light and the σ^- component in absorption. The second peak at 8 kG arises from the resonance between the σ^+ component in the exciting light and the π component in absorption. The shapes of the σ^- and σ^+ components in the exciting light are identical and thus the observed differences in the profiles of the peaks in Fig. 10(a) should arise from the differences in the rates of increase in $\Delta\gamma$ with magnetic field for the σ and π components, as shown in Fig. 10(b). These rates are in the ratio $\frac{4}{3}:\frac{2}{3}$ and, consequently, the half-width of the second peak is twice that of the first peak. This relation has been shown experimentally not to depend on the magnitude of the magnetic field.

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S-Wave Cross Section for $D(p,\gamma)He^3$†

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Nonadiabatic theory has been applied to calculate an accurate wave function for the $p\mu d$ muonic molecule. The value of the wave function describing the nuclear motion evaluated at an internuclear distance equal to zero yields a cross section for the $D(p,\gamma)He^3$ reaction in agreement with the experimental value.

I. INTRODUCTION

FROM the total fusion rate of a proton and deuteron bound in an S state by a muon, one can get,[1,2] under certain assumptions, the radiative fusion rate λ_r, which can be expressed as

$$\tfrac{1}{3}\lambda_r = R|G(0)|^2, \quad (1)$$

where R denotes the reaction constant, the $\frac{1}{3}$ factor is the probability that the pd system is in the doublet state, and $G(0)$ is the value of the wave function describing the nuclear motion in the muonic molecule $p\mu d$, evaluated with the internuclear distance equal to zero. On the other hand, the low-energy S-wave cross section for the $D(p,\gamma)He^3$ reaction is[1]

$$\sigma_s = 2\pi\eta[\exp(2\pi\eta)-1]^{-1}R/v, \quad (2)$$

where v denotes the velocity of the nuclei at infinity, and $\eta = e^2/\hbar v$. Assuming the same rate constant R in (1) and (2), one can eliminate it from the above equations thus getting a relationship between λ_r, σ_s, and $G(0)$. Usually the experimental value of λ_r and the theoretical value of $G(0)$ are used to evaluate σ_s, and the result is compared with the experimental cross section. However, previous theoretical values of $G(0)$ yielded the cross section σ_s, differing from the experimental value by a factor of 10 or more.[3] Recently, Carter[2] reported for σ_s a more accurate value which, however, was still about 2.5 times smaller than the experimental one. To clarify this matter, extensive computations on the $p\mu d$ system have been carried out. The method of computation is briefly sketched in Sec. II, and the results are presented and discussed in Sec. III.

II. METHOD

The $p\mu d$ system is similar to the HD^+ molecular ion, the only difference being in the mass of the light particle. However, since the muon is almost 207 times heavier than the electron, the adiabatic approximation, successful in molecular calculations, breaks down, and the muonic molecule must be treated as a three-particle system. Previous nonadiabatic calculations[4–9] for muonic molecules have usually been limited to symmetric systems, as, e.g., $p\mu p$ or $d\mu d$. For $p\mu d$, however,

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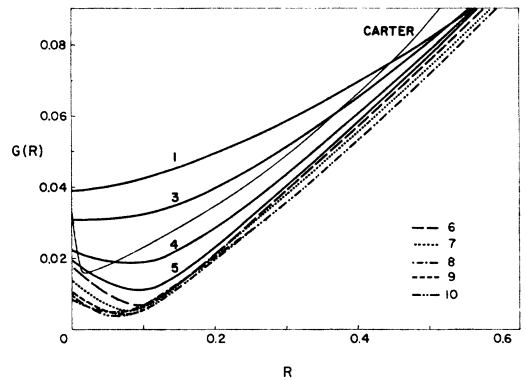

FIG. 1. Pseudowave-function $G(R)$ for $p\mu d$ computed from various complete wave functions as defined in Table I; both G and R are in muonic units.

several calculations have also been carried out.[2,10,11] The main difference between the various calculations consists in using different basis sets to approximate the exact solution of the three-particle Schrödinger equation and in taking different numbers of terms in the expansion, which critically affects the accuracy of the results.

