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Variational Monte Carlo calculations of the ^{2}H$(d,\gamma)^4$He reaction at low energies

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The ^{2}H$(d,\gamma)^4$He reaction is studied at center-of-mass energies below 500 keV, where it is dominated by the $E2$ transition from the $^5S_2$ continuum state to the ground state of the α particle. Both the $^5S_2$ continuum and the ground states are calculated with the variational Monte Carlo method using the realistic Argonne-v_{14} two-nucleon and Urbana model-VII three-nucleon interactions. A qualitative agreement with the observed cross section is obtained. This reaction can proceed only through the D states in the deuteron and/or in the α particle. It is found that, depending upon the continuum wave function, the contributions of the deuteron and α-particle D states can either add to produce a large cross section, or cancel. The reaction is thus very sensitive to the continuum wave function.

I. INTRODUCTION

The study of radiative capture reactions has occupied a privileged place in few-body physics due to our understanding of the electromagnetic interaction. Particulary at low energies, the associated selection rules restrict the number of relevant partial waves, thus scaling down the computational effort and permitting a clearer interpretation of the physical processes involved. Another important feature of these reactions is that some of them occur due to the D-state components in the nuclear wave functions which are generated by the two-nucleon tensor interaction.

Among the radiative capture reactions, the ^{2}H$(d,\gamma)^4$He reaction is especially important due to its implications in several domains of physics. The radiative fusion of two low-energy deuterons is important in astrophysics, since it can influence the predictions for the abundances of the primordial elements in the Universe.[1] The detailed knowledge of the reaction mechanism may also have applications in fusion reasearch.[2] Finally, this reaction can provide information on the D-state components of the deuteron and α-particle wave functions, of interest in nuclear physics.

Since the early 1950s, the cross section of the ^{2}H$(d,\gamma)^4$He reaction has been the object of both theoretical and experimental studies.[3–6] More recently, in the last decade, the access to more sophisticated experimental apparatus and the possibility of polarizing the ion beams have produced a renewed interest in the study of this fusion reaction. Measurements of the cross section and polarization observables have been carried out at relative d-d energies ranging from 25 keV up to 47.5 MeV.[7–14] From the theoretical point of view, more and more elaborate models have been presented in an attempt to overcome inconsistent interpretations of the experimental data.[7,10,11,14–21] Substantial progress has been made with the resonating-group method (RGM) to include the effects of the coupling of the scattering channel to the $t+p$ and ^{3}He$+n$ channels.[21] However, none of the theories used so far consistently describes the initial and final states, starting from realistic models of the nuclear forces.

We discuss here a calculation of the ^{2}H$(d,\gamma)^4$He reaction performed with bound- and continuum-state wave functions obtained from the Argonne-v_{14} two-nucleon and Urbana-VII three-nucleon interactions. We are especially interested in very low energies, $E_{\rm c.m.} \leq 500$ keV, where the reaction, as mentioned before, seems to have implications in astrophysics and fusion research, and where the D-state components of both deuteron and α particle play a determinant role.

It is known that the symmetry between the two deuterons restricts the entrance channels to those in which the orbital angular momentum and the spin are both even or odd. The allowed electromagnetic transitions, for multipoles $l \leq 2$, are then[15]

$$(E1;{}^3P_1),\ (M1,{}^5D_1),\ (E2;{}^1D_2),\ (E2;{}^5S_2)\ ,$$
$$(E2;{}^5D_2),\ (E2;{}^5G_2),\ (M2;{}^3P_2),\ (M2;{}^3F_2)\ .$$

At very low energies ($E_{\rm c.m.} < 0.5$ MeV), the centrifugal barrier tends to suppress all transitions except the one from the $^5S_2$ channel. Hence, in this work we only consider the $E2$ transition from this continuum state. Isospin conservation rules imply that the $E2$ transition from the $^1D_2$ channel dominates in the $E_{\rm c.m.} \sim 2-5$-MeV region;[20] however, it has been shown that both the $E1$ and

$M2$ transitions are important at $E_{\text{c.m.}} \sim 0.6$ MeV.[14,21]

In Sec. II we give a short description of the α-particle wave function calculated by Schiavilla *et al.*[22] with the variational Monte Carlo (VMC) method and used in the present work. The initial d-d scattering state wave function is also calculated using the VMC methods developed by Carlson *et al.*[23] as discussed in Sec. III. In Sec. IV we describe the calculation of the transition matrix element and, finally, in Sec. V we present and discuss the results for the astrophysical factor. In the last two sections we also analyze the contributions of the S- and D-state components of the deuteron and α-particle wave functions to this transition.

