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Muon, positron and antiproton interactions with atoms and molecules

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Abstract. In this paper, a description is given of some interesting processes involving the interaction of a muon, a positron, or an antiproton with atoms and molecules. The process involving a muon is the resonant formation of the muonic molecular ion, $dt\mu$, in the muon catalyzed fusion cycle. In the case of a positron, the process considered is positron annihilation in low-energy positron scattering by the hydrogen molecule. The antiproton is considered as the nucleus of an antihydrogen atom interacting with simple atoms. Attention is given to antiproton annihilation through the strong interaction. An outline is given of proposed tests of fundamental physics to be carried out using antihydrogen.

1. Introduction

In my talk at the Advanced Science Research 2009 Symposium at Tokai, I described particular interactions of muons, positrons and antiprotons with atoms and molecules.

2. Muon catalyzed fusion

The particle the muon that is central to muon catalyzed fusion was discovered by Anderson and his first graduate student, Neddermeyer, in 1936 when studying cosmic rays [1]. The muon has a mass of $207m_e$, where m_e is the mass of the electron. It has a mean lifetime of 2.2 microseconds. See, for example, [2]. The muon may have a positive or a negative charge. In what follows, I will assume that the muon being considered is negatively charged.

If the electron in a hydrogen atom (H) is replaced by a muon, the result is a hydrogen-like atom $p\mu$. The reduced mass of this atom is $186m_e$. Thus its bohr radius is $\frac{a_0}{186}$, where a_0 is the bohr radius of H. The binding energy of each of its bound states is $186\times$ (the corresponding value for the H atom). $p\mu$ is thus very compact and strongly bound.

An electron can bind two protons to form a weakly bound ion, H_2^+, the hydrogen molecular ion. If the electron in this ion is replaced by a muon, the resulting ion in its ground state is very compact and strongly bound like $p\mu$. As is to be expected, these properties remain if either or both protons are replaced by a deuteron (d) or a triton (t).

A natural question to ask is whether any way could be found of bringing about fusion that did not require very high temperatures, such as are necessary for fusion in the core of the sun and in the ITER project. In 1947, Frank [3] suggested that in the presence of protons and deuterons a slow muon might bind to a p to form $p\mu$. This could come close to a d and form $pd\mu$ which we have seen is tightly bound. Frank thought that it was sufficiently tightly bound

that *p*-*d* fusion might occur. With luck, this would leave the muon free to catalyze further fusions, i.e. bring about *p*-*d* fusion while remaining unchanged at the end of the reaction. Experiments on *d*-*d* fusion catalyzed by a muon carried out by Dzhelepov et al. [4] at the Joint Institute for Nuclear Research (JINR) in Dubna, north of Moscow, in 1966 revealed a strong and unexpected temperature dependence in the rate of formation of $dd\mu$. This was a very exciting discovery. It strongly suggested that a resonant process was involved and held out the possibility of a large increase in the fusion rate under suitable conditions.
It was not long before a form was suggested for this resonant process. In 1967, Vesman [5] proposed that the formation of $dd\mu$ could occur by the reaction

$$d\mu + \mathrm{D}_2 \rightarrow [(dd\mu)^* dee] \tag{1}$$

where the species on the right-hand side is a muonic molecular complex in which $dd\mu$, in a weakly bound excited state, forms one of the nuclei. Such a mechanism depends crucially on the existence of a weakly bound state with binding energy less than the 4.5 eV dissociation energy of D_2. Gershtein and Ponomarev and their group [6, 7] showed that $dd\mu$ did indeed have a weakly bound state which had rotational and 'vibrational' quantum numbers $(J, v) = (1, 1)$ and binding energy $\sim$2 eV. They were also able to show that a corresponding weakly bound state of $dt\mu$ exists with binding energy $\sim$1 eV.
The most favourable muonic molecular ion for muon catalyzed fusion is $dt\mu$. For example, the *d*-*t* fusion rate for this ion is more than 1000 times larger than for any other ion. Also, it produces nearly the highest energy per fusion (17.6 MeV). See, for example, [8].
In the resonant reaction

$$t\mu + \mathrm{D}_2 \rightarrow [(dt\mu)_{11} dee] \tag{2}$$

$dt\mu$ is formed in its $J = 1$, $v = 1$ state. However, rapid fusion only takes place if $dt\mu$ is in a state with $J = 0$. It is thus important to know the binding energies and wave functions of the various states of $dt\mu$ below the very weakly bound $(1, 1)$ state. These binding energies are given in [9]. Deexcitation to these lower states is brought about by Auger decay.
Reaction (2) is incomplete without an indication of what results from the formation of the $[(dt\mu)_{11} dee]$ complex. With inclusion of the most important decay products, it becomes

