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Exact matrix elements of the Uehling potential in a basis of explicitly correlated two-particle functions

Piotr Petelenz* and Vedene H. Smith, Jr.
Department of Chemistry, Queen's University, Kingston, Ontario, Canada K7L 3N6

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Exact analytical expressions are derived for the matrix elements of the Uehling potential in a basis of explicitly correlated two-particle wave functions (geminals) used for the approximate solution of the quantum-mechanical three-body problem within the framework of the integral transform method. The derived formulas may be used to include corrections due to polarization of the vacuum in calculations of the binding energies of muonic molecules.

I. INTRODUCTION

Due to the involvement of $dd\mu$ and $dt\mu$ molecules in nuclear fusion as fusion catalysts, there is an increasing interest in the literature in the calculation of the energy levels of small muonic molecules.[1-8] The salient feature of the problem is the high accuracy required, which is of the order of 10^{-3} eV.[1]

In several recent works on this topic,[1,2] a version of the integral-transform method, very close to that developed in this laboratory,[9,10] has been applied and found successful. The authors seem to have achieved impressive numerical accuracy.

However, the physical relevance of their results still remains open to discussion, due to the purely Coulomb form of the interaction potentials used. In fact, the interaction between the muons and nucleons is known to deviate from purely Coulombic, due to the polarization of the vacuum.[11] The first correction to the interaction potential (quadratic in the fine-structure constant α) is usually referred to as the Uehling potential.[12]

As follows from previous calculations,[8,13,14] less elaborate than those of Frolov and Efros,[1,2] the polarization contribution to the interaction energy is the leading correction to the binding energies of muonic molecules. It may amount to as much as 0.4 eV in some states, and in all the states of interest it exceeds 0.001 eV, which is the requested accuracy of the results. This seems to indicate that, in order to obtain results of physical relevance, it is imperative to include the Uehling term in the calculations.

However, the Uehling potential is given as a nonelementary integral over a parameter.[11,12] A series expansion of this potential is available,[11] as well as a representation in terms of transcendental functions,[13] and there are various numerical approaches which allow one to evaluate it.[15-18] Nevertheless, the fact that the potential is not available in a closed form greatly complicates its application in actual calculations which necessitate the computation of the matrix elements.

Fortunately enough, the matrix elements of the Uehling potential in the basis set used in this particular implementation of the integral-transform method[1,2,9,10] may be expressed in an analytical form, although the potential itself may not. In this paper we will present their derivation.

II. UEHLING POTENTIAL AND ITS MATRIX ELEMENTS

The Uehling potential, describing the vacuum polarization contribution to the interaction between two-point particles, reads[12]

$$V_U(r)=-2\alpha e^2/(3\pi r)\times\int_1^\infty dx\,(x^2-1)^{1/2}[1+1/(2x^2)]e^{-2\gamma x r}/x^2\ , \tag{1}$$

where α is the fine-structure constant, and $\gamma=m_e c/\hbar$, with m_e standing for electron mass.

In the approach to the integral-transform method usually applied to solve the quantum-mechanical three-body problem,[1,2,9,10] the radial part of the wave function is expressed as a superposition of the explicitly correlated two-particle functions (geminals):

$$\psi_k=r_1^i r_2^j\exp(-\alpha_k r_1-\beta_k r_2-\gamma_k r)\ , \tag{2}$$

where α_k, β_k, and γ_k are nonlinear variational parameters, and i,j are integer numbers. In the case of a muonic molecule such as $dd\mu$ or $dt\mu$, r_1 denotes the distance between the first nucleon and the muon, r_2 the distance between the second nucleon and the muon, and r the distance between the two nucleons.

The Hamiltonian of the molecule contains terms describing the nucleon-nucleon and nucleon-muon interactions, and the corresponding matrix elements are necessary for the calculation of binding energies and wave functions. The integrals for the Coulomb part of the interaction potential are well known.[19,20] All the matrix elements of the Uehling potential in the basis set described above consist of integrals of the form

$$\tilde{I}(l,m,n)=\int\int dv_1 dv_2 r_1^l r_2^m r^n \exp(-ar_1-br_2-cr)\int_1^\infty dx(x^2-1)^{1/2}[1+1/(2x^2)]e^{-2\gamma x r}/x^2\ , \tag{3}$$

where l,m are natural numbers or -1 and $n=0,-1$. dv_1 and dv_2 denote the infinitesimal volumes corresponding to r_1 and r_2.