II. THE FINAL STATE

A variational calculation of the α particle has been previously carried out by Schiavilla *et al.*[22] using the following ansatz for the wave function

$$|\psi_\alpha\rangle = S \prod_{i<j} F_{ij} |\Phi\rangle \ , \tag{1}$$

where $|\Phi\rangle$ is an antisymmetric four-nucleon spin-isospin state and S symmetrizes the product of the correlation operators F_{ij}. These are given by

$$F_{ij} = f^c(r_{ij}) + \left[\prod_{k\neq i,j} f^{\sigma}_{ijk}\right] f^{\sigma}(r_{ij}) \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + \left[\prod_{k\neq i,j} f^{t\tau}_{ijk}\right] f^{t\tau}(r_{ij}) S_{ij} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \ . \tag{2}$$

In the above equation $f^c(r_{ij})$, $f^{\sigma}(r_{ij})$, and $f^{t\tau}(r_{ij})$ are, respectively, the central, spin, and tensor correlation functions, S_{ij} is the tensor operator, and f^p_{ijk}, $p=\sigma, t\tau$, are three-body correlation functions having the following form:

$$f^p_{ijk} = 1 - t_{1,p} \left[\frac{r_{ij}}{R_{ijk}}\right]^{t_{2,p}} \exp(-t_{3,p} R_{ijk}) \ , \tag{3}$$

where

$$R_{ijk} = r_{ij} + r_{jk} + r_{ki} \ . \tag{4}$$

The functions $f^c(r_{ij})$, $f^{\sigma}(r_{ij})$, and $f^{t\tau}(r_{ij})$ and the parameters $t_{1,p}$, $t_{2,p}$, and $t_{3,p}$ were determined by minimizing the energy obtained with the Argonne-v_{14} two-nucleon and Urbana-VII three-nucleon interactions. The calculated α-particle binding energy and D_2 parameter were found to be, respectively, $E_\alpha = -27.8 \pm 0.4$ MeV and $D_2 = -0.16$ fm^2. The D_2 parameter is defined as

$$D_2 = \lim_{k\to 0} \frac{1}{k^2} \frac{u_2(k)}{u_0(k)} \ ,$$

where u_0 and u_2 are the S and D components of the relative wave function between the two deuteron clusters in the α particle.

III. THE INITIAL STATE

A. Ansatz for the *d-d* wave function

Our anstaz for the initial d-d state wave function lies on the basic assumption that the average d-d interaction effects can be represented by an effective d-d potential, and that the effects associated with the strong N-N interaction, important at short distances and not included in the effective potential, can be taken into account by means of two- and three-body correlation operators. Within this approximation, the expression for the d-d wave function is given by

$$|\psi_{dd}\rangle = A |\psi^{JM_j}_{LS}\rangle \tag{5}$$

with

$$\langle \mathbf{r}\mathbf{r}_{12}\mathbf{r}_{34} | \psi^{JM_j}_{LS}\rangle = \sum (L\lambda S\sigma | JM_j)(1\sigma_{12} 1\sigma_{34} | S\sigma) \times \left[S \prod{}' G_{ij}\right] Y_{L\lambda}(\hat{r}) \psi_{LS}(r) \times \psi_d^{\sigma_{12}}(\mathbf{r}_{12}) \psi_d^{\sigma_{34}}(\mathbf{r}_{34}) \ , \tag{6}$$

where $\mathbf{r}_{12}$ and $\mathbf{r}_{34}$ are, respectively, the internal coordinates of the deuterons formed by particles 1 and 2, and by particles 3 and 4, and $\mathbf{r}$ is the distance between their centers of mass

$$\mathbf{r} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2} - \frac{\mathbf{r}_3 + \mathbf{r}_4}{2} \ . \tag{7}$$

σ_{12} and σ_{34} are the spin projections of the two deuterons, coupled to total spin S with projection σ, and $L\lambda$ and JM_j denote the relative and total angular momenta. In Eq. (5), A is the full antisymmetrization operator. As the deuteron wave functions are already antisymmetric, we have to consider only the permutation of particles between the two deuterons, hence,

$$A = \frac{1}{\sqrt{6}} (1 - P^{13} - P^{14} - P^{23} - P^{24} + P^{13} P^{24}) \ . \tag{8}$$

This operator can be written in a more convenient way as

$$A = \mathcal{A} S_{dd} \ , \tag{9}$$

where $\mathcal{A}$ is given by

$$\mathcal{A} = \frac{1}{\sqrt{3}} (1 - P^{13} - P^{14}) \ . \tag{10}$$

and S_{dd} projects out the states symmetric under the exchange of the two identical deuterons:

$$S_{dd} = \frac{1}{\sqrt{2}} (1 + P^{13} P^{24}) \ . \tag{11}$$

It is obvious that $S_{dd} = \sqrt{2}$ when $L+S$ is even and zero otherwise, and therefore

$$|\psi_{dd}\rangle = \sqrt{2} \mathcal{A} |\psi^{JM_j}_{LS}\rangle \ , \tag{12}$$

with $L+S=$even as a constraint.

The symmetrized product $S\prod{}' G_{ij}$ of the four pair-correlation operators between nucleons belonging to different deuterons is meant to take into account the short-range effects of the N-N interaction not included in the effective deuteron-deuteron potential used to calculate the relative wave function $\psi_{LS}(r)$. The G_{ij} operators are taken as

$$G_{ij}=g^c(r_{ij})+\sum_{p=2}^{3} g^p(r_{ij})O_{ij}^p+\sum_{p=4}^{6}\left[\prod_{k\neq i,j} g_{ijk}^p\right]g^p(r_{ij})O_{ij}^p \qquad (13)$$

with

$$O_{ij}^{p=2,6}=\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j,\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j,(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j),S_{ij},S_{ij}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j \ . \qquad (14)$$

The $g^c(r_{ij})$ and $g^p(r_{ij})$ are obtained from the solutions of N-N Schrödinger-like equations[24] and satisfy the boundary conditions

$$g^c(r)=1 \quad \text{for } r\geq d_c \ , \qquad (15a)$$

$$g^p(r)=\begin{cases}0 & \text{for } r\geq d_c \text{ and } p=\tau,\sigma,\sigma\tau \ , & (15b)\\ 0 & \text{for } r\geq d_t \text{ and } p=t,t\tau \ . & (15c)\end{cases}$$