$$t\mu + \mathrm{D}_2 \rightleftarrows [(dt\mu)_{11} dee] \longrightarrow [(dt\mu)_{Jv} de]^+ + e, \tag{3}$$

where $(J, v) = (0, 1)$, $(2, 0)$, $(1, 0)$ or $(0, 0)$. If the total angular momentum of the $t\mu + \mathrm{D}_2$ is taken to be zero for simplicity, the cross section $\sigma_r(E)$ for this resonant process is determined by the Breit–Wigner formula [10].

$$\sigma_r(E) = \frac{\pi}{k^2} \frac{\Gamma_e \Gamma_a}{(E - E_r)^2 + \frac{1}{4}(\Gamma_e + \Gamma_a)^2}, \tag{4}$$

where k is the wave number of the relative motion of $t\mu$ and D_2,

E = the energy of the system, E_r = the energy of the resonant state,
Γ_e = partial width for back decay into $t\mu + \mathrm{D}_2$, and Γ_a = partial width for Auger decay.

Fig 1 shows how $dt\mu$ formation fits into the overall muon catalyzed fusion cycle.
Cohen at Los Alamos, who has made many contributions to the theory of muon catalyzed fusion over the years, encouraged me to apply the methods of quantum reactive scattering to reaction (3). This reaction has some similarities with the chemical reaction

$$\mathrm{H} + \mathrm{D}_2 \rightarrow \mathrm{H} + \mathrm{D}_2 \text{ or } \mathrm{HD} + \mathrm{D}. \tag{5}$$

This and other chemical reactions have been extensively studied by these methods. See, for example, [12].
However, comparison of reactions (3) and (5) shows that (3) has a special feature not present in (5), namely the Auger decay process which leads to the loss of the electron. Reaction (5) corresponds quite closely to the much slower side reaction

$$t\mu + \mathrm{D}_2 \leftrightarrows [(dt\mu)_{11} dee] \rightarrow [(dt\mu)_{Jv} e] + \mathrm{D} \tag{6}$$

where $(J, v) = (0, 1)$, $(2, 0)$, $(1, 0)$ or $(0, 0)$.
This reaction proceeds through the *same* resonances as reaction (3). In this case, the resonant complex decays forward into the muonic molecule $[(dt\mu)_{Jv} e]$ and a D atom or backward into $t\mu + \mathrm{D}_2$.
One of the methods that has been applied to reaction (5) is the method of Pack and Parker [13]. They use adiabatically adjusting, principal axes hyperspherical coordinates (APH) in their calculations. These are elegant coordinates that transform smoothly between different channels such as $\mathrm{H} + \mathrm{D}_2$ and $\mathrm{HD} + \mathrm{D}$. Together with Pack, my postdoc Zeman and I applied this method to reaction (6) [14–16].
Unfortunately, there was no easy way of including the Auger decay channel directly in our treatment. However, as pointed out by Men'shikov and Faifman [10], the coupling between the resonant channels is small as the lifetime of the resonant complex is much longer than the time the complex takes to complete a vibration. Thus the various decay processes operate essentially independently. This made it possible for us to obtain what we expect to be accurate values for Γ_e and Γ_n, the partial widths for back decay and for the decay of the complex into $[(dt\mu)_{Jv} e] + \mathrm{D}$, by analysing our results for the cross section for the resonant reaction (6) using the Breit–Wigner formula. Details of our calculation are given in [15].
It was found, as expected, that the reaction proceeded only through the resonances. The resonant states were found to be the vibrational states of the complex with vibrational quantum number $v_c = 3$ and 4. The center of the $v_c = 2$ resonance was calculated to be just slightly below threshold.
Somewhat to our surprise, we found that our calculated value of the back decay rate [16] was much larger than the value obtained for it by Lane [17] and comparable with the calculated values of the Auger decay rate in [18]. Further work is necessary to resolve this discrepancy.