The method employed in the present calculation was that developed previously by Wolniewicz and the present author[12,13] for nonadiabatic treatment of diatomic molecules. It consists in transforming the complete Hamiltonian to the angular momentum representation, separating off the rotations, and solving, by the variational method, the equation, or system of equations, for functions depending only on the relative coordinates of the particles. For the nonrotational ground state of $p\mu d$, we assume the variational wave function in the form

$$\Psi=(2\pi)^{-1/2}\sum_{in}c_{in}\Phi_i\chi_n, \tag{3}$$

TABLE I. Convergence of energy and of $G(0)$ for $p\mu d$ with increasing number of terms in expansion (3).

Run	No. of terms	$(r+s)_{\max}$	$n_{\max}$	E (m.u.)	E (eV)	$G(0)$
1	59	4	4	−0.5106636	−2873.29	0.03902
2	67	4	5	−0.5113848	−2877.35	0.02484
3	84	5	5	−0.5115945	−2878.53	0.03125
4	97	5	6	−0.5120430	−2881.05	0.02251
5	106	5	7	−0.5122567	−2882.26	0.01948
6	113	5	8	−0.5123528	−2882.80	0.01787
7	116	5	9	−0.5123824	−2882.96	0.01385
8	120	5	10	−0.5123950	−2883.03	0.00914
9	128	6	10	−0.5124270	−2883.21	0.01091
10	133	6	11		−2883.26	

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TABLE II. Variation of γR_e and R_e in the 133-term expansion for $p\mu d$.

γR_e	R_e	E	$V/2E$	$G(0)$
1.417	2.382	−0.5124329	0.9998992	0.01013
1.517	2.382	−0.5124359	0.9999947	0.00993
1.617	2.382	−0.5124303	1.0000968	0.00940
1.502	2.382	−0.5124354	0.9999583	0.00964
1.502	2.332	−0.5124356	0.9999772	0.00921
1.502	2.307	−0.5124350	1.0000550	0.00923
1.502	2.282	−0.5124378	1.0000920	0.00913
1.502	2.232	−0.5124336	1.0001374	0.00953

where

$$\begin{aligned}\Phi_i&=\phi_{r_is_i}(\alpha_1,\beta;\,\xi,\eta)+\lambda\phi_{r_is_i}(\alpha_2,\,-\beta;\,\xi,\,\eta),\\ \phi_{rs}&=\exp(-\alpha\xi-\beta\eta)\xi^r\eta^s,\\ \chi_n&=(4\pi)^{-1/2}R^{-3/2}H_n(x)\exp(-x^2/2),\end{aligned} \tag{4}$$

ξ and η are elliptic coordinates of the muon, R is the distance between the two nuclei,[14] H_n denotes the nth Hermite polynomial, and $x=\gamma(R-R_e)$. Thus, in addition to the linear parameters c_{in}, we have α_1, α_2, β, γ, R_e, and λ to be optimized by using the variational principle.

Note that the ϕ_{rs} functions depend implicitly on the internuclear distance R, and in the calculation of the matrix elements the $R^{-3/2}$ factor in χ_n merely cancels the R^3 factor from the volume element in elliptic coordinates.

The basis set (4) results in matrix elements analogous to those derived previously[12] for the hydrogen molecule, and they will not be given here explicitly.

Following Carter,[2] the calculated three-particle wave functions were used to compute the pseudo-wave-functions for nuclear motion defined as

$$G(R)=\left[\int|\Psi|^2d\tau_\mu\right]^{1/2}, \tag{5}$$

where the integration extends only over the elliptic coordinates of the muon. The values of $G(0)$ were then used in Eq. (1), which combined with Eq. (2) yielded the value of σ_s.

TABLE III. Nonadiabatic energies of $p\mu d$ calculated with various wave functions.