III. AUXILLIARY INTEGRAL

All integrals defined by Eq. (3) may be generated from $\tilde{I}(-1,-1,-1)$ by partial differentiation with respect to a, b, and c, just as it is usually done in the case of the Coulomb potential.[19] Consequently, the basic integral to be calculated is

$$\tilde{I}(-1,-1,-1)=\int\int dv_1 dv_2 (r_1 r_2 r)^{-1}\exp(-ar_1-br_2-cr)\int_1^\infty dx(x^2-1)^{1/2}[1+1/(2x^2)]\exp(-2\gamma x r)/x^2 \;, \tag{4}$$

which, by changing the order of integrations over x and v_1, v_2, may be recast into the form

$$\tilde{I}(-1,-1,-1)=\int_1^\infty dx[1+1/(2x^2)](x^2-1)^{1/2}x^{-2}\int\int dv_1 dv_2 (r_1 r_2 r)\exp[-ar_1-br_2-(c+2\gamma x)r] \;. \tag{5}$$

The integral over v_1 and v_2 may be calculated analytically and reads[19]

$$16\pi^2/[(a+b)(a+c+2\gamma x)(b+c+2\gamma x)] \;,$$

so that

$$\tilde{I}(-1,-1,-1)=16\pi^2/(a+b)\int_1^\infty \frac{[1+1/(2x^2)](x^2-1)^{1/2}dx}{x^2(a+c+2\gamma x)(b+c+2\gamma x)}=16\pi^2/(a+b)I(-1,-1,-1) \;. \tag{6}$$

By the standard substitution

$$(x^2-1)^{1/2}=t(x-1) \;, \tag{7}$$

the integral $I(-1,-1,-1)$, defined by (6), is reduced to the form

$$I(-1,-1,-1)=\frac{4}{(a+c+2\gamma)(b+c+2\gamma)}(4B-3A) \;, \tag{8a}$$

where

$$A=\int_\infty^1 \frac{(t^4-t^2)dt}{(t^2+1)^2(t^2-p)(t^2-q)} \;, \tag{8b}$$

$$B=\int_\infty^1 \frac{t^4(t^2-1)dt}{(t^2+1)^4(t^2-p)(t^2-q)} \;, \tag{8c}$$

with $p=-(2\gamma-a-c)/(2\gamma+a+c)$ and $q=-(2\gamma-b-c)/(2\gamma+b+c)$.

As integrals of rational functions may always be expressed by elementary functions, it is readily seen from Eq. (8) that $I(-1,-1,-1)$ may be calculated analytically. In order to do that, we decomposed the integrands into sums of partial quotients with respect to t, and integrated term by term. After some straightforward although tedious algebra, this yielded

$$\begin{aligned} A=&\frac{(3+p+q-pq)}{(q+1)^2(p+1)^2}[\arctan(1)-\pi/2]+\frac{1}{2(p+1)(q+1)}\\ &+C\ln\left|\frac{1-p^{1/2}}{1+p^{1/2}}\right|+E\ln\left|\frac{1-q^{1/2}}{1+q^{1/2}}\right|+K\{\arctan[(-p)^{-1/2}]-\pi/2\}\\ &+L\{\arctan[(-q)^{-1/2}]-\pi/2\} \;, \end{aligned} \tag{9}$$

where

$$C=\begin{cases}0 & \text{if } p<0\\ \dfrac{(p-1)p^{1/2}}{2(p+1)^2(p-q)} & \text{if } p>0,\end{cases} \qquad E=\begin{cases}0 & \text{if } q<0\\ \dfrac{(1-q)q^{1/2}}{2(q+1)^2(p-q)} & \text{if } q>0 \;,\end{cases}$$