3. Low-energy positron-hydrogen-molecule scattering

In this section, I wish to consider low-energy scattering of a positron, the antiparticle corresponding to the electron, by the hydrogen molecule.
The calculations I wish to describe were carried out with the nuclei in a fixed position. The quantity that we have calculated is $Z_{\mathrm{eff}}(k)$, the effective number of electrons in the H_2 target that are available to the incident positron for annihilation. k is the wave number of the positron. The positron annihilation rate, λ, is given by

$$\lambda = \pi r_0^2 c D Z_{\mathrm{eff}}(k), \tag{7}$$

where r_0 is the classical radius of the electron and D is the density of H_2 molecules in the vicinity of the positron.
There is currently great interest in the very large positron annihilation rates, and hence $Z_{\mathrm{eff}}(k)$ values, that have been observed in low-energy positron scattering by some organic molecules. These are observed experimentally to occur at energies just below those of excited vibrational states of the molecule concerned [19]. This has been explained by Gribakin [20] as being due to resonant behaviour involving a positron-molecule quasi-bound state. It is hoped that useful information about this process can be obtained from our study of $e^+\mathrm{H}_2$ scattering.

The protons are fixed at A and B, which have coordinates $(0, 0, -\frac{R}{2})$ and $(0, 0, \frac{R}{2})$, respectively, w.r.t. Cartesian axes. R is the internuclear distance. The prolate spheroidal coordinates (λ, μ, ϕ) used in the calculations are of the form

$$\lambda = \frac{r_A + r_B}{R} \quad \text{and} \quad \mu = \frac{r_A - r_B}{R},$$

where r_A and r_B are the distances of the point with coordinates (λ, μ, ϕ) from A and B, respectively. ϕ is the usual azimuthal angle of spherical polar coordinates. Unless stated otherwise, the internuclear distance R was fixed at $1.4a_0$, the equilibrium value for the H_2 molecule.
The Kohn trial function was taken to be of the form

$$\Psi_{\text{trial}} = \psi_p \phi_{\text{target}} + \sum_{i=0}^{n} g_i \chi_i. \tag{8}$$

The open channel function ψ_p was taken to have the form

$$S + a_t T$$

where

$$T = S + iC \tag{9}$$

$$S = N \frac{\sin[c(\lambda_1 - 1)]}{\lambda_1 - 1} \tag{10}$$

$$C = N \frac{\cos[c(\lambda_1 - 1)]}{\lambda_1 - 1} \quad (1 - \exp[-\gamma(\lambda_1 - 1)]) \tag{11}$$

where λ_1 is the ellipsoidal prolate spheroidal coordinate for the positron,

$$c = \tfrac{1}{2} kR,$$

N is a normalisation constant, γ is a non-linear parameter and ϕ_{target} is the H_2 target wave function. A linear combination of S and C, as above, is the simplest form for the function, ψ_p. It represents the s-wave component of the part of the overall scattering wave function that is of $\sum_g^+$ symmetry. $\{\chi_i\}_{i=0}^n$ are short-range correlation functions and a_t and $\{g_i\}$ are linear parameters to be determined by the complex Kohn method.
The short-range correlation functions are of the form

$$\chi_0 = C \exp[-\gamma(\lambda_1 - 1)] \phi_{\text{target}} \tag{12}$$

$$\chi_i = S_{23} \bar{N} \lambda_1^{a_i} \lambda_2^{b_i} \lambda_3^{c_i} \mu_1^{d_i} \mu_2^{e_i} \mu_3^{f_i} C(s_i, t_i) \exp[-\alpha\lambda_1 - \beta(\lambda_2 + \lambda_3)] \Omega, \quad (i \neq 0), \tag{13}$$

where particle 1 is the positron and particles 2 and 3 the electrons, S_{23} is the electron symmetriser, α and β are positive, non-linear parameters and $\bar{N}$ is a normalisation constant. $a_i, b_i, c_i, d_i, e_i, f_i$ are non-negative integers. The forms used for $C(s_i, t_i)$ are given in Table 1. If the method of models [21] is used

$$\Omega = \phi_{\text{target}}.$$

Otherwise Ω is taken to be equal to one.
Details of the first calculations carried out without using the method of models are given in [22]. Earlier calculations by the generalised Kohn method used the method of models [23]. In this method, the target Hamiltonian, $\hat{H}_t$, is taken to be

$$\hat{H}_t = -\tfrac{1}{2}\nabla_2^2 - \tfrac{1}{2}\nabla_3^2 + V_{\text{mod}} \tag{14}$$