As a consequence, G_{ij} has the property

$$G_{ij}=1 \quad \text{for } r_{ij}\geq \max(d_c,d_t) \ . \qquad (16)$$

In principle, d_c and d_t should be treated as variational parameters. However, we have used the values $d_c=1.4$ fm and $d_t=1.9$ fm from Ref. 24. In previous studies the energies were not found to be very sensitive to variations of d_c and d_t around these values. g_{ijk}^p for S_{ij} and $S_{ij}\ \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$ correlations are taken to be $f_{ijk}^{t\tau}$ in the wave function ψ_α, while g_{ijk}^p for the $(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j)$ correlation is f_{ijk}^{σ} of the same wave function.

$\psi_d^{\sigma_{ij}}$ is the deuteron wave function, generated with the Argonne-v_{14} two-body potential. For an isolated deuteron it can be written as

$$\Phi_d^{\sigma_{ij}}(r_{ij})=[f_d^c(r_{ij})+f_d^t(r_{ij})S_{ij}]\phi_d^{\sigma_{ij}} \ , \qquad (17)$$

where $f_d^c(r_{ij})=u(r_{ij})$ and

$$f_d^t(r_{ij})=\omega(r_{ij})/\sqrt{8} \ ,$$

and $\phi_d^{\sigma_{ij}}$ is a two-nucleon spin-isospin state having isospin $T=0$, spin $S=1$, and projection σ_{ij}. In the present work, the $\psi_d^{\sigma_{ij}}$ in the d-d state is taken as

$$\psi_d^{\sigma_{ij}}(r_{ij})=\left[f_d^c(r_{ij})+\left[\prod_{k\neq i,j} f_{ijk}^{t\tau}\right]f_d^t(r_{ij})S_{ij}\right]\phi_d^{\sigma_{ij}} \ . \qquad (18)$$

When the deuterons are far apart, $f_{ijk}^{t\tau}$ [Eq. (3)] tend to unity and the above $\psi_d^{\sigma_{ij}}$ becomes the wave function of an isolated deuteron [Eq. (17)].

Finally, the wave function $\psi_{LS}(r)$ describes the relative motion of the two deuterons and is generated from an effective deuteron-deuteron potential containing two terms:

$$V_{dd}(r)=V_s(r)+V_{\rm Coul}(r) \ . \qquad (19)$$

The effective Coulomb potential $V_{\rm Coul}(r)$ is obtained from the charge density of the deuterons:

$$V_{\rm Coul}(r)=\frac{1}{(2\pi)^3}\int e^{-i\mathbf{K}\cdot\mathbf{r}}[\tilde{F}_c(K)]^2\tilde{V}(K)d\mathbf{K} \ , \qquad (20)$$

where $\tilde{F}_c(K)$ is the Fourier transform of the deuteron charge density and $\tilde{V}(K)$ the Fourier transform of the Coulomb potential between point charges. $V_s(r)$ represents the average strong interaction between the deuterons. We neglected its tensor and spin-orbit terms based on the experimental observation that the vector and tensor analyzing powers for d-d scattering are small[25] at low energies. This approximation implies that the relative wave function does not depend upon J and that there is no coupling between channels with different orbital angular momenta.

The present model also neglects the coupling of the d-d channel to the on-shell ^{3}H$+p$ and ^{3}He$+n$ channels. This approximation is supported by the fact that the $^5S_2$ partial wave, the only initial state we are considering, has spin 2 and therefore the coupling to these reaction channels can only proceed via the tensor force. Furthermore, the conservation of J and parity implies that the lowest orbital angular momentum of the (3+1) channels is 2, and, at low energies, the D waves are suppressed by the centrifugal barrier. Thus, coupling to the on-shell (3+1) channels is expected to play a minor role. The effects of the coupling to the virtual (3+1) partitions are, to some extent, taken into account by means of the G_{ij} correlation operators.

B. The variational calculation

The main aim of the variational calculation is to determine the relative wave function in the $^5S_2$ channel from the realistic nuclear forces. It is strongly distorted by the Pauli repulsion due to which all the theoretical phase shifts, generated mainly with RGM calculations[26–28] are negative. Since all these calculations give very similar results, we assume in the present work that the correct asymptotic behavior of this partial wave is known and use it to simplify our calculation. The consistency of this assumption is verified in the calculation.

The possible existence of inner oscillations, almost independent of energy, in the relative wave functions of clusters of nucleons was pointed out by Tamagaki and Tanaka[29] and by Okai and Park,[30] as a consequence of the Pauli principle. Analyzing the effective equation that determines the relative wave function within the RGM formalism, these authors observed that those Pauli oscillations were determined by the exchange kernels.