$$K=\begin{cases}0 & \text{if } p>0\\ \dfrac{p(p-1)}{(p+1)^2(p-q)} & \text{if } p<0,\end{cases} \qquad L=\begin{cases}0 & \text{if } q>0\\ \dfrac{q(1-q)}{(q+1)^2(p-q)} & \text{if } q<0 \;,\end{cases}$$

and

$$B=P[\arctan(1)-\pi/2]+R\ln\left[\frac{1-p^{1/2}}{1+p^{1/2}}\right]+S\ln\left[\frac{1-q^{1/2}}{1+q^{1/2}}\right]$$
$$+T\{\arctan[(-p)^{-1/2}]-\pi/2\}+U\{\arctan[(-q)^{-1/2}]-\pi/2\}+Q\ , \qquad (10)$$

where

$$P=\frac{2p+2q+5pq-1}{4(p+1)^2(q+1)^2}+\frac{1}{2(p-q)}\left[\frac{q^2(q-1)(q+3)}{(q+1)^4}-\frac{p^2(p-1)(p+3)}{(p+1)^4}\right],$$

$$Q=\frac{1}{24}\frac{7p+7q+19pq-5}{(p+1)^2(q+1)^2}+\frac{1}{2(p-q)}\left[\frac{q^2(q-1)}{(q+1)^3}-\frac{p^2(p-1)}{(p+1)^3}\right],$$

$$R=\begin{cases}0 \text{ if } p<0\\ \dfrac{p^{3/2}(p-1)}{2(p+1)^4(p-q)} \text{ if } p>0\ ,\end{cases} \qquad S=\begin{cases}0 \text{ if } q<0\\ -\dfrac{q^{3/2}(q-1)}{2(q+1)^4(p-q)} \text{ if } q>0\ ,\end{cases}$$

$$T=\begin{cases}0 \text{ if } p>0\\ \dfrac{p^2(p-1)}{(p+1)^4(p-q)} \text{ if } p<0\ ,\end{cases} \qquad U=\begin{cases}0 \text{ if } q>0\\ -\dfrac{q^2(q-1)}{(q+1)^4(p-q)} \text{ if } q<0\ .\end{cases}$$

The above formulas, along with Eqs. (6) and (8a), are the sought analytical expressions for the basic integral $\widetilde{I}(-1,-1,-1)$.

IV. GENERATION OF OTHER INTEGRALS

As has been mentioned at the beginning of Sec. III, other integrals involving the Uehling potential may be generated from $\widetilde{I}(-1,-1,-1)$ by differentiation with respect to a, b, and c. Once again, the procedure is tedious but straightforward.

For instance, the integral $\widetilde{I}(0,0,-1)$, generated in this way, reads

$$\widetilde{I}(0,0,-1)=\frac{\partial^2\widetilde{I}(-1,-1,-1)}{\partial a\partial b}$$
$$=4F(0,0,-1)\left[\frac{1}{(p-q)}[g_1(q)-g_1(p)]+\frac{(8\rho+\frac{5}{3})pq-(\rho+\frac{1}{3})p-(\rho+\frac{1}{3})q-(10\rho+\frac{7}{3})}{(q+1)^2(p+1)^2}\right]$$
$$+4q'F(0,-1,-1)\left[\frac{[g_1(q)-g_1(p)]}{(p-q)^2}+\frac{g_1'(q)}{(p-q)}-\frac{(8\rho+\frac{5}{3})pq-(10\rho+\frac{7}{3})p-(\rho+\frac{1}{3})q-(19\rho+\frac{13}{3})}{(q+1)^3(p+1)^2}\right]$$
$$+4p'F(-1,0,-1)\left[\frac{[g_1(q)-g_1(p)]}{(p-q)^2}-\frac{g_1'(p)}{(p-q)^2}-\frac{(8\rho+\frac{5}{3})pq-(\rho+\frac{1}{3})p-(10\rho+\frac{7}{3})q-(19\rho+\frac{13}{3})}{(q+1)^2(p+1)^3}\right]$$
$$+4p'q'F(-1,-1,-1)\left[-2\frac{g_1(q)-g_1(p)}{(p-q)^3}-\frac{g_1'(p)+g_1'(q)}{(p-q)^2}\right.$$
$$\left.+\frac{(8\rho+\frac{5}{3})pq-(10\rho+\frac{7}{3})p-(10\rho+\frac{7}{3})q-(28\rho+\frac{37}{3})}{(q+1)^3(p+1)^3}\right], \qquad (11)$$