where $V_{\rm mod}$ is such that

$$\hat{H}_t\phi_{\rm target} = E_t\phi_{\rm target} \tag{15}$$

where E_t is the expectation value of the energy of $\phi_{\rm target}$. No knowledge of $V_{\rm mod}$ is required when carrying out Kohn calculations. Also we do not have to consider the $\frac{1}{r_{23}}$ electron repulsion term in the exact form of the target potential.
This method had the very considerable advantage that it was possible to include the key correlation functions in Table 1 containing $C(1,1) = \rho_{12} = \frac{2}{R}r_{12}$ without calculating integrals involving $\frac{\rho_{12}\rho_{13}}{\rho_{23}}$. These functions are Hylleraas-type functions that correlate the positron and the electrons. They play a very important role in improving the accuracy of the wave function at points at which the positron and an electron coincide that are the key to calculating $Z_{\rm eff}(k)$ accurately. However, the complexity of the calculation prevented us from using a very accurate target wave function.
Recently, we have taken account of the motion of the nuclei in our calculations as R has been fixed at its equilibrium value, 1.4 a_0. As a first step we have determined how $Z_{\rm eff}(k)$ at $k = 0.04$ varies with the internuclear distance, R. The results obtained both with and without the use of the method of models are given in Table 2. It can be seen that the results obtained using the method of modules are larger than those obtained without using this method. The vibrationally averaged value of $Z_{\rm eff}(k)$, obtained using a Morse function, is 13.5 when obtained using the method of models and 9.7 without using this method [24, 25].
Thus the value obtained with the method of models is closer to the experimental value of 14.6 [26] than that obtained without using it. In a very recent, very accurate calculation of $Z_{\rm eff}(k)$ at very low energies, Zhang et al. [27] find similar behaviour to the behaviour we find using the method of models as R increases beyond $1.6a_0$. The more accurate value obtained by the method of models, despite using a less accurate target wave function, may be due to the better convergence behaviour that is obtained using this method [28, 22].

4. Antihydrogen

There is great current interest in the preparation of cold antihydrogen ($\bar{\rm H}$), the simplest antiatom made up of an antiproton and a positron. This work is being carried out by the ALPHA and ATRAP collaborations at CERN [29, 30]. It is proposed to carry out tests of fundamental principles of physics using trapped antihydrogen. There is a very good article on the underlying theory by Shore [31]. For my summary with comments, see [32].
To this end, it is proposed to carry out the following experiments at CERN.

(1) Examination of the spectrum of $\bar{\rm H}$ to test the CPT and Lorentz invariance of relativistic quantum field theory.
(2) The weak form of Einstein's principle of equivalence predicts that $\bar{\rm H}$ should fall at the same rate as H in a gravitational field. This is to be tested by an experiment to be carried out by Kellerbauer et al. [33].

The proton and the antiproton are hadrons. Thus they can interact through the strong interaction that brings about proton-antiproton annihilation. This interaction is much stronger than the electromagnetic interaction that brings about electron-positron annihilation. The strong interaction is described by Quantum Chromodynamics (QCD). Current applications treat QCD as a perturbation. However, the coupling constant for QCD at very low energies is too large for perturbation theory to be applicable. This situation is not very satisfactory. However, the underlying problem 'is a very difficult, long standing problem in QCD' [34].
The most accurate practical treatment is to use a complex phenomenological potential taking into account the following: the meson exchange part of the strong interaction, proton-antiproton annihilation, the dipole interaction between the nuclear spins and spin-orbit

coupling between nucleon spins and partial waves. The form of the terms in the potential is determined from experiment. A detailed treatment of this type is possible for $H + \bar{H}$ [35], but, as far as I am aware, not for more complicated systems.
Calculations that we have carried for $H\bar{H}$ scattering [36] show that cross sections for $\bar{H}$ loss through the rearrangement reaction with product $p\bar{p} + Ps$ are larger than for $\bar{H}$ loss by antiproton annihilation [35]. However, this is not the case for $He\bar{H}$ scattering. Cross sections for $\bar{H}$ loss through the three rearrangement reactions with products $He^+\bar{p} + Ps$, $He\bar{p} + e^+$ and $\alpha\bar{p} + Ps^-$, respectively, are much smaller than for $\bar{H}$ loss by antiproton annihilation [37, 25].

5. Conclusion

I have described interesting ways in which a muon, a positron and antihydrogen, which contains an antiproton, can interact with simple atoms and molecules. It is to be expected that new facilities such as J-PARC and further work at CERN will make possible many more studies of interactions of this type.
I have also outlined proposed tests of fundamental physics to be carried out using antihydrogen. These should either reinforce our present understanding of physics or show that modifications to this understanding are necessary. A need for modifications would be a very exciting outcome.