Under these circumstances, we consider $V_s(r)$ as a sum of two Woods-Saxon potentials, one of them attractive and the other repulsive. The parameters of these potentials are chosen so as to reproduce the phase shifts obtained by the RGM calculation of Ref. 28 up to 4 MeV, and to generate wave functions with different short-range behaviors, namely, with Pauli oscillations having different characteristics or even without Pauli oscillations. In Fig. 1 we show the five trial relative wave functions $U_{02}(r)$ defined by

$$\psi_{02}(r)=\mathcal{N}\exp(i\delta_{02})U_{02}(r) \qquad (21)$$

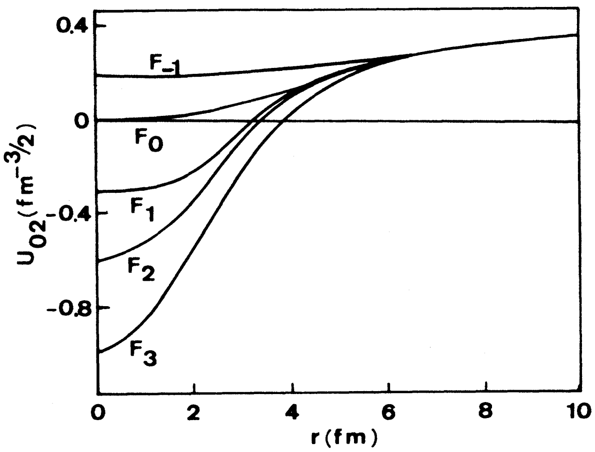

FIG. 1. Relative *d-d* wave functions generated with the effective *d-d* potentials, for a kinetic energy of 100 keV. All the wave functions have the same phase shift: $\delta(100\ \text{keV}) = -2.8518°$.

that have been considered in this work. In the above equation $\mathcal{N}$ is a normalization constant chosen such that, in the absence of the effective potential, the scattering wave function becomes the incident plane wave. The wave functions in Fig. 1 are obtained for $E_{\text{c.m.}} = 100$ keV, from potentials whose parameters are given in Table I. For convenience, the wave functions and the potentials are labeled F-1, $F0$, $F1$, $F2$ $F3$, and $V_s - 1$, V_s0, V_s1, V_s2, V_s3.

The expectation value of the Hamiltonian $\langle H \rangle$ is then calculated from the variational wave function [Eq. (6)] containing these relative wave functions. We confine the system in a box with a radius of 9 fm, where the wave functions are in the asymptotic regime, and therefore the boundary condition is clearly imposed. The best *d-d* wave function is the one that gives the lowest value for $\langle H \rangle$, which is calculated from 48 000 Monte Carlo samples, using the same Argonne-v_{14} two-nucleon and Urbana-VII three-nucleon interactions used in the variational calculation of the α particle. If the assumed phase shift is consistent with the microscopic Hamiltonian, then the minimum value $\langle H \rangle_0$ should satisfy

$$\langle H \rangle_0 \geq 2E_d + 100 \text{ keV} \tag{22}$$

with $E_d = -2.225$ MeV the deuteron binding energy.

TABLE I. Woods-Saxon well parameters of the five different effective *d-d* potentials, labeled $V_s - 1$, V_s0, V_s1, V_s2, and V_s3. The subscripts r and a refer to the repulsive and attractive potentials, respectively.

Potential label	Woods-Saxon well parameters (MeV)	(fm)	(fm)
$V_s - 1$	$V_{0r} = 0.845$	$R_{0r} = 7.556$	$a_r = 0.299$
	$V_{0a} = 0.0$		
V_s0	$V_{0r} = 75.369$	$R_{0r} = 1.874$	$a_r = 0.743$
	$V_{0a} = 0.0$		
V_s1	$V_{0r} = 27.670$	$R_{04} = 1.610$	$a_r = 0.150$
	$V_{0a} = 32.349$	$R_{0a} = 3.254$	$a_a = 0.150$
V_s2	$V_{0r} = 11.842$	$R_{0r} = 1.539$	$a_r = 0.249$
	$V_{0a} = 26.162$	$R_{0a} = 3.015$	$a_r = 0.539$
V_s3	$V_{0r} = 8.355$	$R_{0r} = 1.855$	$a_r = 1.373$
	$V_{0a} = 27.595$	$R_{0a} = 2.643$	$a_a = 1.084$

In Table II we present the results for $\langle H \rangle$ obtained with the various trial functions for 48 000 configurations with and without the three-body correlations g^{p}_{ijk} and $f^{t\tau}_{ijk}$. The Monte Carlo sampling error is estimated from average values $\langle H \rangle_i$ of either 1000 or 2000 samples, so that

$$\delta_{48} = \left[\frac{1}{48} \sum_{i=1}^{48} (\langle H \rangle_i)^2 - \left[\frac{1}{48} \sum_{i=1}^{48} \langle H \rangle_i \right]^2 \right]^{1/2} \Big/ \sqrt{48} , \tag{23}$$

$$\delta_{24} = \left[\frac{1}{24} \sum_{i=1}^{24} (\langle H \rangle_i)^2 - \left[\frac{1}{24} \sum_{i=1}^{24} \langle H \rangle_i \right]^2 \right]^{1/2} \Big/ \sqrt{24} . \tag{24}$$

These two estimates of the standard deviation give similar results.

From the results presented in Table II, we see that the estimated standard deviation δ is quite small and that the $\langle H \rangle$ is well determined so that we can clearly locate the minimum. As a matter of fact, the minimum of the energy is achieved with the wave function $F0$, and when the three-body correlations are included. The minimum $\langle H \rangle_0 = -4.32$ MeV is very close to the physically correct energy of -4.35 MeV from Eq. (22).

