 0.138 | | 0.105 | | | | Ref.[1] |
| | | 0.1058 | | 0.0220 | | | | Ref.[5] |
| | $pt\mu$ | 0.157 | | 0.130 | | | | Ref.[1] |
| | | 0.1040 | | 0.0212 | | | | Ref.[5] |
| | $dt\mu$ | 0.137 | 0.18 | 0.117 | -0.5 | 0.064 | | Ref.[1] |
| | | 0.1261 | 0.0807 | 0.1005 | -2.51 | | | Ref.[5] |

For each bound state the results of the two-level PSS calculation by Melezhik and Ponomarev [1] (first lines) and of the variational one by Assing and Monkhorst [5] (second lines) are presented. The table is compiled on the basis of the data of papers [1], [5] for VP-shifts $\Delta\varepsilon_{J\vartheta}^{VP}$ and papers [6] for non-relativistic binding energies $\varepsilon_{J\vartheta}$.

expansion

$$\Psi_\varepsilon(\vec{r},\vec{R}) = \varphi_a(\vec{r};R)\cdot\chi_a^\varepsilon(R) + \varphi_b(\vec{r};R)\cdot\chi_b^\varepsilon(R) \qquad (2)$$

over the eigenfunctions $\varphi_{1s\sigma,2p\sigma}(\vec{r};R)$ of the two-center problem ( a muon in the field of two Coulomb centers separated by $R$ ). Where $\varphi_{a,b} = \frac{1}{\sqrt{2}}(\varphi_{1s\sigma} \pm \varphi_{2p\sigma})$ are the symmetrized "muon" wave functions and "nuclear" functions $\chi_{a,b}(R)$ represent in an asymptotic region $R \to \infty$ two possible asymptotic states $a\mu + b$ and $b\mu + a$ of the system $a\mu - b$. Hereafter only symmetrization formulas for the asymmetric case are used; an extension to the more complicated ( due to including the spins ) symmetric case can be found in [12],[8]. The initial three-body Shrödinger equation is reduced by averaging over muon coordinates $\vec{r}$ to a system of two ordinary differential equations:

$$\begin{aligned}
&\{\frac{1}{2M}\frac{d^2}{dR^2} + \varepsilon - W_a(R) - \Delta V_a^{VP}(R)\}\chi_a(R)\\
&\quad -\{W_{ab}(R) + \Delta V_{ab}^{VP}(R)\}\chi_b(R) = 0,\\
&\{\frac{1}{2M}\frac{d^2}{dR^2} + \varepsilon - W_b(R) - \Delta V_b^{VP}(R)\}\chi_b(R)\\
&\quad -\{W_{ba}(R) + \Delta V_{ba}^{VP}(R)\}\chi_a(R) = 0,
\end{aligned} \qquad (3)$$

where

$$W_{a,b}(R) = \frac{1}{2}(E_{1s\sigma}(R) + E_{2p\sigma}(R)) + \frac{1}{R} + \frac{1}{2M}H_{a,b}(R),$$

$$W_{ab,ba}(R) = \frac{1}{2}(E_{1s\sigma}(R) - E_{2p\sigma}(R)) + \frac{1}{2M}H_{ab,ba}(R),$$

and $E_{1s\sigma,2p\sigma}(R)$ are the eigenvalues of the two-center problem, $1/M = m_\mu/(M_a + m_\mu) + m_\mu/M_b$ . In this representation the $VP$-interaction (1) is transformed to the effective potentials $\Delta V^{VP}(R)$ by averaging with functions $\varphi_{a,b}(\vec{r};R)$. The problem may be simplified further by omitting the non-adiabatic terms $H(R)/2M \sim 10^{-1}$ in Eq. (3) ( the effective potentials of the three-body problems [3] ) to two uncoupled equations for the amplitudes $\chi_{1s\sigma}$ and $\chi_{2p\sigma}$, i.e. to the Born-Oppenheimer (BO) approximation broadly applied in atomic calculations. Recently an application of this approach to the muonic three-body system has been analyzed by J.D. Jackson [13] both for bound and scattering states and compared with existing data [8]. He showed that despite increasing the non-adiabatic parameter $1/2M \sim 10^{-1}$ of the muonic system by a factor $m_\mu/m_e \approx 200$ as compared to a normal one, the BO approximation still gives a quite good description of the muonic system ( especially the S-states ), "containing all the essential physics". We use the usual BO picture of the quantum dynamics of a particle in the effective potential well $W(R)$ as a clarifying illustration of our analysis ( see Fig.1 ). In [14] it has been shown that the presence in the field $W(R)$ of a resonance ( bound) state with an anomausly small energy $|\varepsilon_\vartheta| \rightarrow 0$ leads to an amplification of the eigenfunction amplitude $\chi_\varepsilon(R \rightarrow 0) \sim A_\varepsilon$ for an eigenstate in the region $|\varepsilon| \sim |\varepsilon_\vartheta|$. This leads in turn to increase of the VP-shift $\Delta\varepsilon_\vartheta^{VP}$ of the Coulomb binding energy of the state $\varepsilon_\vartheta \rightarrow 0$:

$$\Delta\varepsilon_\vartheta^{VP} \simeq \int_0^\infty [\chi^\vartheta(R)]^2 \Delta V^{VP}(R) R^2 dR \sim A_\vartheta^2 \int_0^{a_\mu} R^2 \Delta V^{VP}(R) dR, \quad (4)$$

according to the short-range character of the effective VP-interaction $\Delta V^{VP}(R)$. Table 1 demonstrates this effect in the case of loosely bound states $J = \vartheta = 1$ of $dd\mu$ and $dt\mu$ muonic molecules with the anomalously small Coulomb binding energies $\varepsilon_{11}(dd\mu) = -1.975eV$ and $\varepsilon_{11}(dt\mu) = -0.660eV$. ( The binding energies of all other bound states are in the neighborhood of $50eV \leq |\varepsilon_{J\vartheta}| \leq 350eV$, quite far from the border $\varepsilon = 0$ .) It is natural to expect an analogous amplification of the VP-effect in the scattering amplitude $\Delta f_{FF'}^{VP}(\varepsilon)/f_{FF'}(\varepsilon) \simeq \Delta\sigma_{FF'}^{VP}(\varepsilon)/(2\sigma_{FF'}) = (\sigma_{FF'}^{VP} - \sigma_{FF'})/(2\sigma_{FF'})$ as well for positive energy $\varepsilon \sim |\varepsilon_\vartheta|$. There it was found [14] that there is resonance amplification of the wave function amplitude $A_\varepsilon \simeq \chi_\varepsilon(R \rightarrow 0)$ for $p\mu + p$ low-energy S-wave scattering. The amplification of $A_\varepsilon(p\mu + p)$ reaches a factor $\sim 10$ as compared to other muonic systems at $\varepsilon \rightarrow 0$ ( see Eq. (17) in [14] ) , and is a consequence of the near-zero virtual state in $p\mu(F = 1) + p$ scattering ( F is a $\mu$-atom spin ). Rough estimation by the formula $cot\delta(\varepsilon) = -\sqrt{\varepsilon_\vartheta/\varepsilon}$ with the phase shifts $\delta(\varepsilon)$ from [8] gives the estimate $\varepsilon_\vartheta \sim 10eV$ for the state. In Fig. 2 the relative amplification of the elastic scattering ( $F = F'$ ) and spin-flip ( $F \neq F'$ ) cross sections in $p\mu + p$ collisions is demonstrated by comparison with the usual case of $d\mu + d$ without singularities in the scattering. It is interesting to note that the VP-effect in scattering and in bound states has the same order of magnitude, $\sim 0.1\%$, if the positions of the resonant and bound states are far enough from the boundary of the continuum. The presence of a near-threshold singularity either in scattering or bound states produces noticeable amplification of the effect.

It is also interesting to check the VP-effect in the regions where the pure Coulomb scattering amplitude is rather small . Two such cases are demonstrated in Figs. 3 and 4, where the VP-scattering amplitudes become comparable to pure Coulomb amplitudes in the regions of anomalously weak elastic low-energy $t\mu(F = 0) + t$ scattering, and in the region of Ramsauer-Townsend (RT) minimum in the $d\mu + p$ elastic scattering. The same effect is in $t\mu + p$ collisions where the RT minimum is shifted to $\varepsilon_{min} \simeq 2.5eV$ [8].