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Table 1. Forms used for the factor $C(s_i, t_i)$ in the short-range correlation functions.

s_i	t_i	$C(s_i, t_i)$	Type of basis function
0	0	1	Product of σ functions
1	1	ρ_{12}	Positron-electron Hylleraas-type
1	2	ρ_{23}	Electron-electron Hylleraas-type
2	1	$\frac{2}{R}(x_1x_2 + y_1y_2)$	Positron-electron configuration interaction (CI) product of π functions
2	2	$\frac{2}{R}(x_2x_3 + y_2y_3)$	Electron-electron CI, product of π functions

R is the internuclear distance.
The distance between particles i and j,

$$r_{ij} = \frac{R}{2}\rho_{ij}.$$

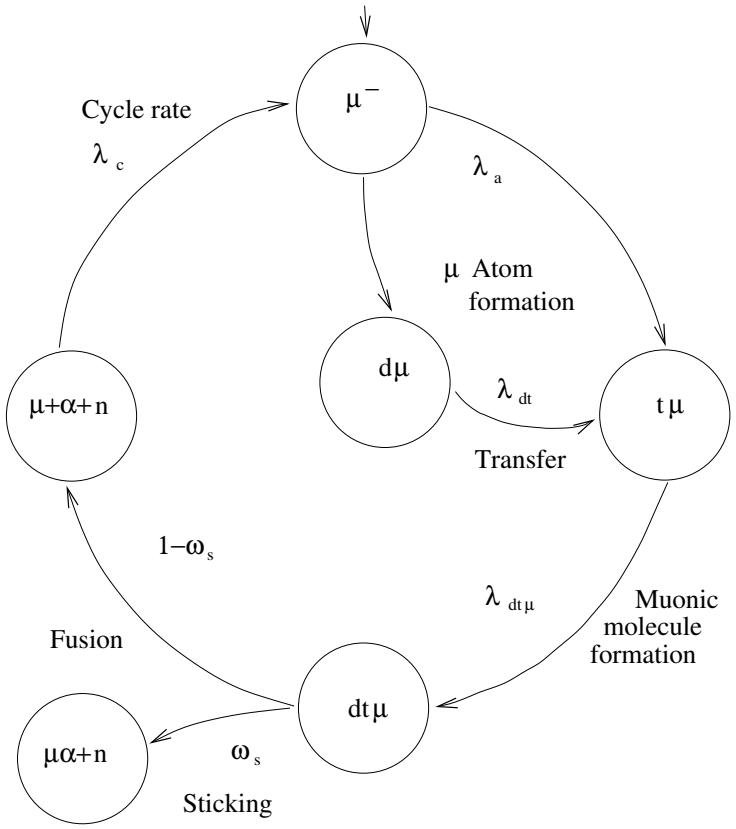

Figure 1. The principal muon catalysis fusion cycle in a deuterium and tritium mixture [8]. Side chains involving *d-d* and *t-t* fusion are not shown. λ_a = muonic atom formation rate $\approx 4 \times 10^{12}\, s^{-1}$; λ_{dt} = muon transfer rate from $(d\mu)_{1s}$ to $(t\mu)_{1s} \approx 3 \times 10^8\, s^{-1}$; $\lambda_{dt\mu}$ = resonant formation rate of $dt\mu \approx 4 \times 10^8\, \mathrm{sec}^{-1}$; ω_s = effective sticking probability $\approx 0.43\%$; λ_c = cycle rate. Values [11] are for $T = 300$K and liquid hydrogen density (4.25×10^{28} atoms m^{-3}).

Table 2. The dependence of $Z_{\mathrm{eff}}(k)$ for $k = 0.04$ on the internuclear distance R.

Internuclear distance, R (a_0)	$Z_{\mathrm{eff}}(k)$	
	Calculated using the method of models †	Calculated without using the method of models *
0.8	6.4	5.0
0.9	7.2	5.8
1.0	8.0	6.5
1.2	10.0	8.1
1.4	12.6	9.6
1.6	15.8	10.6
1.8	19.8	11.1
2.0	24.3	10.8
2.1	26.7	10.5

† Trial function containing 279 short-range correlation functions, 18 of which correlate the positron and the electrons, and a target wave function that takes into account 57.1% of the correlation of energy of H_2 at $R = 1.4a_0$.

∗ Trial function as above but with a target wave function that takes into account 96.8% of

the correlation energy of H_2 at $R = 1.4a_0$.