TABLE II. Results of $\langle H \rangle$, δ_{48}, and δ_{24} (in MeV) for the trial wave functions $F-1$, $F0$, $F1$, $F2$, and $F3$ with and without the three-body correlations g^{p}_{ijk} and $f^{t\tau}_{ijk}$.

d-d-wave function	Without three-body correlation $\langle H \rangle$	δ_{24}	δ_{12}	With three-body correlation $\langle H \rangle$	δ_{24}	δ_{12}
$F-1$	-4.029	0.045	0.040	-4.152	0.027	0.024
$F0$	-4.263	0.029	0.025	-4.323	0.038	0.041
$F1$	-4.075	0.042	0.027	-4.028	0.035	0.035
$F2$	-3.672	0.059	0.062	-3.899	0.067	0.069
$F3$	-2.865	0.144	0.144	-3.189	0.097	0.078

IV. THE MATRIX ELEMENTS AND THE $Y(^{2S+1}L_J,r)$ FUNCTIONS

The transition amplitude between an initial state $|\psi_i\rangle$ and a final state $|\psi_f\rangle$ is given, in first order, by

$$a_{if}=2\pi i\delta(E_i-E_f-E_\gamma)\sqrt{(2\pi\hbar c)/k\Omega}\times\langle\psi_f|H_I(\mathbf{k},\epsilon_n)|\psi_i\rangle \ , \quad (25)$$

where E_i, E_f, and E_γ are, respectively, the energies of the initial and final nuclear states, and of the emitted gamma. Ω is the quantization volume and $H_i(\mathbf{k},\epsilon_n)$ is the Hamiltonian that describes the emission of a photon with a linear momentum $\mathbf{k}$ and a polarization ϵ_n ($n=1,2$). In the present case, $|\psi_f\rangle$ and $|\psi_i\rangle$ are given, respectively, by Eqs. (1)–(4) and (5)–(16) and Eq. (18). Since the operator $H_I(\mathbf{k},\epsilon_n)$ is fully symmetric, it commutes with the antisymmetrization operator, and therefore we can write

$$\langle\psi_f|H_I(\mathbf{k},\epsilon_n)|\psi_i\rangle=\langle\psi_a|H_I(\mathbf{k},\epsilon_n)|\psi_{dd}\rangle=\sqrt{6}\langle\psi_\alpha|H_I(\mathbf{k},\epsilon_n)|\psi_{LS}^{JM_j}\rangle \ . \quad (26)$$

We use the standard multipole expansion[17,31] of $H_i(\mathbf{k},\epsilon_n)$ and the Wigner-Eckart theorem to obtain for the above matrix element,

$$\langle\psi_\alpha|T_{lM}^\dagger(\beta)|\psi_{LS}^{JM_j}\rangle=-\frac{1}{\sqrt{2J+1}}\delta_{lJ}\delta_{MM_j}\langle\psi_\alpha\|T_l^\dagger(\beta)\|\psi_{LS}^J\rangle \ , \quad (27)$$

where $T_{lM}^\dagger(\beta)$ are the multipolar operators and $\beta=0,1$, respectively, for electric and magnetic transitions. This equation shows that the amplitude vanishes unless $J=l$ and $M_j=M$, and it may be evaluated for the most convenient value of M.

In the long-wavelength approximation (LWA) the electric operators have the form[20]

$$T_{lM}^\dagger(0)=\alpha_l^*(0)e\sum_j\sqrt{4\pi/(2l+1)}e_jr_j^lY_{lM}^*(\hat{r}) \quad (28)$$

with $a_l(0)$ a constant given in Ref. 17, e_j the proton projection operator, $e_j=\frac{1}{2}[1+\tau_z(j)]$ [$\tau_z(j)$ is the z component of the isospin operator for the jth nucleon]. In the long-wavelength limit, meson-exchange currents are taken into account for the electric transitions, if the operators are expressed as in Eq. (28), by Siegert's theorem, and the spin terms are negligible.[31]

The matrix elements of Eq. (27) were calculated in two steps. We first calculate the functions

$$Y(^{2S+1}L_J,r)=\langle\psi_\alpha|T_{lM}^\dagger(\beta)|\bar{\psi}_{LS}^{JM_j}\rangle \ , \quad (29)$$

where $|\bar{\psi}_{LS}^{JM_j}\rangle$ is obtained from $|\psi_{LS}^{JM_j}\rangle$ by replacing the relative wave function $\psi_{LS}(r')$ by $\delta(r-r')$. The $Y(^{2S+1}L_J,r)$ functions are calculated on a grid of points spaced by 0.2-fm intervals, by sampling 800 000 configurations with the Monte Carlo method. These functions are independent of $\psi_{LS}(r)$ and thus of $E_{\mathrm{c.m.}}$. In the present work we give only the results for $Y(^5S_2,r)$; the Y functions for the remaining channels $^3P_1$, $^5D_1$, $^1D_2$, $^5D_2$, $^5G_2$, $^3P_2$, and $^3F_2$, are tabulated in Ref. 32.