where $\rho=\arctan(1)-\pi/2$ and

$$F(l,m,n)=\int\int dv_1dv_2r_1^lr_2^mr^n\exp[-ar_1-br_2-(c+2\gamma)r] \qquad (12)$$

is the integral appearing in the standard three-body problem with Coulombic potentials which can be analytically calculated from

$$F(-1,-1,-1)=16\pi^2/[(a+b)(b+c+2\gamma)(a+c+2\gamma)]$$

by differentiation with respect to the parameters.[19,20]

$g_1(x)$ is defined by

$$g_1(x)=(x+1)^{-4}g_2(x)\ ,$$

where

$$g_2(x)=2\rho(x^4+2x^3-3x^2)+2x^4-2x^2+(3x^4-x^3+x^2-3x)\left[\frac{1}{2}\sigma x^{-1/2}\ln\left[\frac{1-x^{1/2}}{1+x^{1/2}}\right]+(1-\sigma)\left[\arctan[(-x)^{-1/2}]-\frac{\pi}{2}\right]\right]$$

with

$$\sigma=\begin{cases}1 & \text{if } x>0\\ 0 & \text{if } x<0\ ,\end{cases}$$

so that the derivatives which appear in Eq. (11) read

$$g_1'(x)=-4(x+1)^{-5}g_2(x)+(x+1)^{-4}g_2'(x)\ ,$$

with

$$\begin{aligned}g_2'(x)={}&2\rho(4x^3+6x^2-6x)+8x^3-4x+\tfrac{1}{4}\sigma(21x^3-5x^2+3x-3)x^{-1/2}\ln\left[\frac{1-x^{1/2}}{1+x^{1/2}}\right]\\&-\tfrac{1}{2}(3x^3-x^2+x-3)x^{1/2}/(1-x)+(1-\sigma)(12x^3-3x^3+2x-3)\left[\arctan[(-x)^{-1/2}]-\frac{\pi}{2}\right]\ .\end{aligned}$$

p' and q' denote the derivatives of p and q with respect to a and b, respectively, and read

$$p'=(2\gamma+a+c)^{-1}+(2\gamma-a-c)(2\gamma+a+c)^{-2}\ ,$$

$$q'=(2\gamma+b+c)^{-1}+(2\gamma-b-c)(2\gamma+b+c)^{-2}\ .$$

Other integrals necessary for the calculations of the binding energies of $J=0$ states [i.e., $\tilde{I}(-1,0,0)$ and $\tilde{I}(0,-1,0)$] may be readily found by the appropriate interchange of parameters a, b, and c. For the $J=1$ states further integrals are needed. They can again be calculated analytically from the formulas derived from Eq. (11) by subsequent differentiation.

V. CONCLUSIONS

We have shown that the matrix elements of the Uehling potential in the basis of explicitly correlated two-particle functions [defined in Eq. (2)] used in calculations of the binding energies of muonic molecules may be expressed in an analytical form, although the potential itself may not. The resulting expressions are rather complicated. Nevertheless, their evaluation is likely to be less time consuming and possibly more accurate than numerical integration. The derivation of the corresponding expressions for the variational functions with $J>0$ will certainly be very tedious, but may easily be done with computer programs for symbolic operations, like MACSYMA, ALTRAN, or MAPLE. Application of the resulting expressions in actual calculations of the binding energies of muonic molecules would allow one to include the contribution to the binding energy which arises due to the polarization of the vacuum and seems to be the most important correction to the Coulomb model. This would be likely to increase considerably the physical relevance of the results. We intend to undertake such an attempt in the future.

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*Permanent address: Department of Theoretical Chemistry, Jagiellonian University, 30-060 Cracow, Karasia 3, Poland.

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