The percentage correlation energy is given by the percentage of the energy, beyond the SCF energy, taken into account by the wave function under consideration.

References

[1] Neddermeyer S H and Anderson C D, 1937 Phys. Rev. **51**, 884.
[2] Froelich P, 1992 Advances in Physics **41**, 405.
[3] Frank F C, 1947 Nature **160**, 525.
[4] Dzhelepov V P, Ermolov P, Moscalev V I and Filchenkov V V, 1966 Sov. Phys. JETP **23**, 820.
[5] Vesman E A, 1967 Sov. Phys. JETP Lett. **5**, 91.
[6] Gershtein S S and Ponomarev L I, 1977 Phys. Lett. **72 B**, 80.
[7] Vinitsky S I, Ponomarev L I, Puzynin I V, Puzynina T P, Somov L N and Faifman M P, 1978 Sov. Phys. JETP **47**, 444.
[8] Ponomarev L I, 1990 Contemporary Physics **31**, 219.
[9] Bhatia A K and Drachman R J, 1989 Comments At. Mol. Phys. **22**, 281.
[10] Men'shikov L I and Faifman M P, 1986 Sov. J. Nucl. Phys. **43**, 414.
[11] Breunlich W H, Kammel P, Cohen J S and Leon M, 1989 Annu. Rev. Nucl. Part. Sci. **39**, 311.
[12] Manolopoulos D E and Clary D C, 1989 Ann. Rep. Prog. Chem. Sec. C: Phys. Chem. **86**, 95.
[13] Pack R T and Parker G A, 1989 J. Chem. Phys. **87**, 3888 (1987); **90**, 3511.
[14] Armour E A G, 1997 J. Chem. Soc., Faraday Trans. **93**, 1011.
[15] Zeman V, Armour E A G and Pack R T, 2000 Phys. Rev. A **61**, 052713.
[16] Zeman V and Armour E A G, 2001 Hyperfine Interactions **138**, 255.
[17] Lane A M, 1983 Phys. Lett. **98**A, 337.
[18] Bhatia A K, Drachman R J and Chatterjee L, 1988 Phys. Rev. A **38**, 3400.
[19] Gilbert S J, Barnes L D, Sullivan J P and Surko C M, 2002 Phys. Rev. Lett. **88**, 043201
[20] Gribakin G F, 2000 Phys. Rev. A **61**, 022720.
[21] Drachman R J, 1972 J. Phys. B: At. Mol. Opt. Phys. **5** L30.
[22] Cooper J N, Armour E A G and Plummer M, 2008 J. Phys. B: At. Mol. Opt. Phys. **41**, 245201.
[23] Armour E A G, Baker D J and Plummer M, 1990 J. Phys. B: At. Mol. Phys. **23**, 3057.
[24] Cooper J N, 2009 PhD thesis, University of Nottingham, UK.
[25] Armour E A G, Cooper J N, Gregory M R, Jonsell S, Plummer M and Todd A C, 2010 Proceedings of POSMOL 2009, Toronto, J. Phys. Conf. Ser., in press.
[26] Laricchia G, Charlton M, Beling C D and Griffith T C, 1987 J. Phys. B: At. Mol. Phys. **20**, 1865.
[27] Zhang J-Y, Mitroy J and Varga K, 2009 Phys. Rev. Lett. **103**, 223202.
[28] Van Reeth P and Humberston J W, 1995 J. Phys. B: At. Mol. Opt. Phys. **28**, L23.
[29] Fujiwara M et al., 2008 Phys. Rev. Lett. **101**, 053401.
[30] Gabrielse G et al., 2008 Phys. Rev. Lett. **100**, 113001.
[31] Shore G M, 2005 Nuc. Phys. B **717**, 86.
[32] http://www.maths.nott.ac.uk/personal/eaga/
[33] Kellerbauer A et al., 2008 Nuc. Math. and Inst. B **266**, 351.
[34] Signer A, 2006 Private communication.
[35] Armour E A G, Liu Y and Vigier A, 2005 J. Phys. B: At. Mol. Opt. Phys. **38**, L47.
[36] Armour E A G and Chamberlain C W, 2002 J. Phys. B: At. Mol. Opt. Phys. **35** L489.
[37] Armour E A G, Todd A C, Jonsell S, Liu Y, Gregory M R and Plummer M, 2008 Nucl. Instr. and Meth. B **266**, 363; in 'Cold Antimatter Plasmas and Application to Fundamental Physics', 2008 (eds. Kanai Y and Yamazaki Y) AIP CP1037, 333.