Nuclear polarization in $d\mu$ and $t\mu$ atoms and in the $dt\mu$ molecule

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Deuteron polarization in a $d\mu$ atom and triton polarization in a $t\mu$ atom were investigated on the basis of a three- (four-) body model of the d-μ (t-μ) system. Virtual excitation of the deuteron and triton is treated within the second-order perturbation theory. The nuclear polarization energy is obtained as -9.9 meV for the $d\mu$ atom and -1.1 meV for the $t\mu$ atom. We examined the validity of the adiabatic approximation and the dipole approximation which were employed in the literature calculation of the deuteron polarization; the approximations were found to be rather poor. Deuteron and triton polarization potentials were derived and were found to deviate much, in the internal region, from the r^{-4}-type potential, which is given by the adiabatic and dipole approximations. With the use of these potentials, correction to ϵ_{11} due to the nuclear polarization in the $dt\mu$ molecule at the $J=v=1$ state was calculated to be -1.7 meV, which should significantly affect the resonant formation of the state, a key to the muon catalyzed d-t fusion.

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I. INTRODUCTION

Muon-catalyzed d-t fusion is attracting strong attention [1] in nuclear physics and atomic or molecular physics from the viewpoint of the study of the possibility of energy release in hydrogen isotopes at low temperature and the study of physically interesting few-body problems seen in the fusion cycle (a recent review of this subject is given in Ref. [1]. An essentially important key to the fusion cycle is the formation of the muonic molecule $(dt\mu)_{11}$ in a very loosely bound excited state with $J=v=1$ (J is the total angular momentum and v is a quantum number to specify the states with the same J). Energy of this $J=v=1$ state, ε_{11}, is only -660 meV with respect to the $(t\mu)_{1s}$-d breakup threshold which lies 2711 eV below the $d+t+\mu$ three-body breakup threshold. The rate of formation of the muonic molecule $(dt\mu)_{11}$ is known [2] to depend very sensitively on ε_{11}. The value of $\varepsilon_{11}=-0.6603$ eV obtained by variational calculations with the nonadiabatic coupled-rearrangement-channel approach [3,4] was consistent with those obtained by other approaches [5,6].

However, the Coulomb three-body problem was solved with the use of the nonrelativistic pure Coulombic potentials among d, t, and μ. Since at least the accuracy of 1 meV is required, various corrections to ε_{11} should be estimated carefully as far as they are of the order of 0.1–1 meV. Many authors then investigated the corrections extensively, such as those due to relativistic effect ($\approx+1.0$ meV) [7–9], effect of finite size of the charge distribution of nuclei d and t ($\approx+10.4$ meV [8,10,11], effect of the vacuum polarization ($\approx+17.0$ meV) [8,10,11], effect of the nuclear interaction between d and t ($\approx+10^{-4}$ meV [8,10], effect of the electron screening on the $(dt\mu)_{11}$ molecule ($\approx+0.3$ meV) [11], and effect of the deuteron polarization by the muon (≈-2.2 meV) [7].

Among these corrections, the last one due to the deuteron polarization has been the least investigated. Contrary to the other effects, each of which was calculated at least by two different groups, the effect of deuteron polarization in $(dt\mu)_{11}$ has been calculated only by Bakalov [7]. However, his calculation was based on crude approximations. In addition, there is no calculation for the triton polarization effect. Thus, accurate calculation of the nuclear polarization effect in the $(dt\mu)_{11}$ molecule is more desirable from the viewpoint of not only muon-catalyzed fusion problems but also a precise study of few-body problems.

Lack of accurate calculation of the nuclear polarization is due to the difficulty that one has to investigate the three- and four-body systems, $p+n+\mu$ and $p+n+n+\mu$, and treat the nuclear force and the (atomic) Coulomb force simultaneously. The former force is strong and short ranged and the latter one is weak and long ranged. One needs an accurate and tractable method for this purpose. The Gaussian-basis coupled-rearrangement-channel variational method is such a method. It has been developed by Kamimura in the study of muonic molecules such as $(dt\mu)$ [3] and by Kameyama, Fukushima, and Kamimura for three-nucleon bound states (t and ^{3}He) [12]. This method has been found to be suited for describing both the short-range correlations due to the nuclear force and the long-

range behavior due to the Coulomb force.

The purpose of this paper is to apply the Gaussian-basis coupled-rearrangement-channel method to a precise study of the nuclear polarization effects in the $d\mu$ and $t\mu$ atoms and in the $dt\mu$ molecule.

Construction of this paper is as follows. In Sec. II, we study the effect of deuteron polarization by the muon in the $d\mu$ atom on the basis of the three-body $(p+n+\mu)$ model of the d-μ system. We calculate the polarization energy and polarization potential, and examine some approximations which were employed in the literature studies of the effect. In Sec. III, we investigate the triton polarization effect in the $t\mu$ atom using the four-body $(p+n+n+\mu)$ model of the t-μ system. In Sec. IV, the deuteron and triton polarization effects in the $dt\mu$ molecule are studied. Concluding remarks are given in Sec. V.