The matrix elements are then obtained by integrating

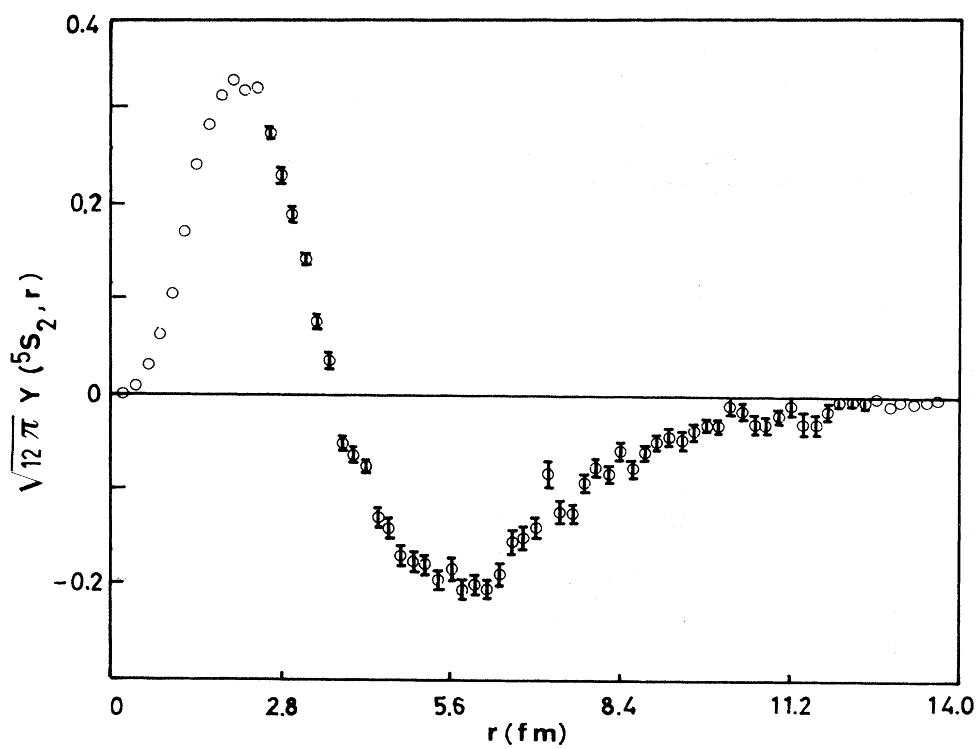

FIG. 2. The $Y(^5S_2,r)$ function. The error bars correspond to the statistical errors associated with the Monte Carlo integrations.

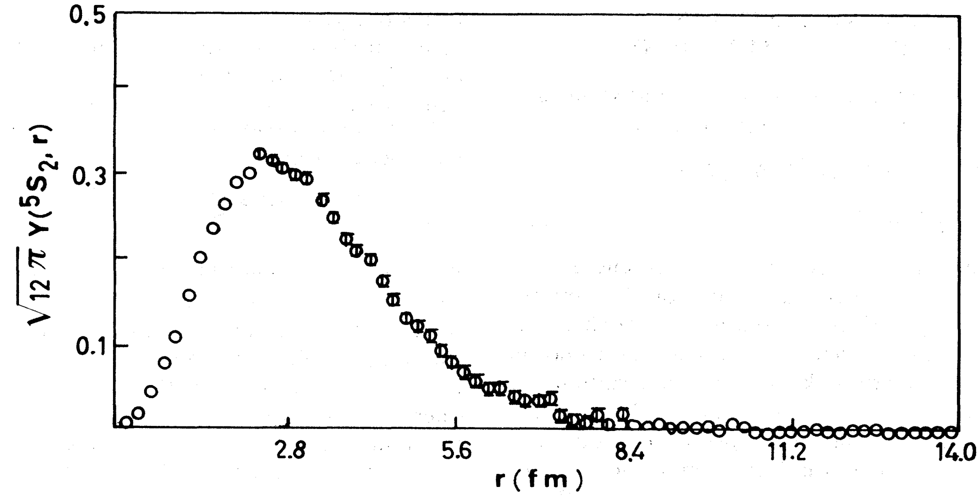

FIG. 3. The $Y(^5S_2,r)$ function without the inclusion of the α-particle D state. The error bars correspond to the statistical errors associated with the Monte Carlo integrations.

$Y(^{2S+1}L_J,r)$ with the corresponding $\psi_{LS}(r)$ function:

$$\langle \psi_\alpha | T^\dagger_{lM}(\beta) | \psi^{JM_j}_{LS} \rangle = \int_0^\infty Y(^{2S+1}L_J,r)\psi_{LS}(r)dr \ . \qquad (30)$$

Following Eq. (29), the Y function for the $E2$ transition from the $^5S_2$ continuum state is defined by the equation

$$Y(^5S_2,r) = \left\langle \psi_\alpha \left| \sum_{j=1}^{4} \tfrac{1}{2} r_j^2 Y^\dagger_{20}(\hat{r}_j) \right| \psi^{20}_{02} \right\rangle , \qquad (31)$$

where we used Eq. (28) for $l=2$ and $M=0$, and ignored the τ_z term in e_j since $T=0$. [The constant involved in Eq. (28) was included in the integration of Eq. (32).] The $Y(^5S_2,r)$ function is shown in Fig. 2, and clearly exhibits a positive and a negative region. This function is zero if only the spin-symmetric S waves are retained in the deuteron and α-particle wave functions. Therefore, it gets contributions from either or both of the D-state components in these wave functions. We can represent the α-particle wave function as a sum of a $^1S_0$ state with no D wave, and a $^5D_0$ state. Essentially, the positive and negative regions of $Y(^5S_2,r)$ are determined, respectively, by the

$$^5S_2 \xrightarrow{E2} {}^1S_0$$

transition, which proceeds only through the deuteron D state, and by the

$$^5S_2 \xrightarrow{E2} {}^5D_0$$

transition. To illustrate this fact, we present in Fig. 3 the $Y(^5S_2,r)$ function calculated without the inclusion of the α-particle D state, which is positive everywhere, and in Fig. 4 that obtained without the inclusion of the deuteron D state, which is essentially negative.