We have shown that muonic atom scattering is sensitive to the short-range VP correction of the Coulomb interaction in the three-body muonic system $a\mu - b$. That circumstance becomes important in connection with experimental analysis of muonic atom scattering at a few eV [9],[15]. We have analyzed qualitatively the physics of this effect, but for more accurate quantitative consideration some additional problems remain. First it is necessary to increase the accuracy of calculation of the pure Coulomb muonic three-body problem $a\mu - b$. This may be realized by further improvement of the multilevel PSS [7],[8] or by other [16] approaches being currently investigated in muonic three-body problems. It is also necessary to take into consideration nuclear finite-size corrections having similar magnitude to the VP for some bound states of muonic molecules [4],[5]. An additional important problem is the separation of the electron screening and molecular effects which become dominant in muonic atom scattering as $\varepsilon \rightarrow 0$. This problem may be solved by using the strong angular dependence of screening effects in this region[17] as compared with isotropic $\mu$-atom scattering by bare nuclei. The rapid development of experimental possibilities in investigating the muonic atom scattering[9],[15] may stimulate solution of the above-mentioned problems.

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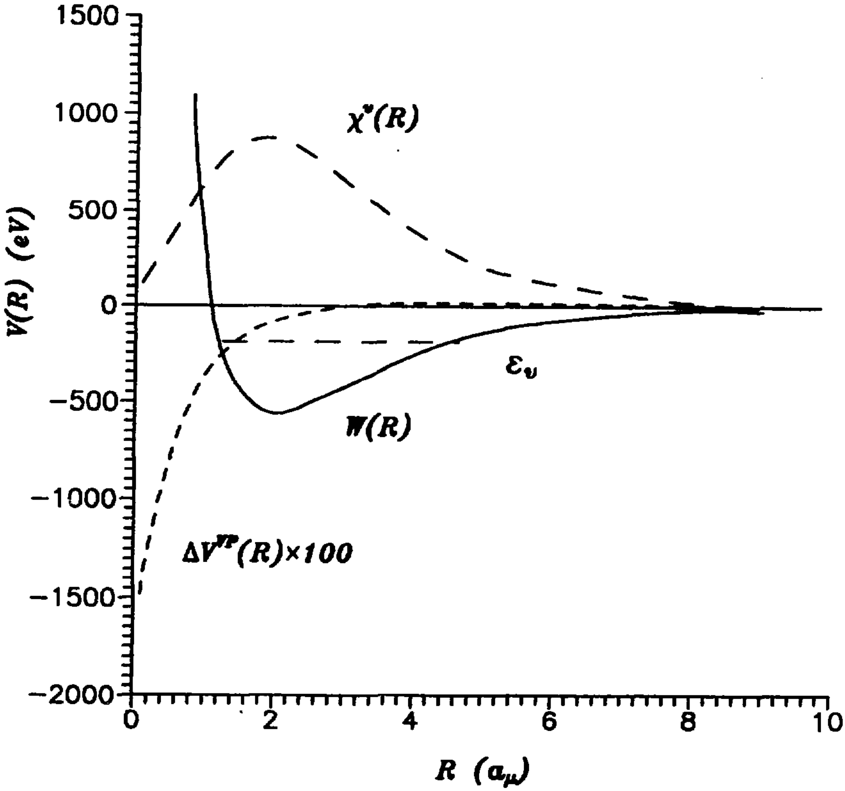


Fig. 1: Born-Oppenheimer potential energy curve $W(R)$ for muonic three-body system $ab\mu$ with effective VP-correction $\Delta V^{VP}(R) = \Delta V^{VP}_{1s\sigma}(R)$.