No. of terms	Energy (eV)	Reference
12	−2856	a
8	−2859	a
84	−2876.5	b
?	−2883.8	c
133	−2883.3	Present work

[a] Reference 10. [b] Reference 11. [c] Reference 2.

[14] Not to be confused with the reaction constant used in Eqs. (1) and (2).

III. RESULTS AND DISCUSSION

The numerical computations were carried out on the IBM 7094 computer at the Computation Center of the University of Chicago. The primitive integrals over the muonic coordinates and the Hermite polynomials were calculated in double-precision and all other quantities in single-precision arithmetic.

The convergence of the results with increasing number of terms in the expansion (3) was rather slow and a systematic approach had to be adopted to select the most important terms. The general procedure was the same as that used previously[13,15] in H_2 computations, i.e., numerous machine runs were made in which the expansion length was gradually increased and those terms that did not improve the energy were dropped in subsequent runs. The nonlinear parameters were first optimized for an arbitrarily selected wave function, and in the course of the systematic selection procedure they were reoptimized.

Table I shows convergence of the energy and of $G(0)$, as defined by (5), with increasing number of terms.[16] The runs 1–8 were all made with the same set of the nonlinear parameters. One can notice that terms with higher powers of ξ and η increase the value of $G(0)$, whereas those with higher degrees of the Hermite polynomials have a diminishing effect. A reoptimization of the nonlinear parameters in each case might make these effects less pronounced.

The $G(R)$ curves are plotted in Fig. 1 which shows that, particularly in the vicinity of $R=0$, they are quite sensitive to the accuracy of the complete wave function. It is also seen that the general shape of our curves is quite different from the shape of the $G(R)$ curve calculated by Carter.[2]

In the last two runs, 9 and 10, we tried to reoptimize the parameters γ and R_e since they seemed to affect most significantly the value of $G(0)$. The optimization was more or less successful for the 128-term expansion but could not be carried out for the 133 terms. With this expansion length for a function of three variables, and working in single precision, we had nearly redundant terms, and the rounding errors were larger than the changes of energy due to the exponent variation. The problem could be overcome by reselecting the terms and omitting those that contributed mainly to the rounding errors, but this did not seem to be worth doing. It was rather unlikely that this would give any sizable energy improvement, and from the results shown in Tables I and II, it was quite clear that the final value of $G(0)$ obtained with our basis set would be between 0.009 and 0.010. Using Eqs. (1) and (2) and Carter's value[2] of the radiative fusion rate $\lambda_r=0.276$ μsec^{-1}, the above bracketing values of $G(0)$ give $\sigma^s=1.30\times10^{32}$ cm^2 and $\sigma_s=1.05\times10^{32}$ cm^2, respectively, for 25-keV protons, and both cross sections agree with the experimental value[17] $\sigma_s=(1.3\pm0.3)\times10^{32}$ cm^2 within the experimental error.

The problem of energy of the $p\mu d$ molecule remains, however, not quite clear. In Table III, we compare our result with nonadiabatic energies computed by other authors, and it is seen that Carter's value[2] is by 0.0001 m.u., where m.u. stands for muonic units (or 0.5 eV), lower than the best result of the present work. Judging from the energies listed in Table I, it does not seem likely that by increasing the expansion length with the basis set (4), which in double precision would be still possible, one could get an energy improvement of 0.5 eV over the best result listed in Table I. The main difference between our basis set and the set used by Carter consists apparently in the fact that he has only linear dependence on R in the exponents. However, in our basis set, we have the factor $\exp[-\frac{1}{2}\gamma^2(R-R_e)^2]$, and since both γ and R_e are variational parameters, we have in principle both the quadratic and the linear dependence on R in the exponent. Carter expands the wave function in terms of products of simple exponentials and uses different exponents in each term of the expansion. Variation of exponents is known to be a powerful tool in determining approximate wave functions, and Carter's basis set with carefully optimized exponents could give a faster convergence of the energy than ours. However, our best results for $G(R)$ as shown in Fig. 1 seem to be better than Carter's; therefore, it is somewhat puzzling that we were unable to reach his energy.

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