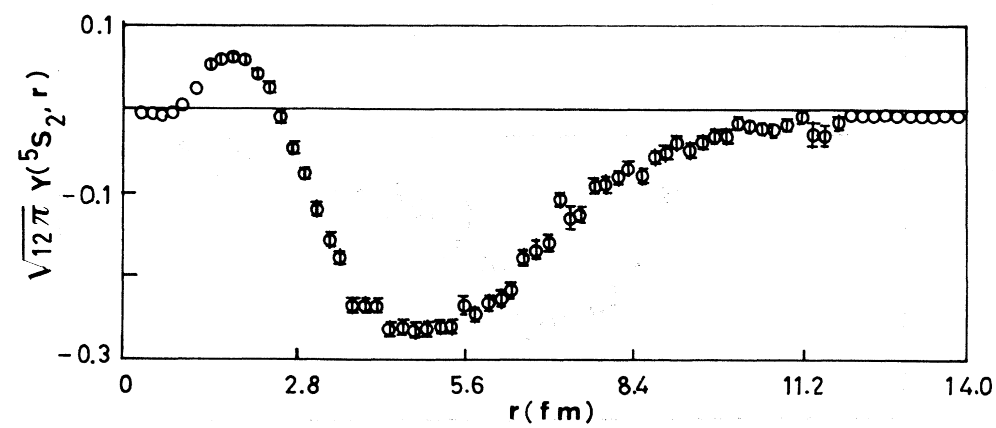

FIG. 4. The $Y(^5S_2,r)$ function withou the inclusion of the deuteron D state. The error bars correspond to the statistical errors associated with the Monte Carlo integrations.

It is known that the deuteron has a prolate shape (cigar shape), hence, its S and D radial wave functions, u and w, have the same sign, generally taken to be positive. On the contrary, some components of the α-particle D state are out of phase, i.e., negative with respect to the positive S state. For this same reason the D_2 and η parameters of the $\langle dd|\alpha\rangle$ overlap function are also negative.[15,20,22,33] This can be easily understood if we consider the α particle as formed by two deuterons with antiparallel spins. The tensor force between them is repulsive when the relative coordinate is along the spin direction, and is attractive when is orthogonal to it. In order to make the latter configuration favorable, the S- and D-state amplitudes of the overlap must interfere destructively. As a consequence, the corresponding radial functions have opposite signs, and the intrinsic deformation of the α particle is oblate.

Finally, for the sake of completeness, the reduced matrix element of the $E2$ transition from the $^5S_2$ state is given by

$$\langle \psi_\alpha \| T_2^\dagger(0) \| \psi_{02}^2 \rangle = -\mathcal{C}(k)\sqrt{\pi/3}\frac{E_\gamma}{\hbar c}e^{i\delta_{02}}\int_0^\infty Y(^5S_2,r)U_{02}(r)dr \quad (32)$$

with

$$\mathcal{C}(k) = -4\pi e k \ . \quad (33)$$

V. RESULTS AND DISCUSSION

In the present work we consider only very low energies where the $E2$ transition dominates. In this case, it can be shown that the total cross section is given by[32]

$$[\sigma^{\rm tot}]_{\rm cap} = \mathcal{F}(E) 6 \| \langle \psi_\alpha | T_{20}^\dagger(0) | \psi_{02}^2 \rangle \|^2 \quad (34)$$

with

$$\mathcal{F}(E) = \frac{1}{3\pi}\frac{mc^2}{(\hbar c)^3}\frac{E_\gamma}{p} \quad (35)$$

and the astrophysical factor by

$$S(E_{\rm c.m.}) = \sigma^{\rm tot} E_{\rm c.m.} \exp(2\pi\eta) \ , \quad (36)$$

where η is the Sommerfeld parameter.

In Figs. 5 and 6 we present the results for the astrophysical factor, respectively, without and with the inclusion of three-body correlation in the $^5S_2$ channel, for the $F-1$, $F0$, $F1$, $F2$, and $F3$ continuum wave functions. We point out that our results are not meaningful for energies higher than 500 keV, where the contributions of the P waves, associated with $E1$ and $M2$ transitions, as well as that due to the $E2$ transition involving the $^1D_2$ channel, become important. Furthermore, the coupling of these continuum states to the ^{3}H$+p$ and ^{3}He$+n$ channels may also become important at higher energies.

Figures 5 and 6 indicate that the best agreement with the data is obtained with the $F1$ wave function when three-body correlation operators are included in the scattering state, despite the fact that, in the variational calculation, the minimum of the energy is obtained with the $F0$ wave function.