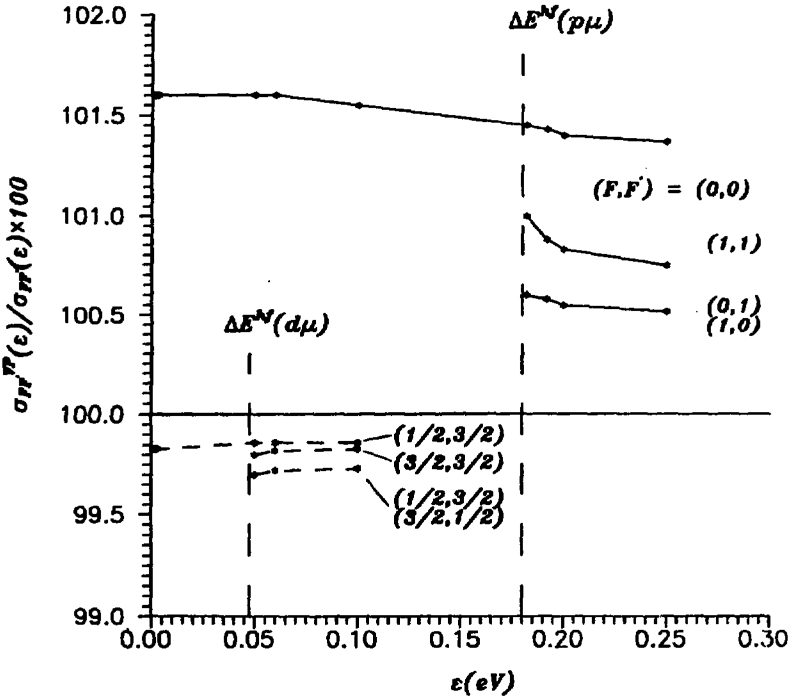


Fig. 2: The VP effects in $d\mu(F) + d \rightarrow d\mu(F') + d$ scattering without singularities in Coulomb scattering amplitude ( dashed curves) and in the case of resonance amplification by the threshold singularity in $p\mu(F) + p \rightarrow p\mu(F') + p$ scattering ( solid curves ). Here $\Delta E^{hf}(d\mu) = E_{1s}(F = 3/2) - E_{1s}(F = 1/2) = 0.049eV$ and $\Delta E^{hf}(p\mu) = E_{1s}(F = 1) - E_{1s}(F = 0) = 0.182eV$ are the hyperfine splitings of the ground states of $d\mu$ and $p\mu$ atoms.

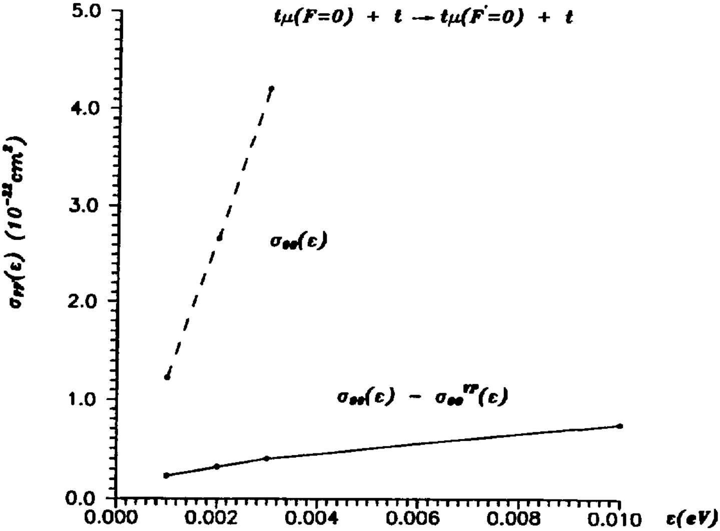


Fig. 3: The VP effect in low energy $t\mu(F=0) + t$ scattering.

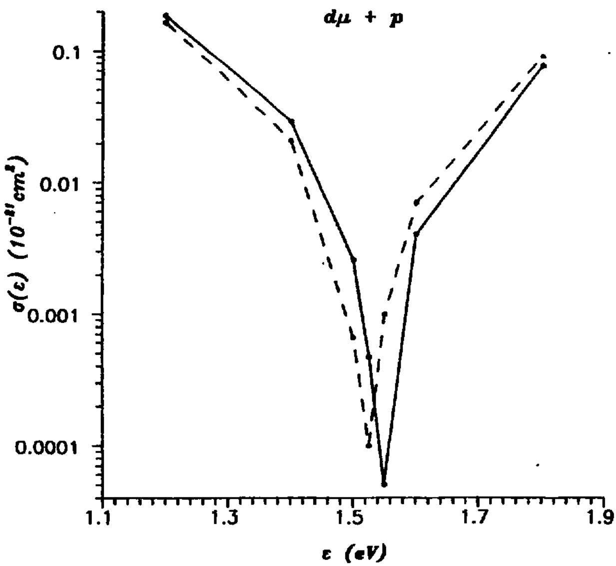


Fig. 4: Shift of the RT minimum in $d\mu + p$ elastic scattering cross sections by VP-interaction. The dashed curve is $\sigma(\varepsilon)$ and the solid curve is $\sigma^{VP}(\varepsilon)$.

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