In Figs. 7 and 8 we show the sensitivity of the astrophysical factor to the D states. Results obtained without the inclusion of the α-particle D state, without the inclusion of the deuteron D state, and including both D

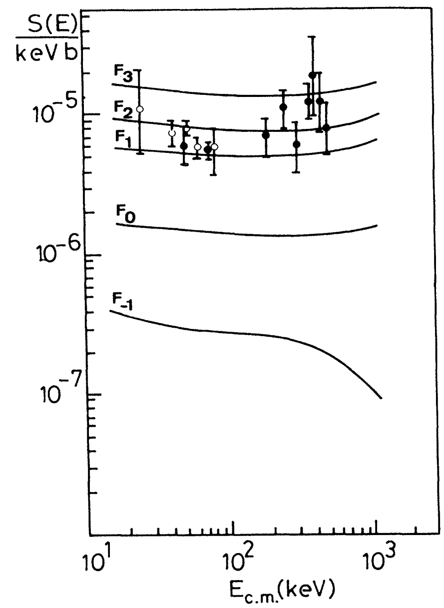

FIG. 5. The astrophysical S factor obtained with the inclusion of three-body correlations in the trial scattering wave functions. The experimental data are from Ref. 8 (full circles) Ref. 13 (open circles), and from Ref. 35 (full triangles).

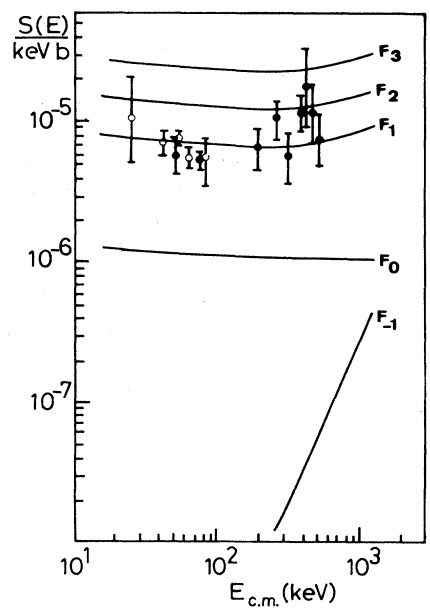

FIG. 6. The astrophysical S factor obtained without the inclusion of three-body correlations in the trial scattering wave functions. The experimental data are from the same references as in Fig. 5.

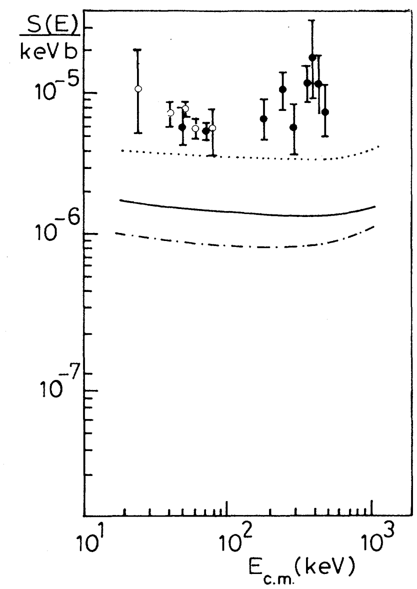

FIG. 7. The astrophysical S factor obtained with the $F0$ wave function when (1) both D states are included (full line), (2) without the D state in the α particle (dash-dotted line), and (3) without the D state in the deuterons (dotted line). The experimental data are from the same references as in Fig. 5.

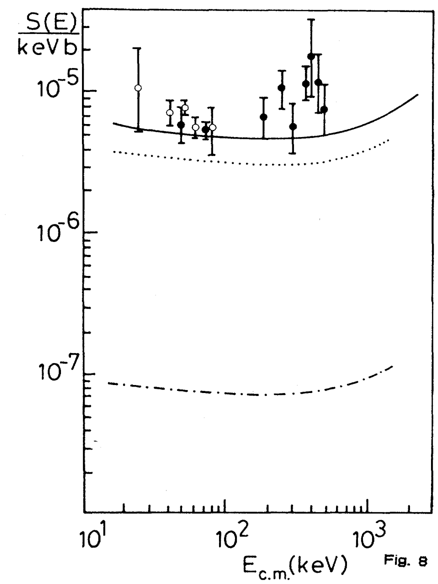

FIG. 8. The astrophysical S factor obtained with the $F1$ wave functions when (1) both D states are included (full line), (2) without the D state in the α particle (dash-dotted line), and (3) without the D states in the deuteron (dotted line). The experimental data are from the same references as in Fig. 5.

states are shown by dash-dotted, dotted, and full lines, respectively. It is evident that both α-particle and deuteron D states contribute to this transition at these very low energies, although the D state in the α particle seems to have a larger contribution. With the wave function $F0$, the two D-state contributions cancel and the result is below the experimental data (Fig. 7). On the other hand, due to the node in the wave function $F1$, the D-state contributions obtained with it add and the total is close to the observed cross section (Fig. 8). We conclude that calculations neglecting either of these two D states in the wave functions are not meaningful.

Since the optimum variational wave function does not explain the data, it is obvious that the present calculation needs to be improved. Firstly, we can use a more recent and accurate α-particle wave function, obtained by Wiringa.[34] Secondly, we can consider the parameters of the two- and three-body correlations in the continuum state as variational parameters in the scattering calculation. Finally, we can change the ansatz of the scattering state [Eq. (6)] by introducing suitable distortions of the deuterons at small r. Nevertheless, the present results are encouraging enough to indicate that the Monte Carlo methods could be used to study the ^{2}H$(d,\gamma)^4$He reaction at low energies with bound and continuum wave functions generated from realistic nuclear forces, and that this reaction shows an interesting interplay among the D states of the deuteron and α particle, both determined by the tensor force, and the d-d continuum wave function.

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