II. DEUTERON POLARIZATION IN THE $d\mu$ ATOM

A. Adiabatic and dipole approximation model

In order to discuss the deuteron polarizability in the $(dt\mu)_{11}$ molecule, we need precise knowledge of deuteron polarizability in the $d\mu$ atom and the induced effective potential between d and μ.

A quantitative calculation of the deuteron polarization in the $d\mu$ atom was made by Startsev, Petrun'kin, and Khomkin [13]. They started with the well-known second-order perturbation formula for the correction to the energy of an atomic level n_0:

$$\Delta E_{d\mu}^{\rm pol}(n_0)=-\sum_{N(\neq 0),n}\frac{|\langle N,n|\Delta V|0,n_0\rangle|^2}{E_N-E_0+\varepsilon_n-\varepsilon_{n_0}}\ , \tag{1}$$

where

$$\Delta V=-\frac{e^2}{|\mathbf{r}-\mathbf{R}/2|}+\left\langle 0\left|\frac{e^2}{|\mathbf{r}-\mathbf{R}/2|}\right|0\right\rangle . \tag{2}$$

Here, N and n are the quantum numbers, respectively, of the deuteron and $(d\mu)$ atomic states ($|0\rangle$ is the deuteron ground state), E_N and ε_n are the energies of the states, $\mathbf{R}$ is the radius vector between proton (p) and neutron (n), and $\mathbf{r}$ is the radius vector of the muon with respect to the c.m. of the $p+n$ system (Fig. 1).

The muon levels $n_0=1s$ and $2s$ were considered. Startsev, Petrun'kin, and Khomkin [13] used two approximations to proceed further; the adiabatic approximation

$$\varepsilon_n-\varepsilon_0\ll E_N-E_0 \tag{3}$$

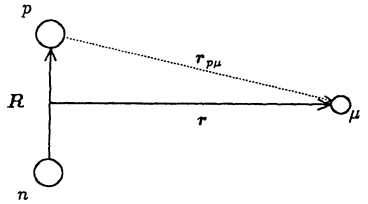

FIG. 1. Jacobian coordinates of the $p+n+\mu$ coordinates.

and the dipole approximation (based on the assumption $R\ll r$)

$$\Delta V=-\frac{e^2(\mathbf{r}\cdot\mathbf{R})}{2r^3}\ . \tag{4}$$

These two approximations make Eq. (1) very simple, and generate

$$\Delta E_{d\mu}^{\rm pol}(n_0)=-\frac{\bar{\alpha}e^2}{2}\left\langle n_0\left|\frac{1}{r^4}\right|n_0\right\rangle , \tag{5}$$

where $\bar{\alpha}$ is the electric dipole polarizability constant of deuteron

$$\bar{\alpha}=\sum_{N(\neq 0)}\frac{|\langle N|\mathbf{R}|0\rangle|^2}{E_N-E_0}\ . \tag{6}$$

The effective deuteron polarization potential induced by the interaction (4) may be written as

$$V_{d\mu}^{\rm pol}(r)=-\frac{\bar{\alpha}e^2}{2r^4}\ . \tag{7}$$

In the case of S states for n_0, however, the correction (5) diverges due to the integration in the region of $r\sim 0$, and introduction of some cutoff is needed. Startsev, Petrun'kin, and Khomkin introduced a prescription for the cutoff and obtained $\Delta E_{d\mu}^{\rm pol}=-9.1$ meV for the $n_0=1s$ state by employing the observed value [14] of $\bar{\alpha}=0.63$ fm^3.

Correction to $\varepsilon_{11}(dt\mu)$ due to the deuteron polarization by muon in the $(dt\mu)$ molecular ion was calculated by Bakalov [7], who referred to the value of $\Delta E_{d\mu}^{\rm pol}=-9.1$ meV. He assumed, instead of Eq. (7), an effective polarization potential between d and μ in the form

$$V_{d\mu}^{\rm pol}(r)=-\frac{\bar{\alpha}e^2}{2r^2(r^2+r_0^2)},\quad r_0=15.8\ \text{fm}\ , \tag{8}$$

where the parameter r_0 was introduced to avoid the divergence of Eq. (4) at small distance and to simulate the $1/r^2$ behavior [15] in the intermediate region; r_0 was so determined as to reproduce $\langle 1s|V_{d\mu}^{\rm pol}|1s\rangle=-9.1$ meV with no cutoff in the integration. Bakalov then calculated the deuteron polarization correction, $\Delta\varepsilon_{11}^{\rm pol}(dt\mu)$, to the energy $\varepsilon_{11}(dt\mu)$ within the first-order perturbation and obtained

$$\Delta\varepsilon_{11}^{\rm pol}(dt\mu)\equiv\langle\Psi_{11}(dt\mu)|V_{d\mu}^{\rm pol}|\Psi_{11}(dt\mu)\rangle =-2.2\ \text{meV}\ , \tag{9}$$

where $\Psi_{11}(dt\mu)$ is the wave function [16] of the $J=v=1$ state of the $dt\mu$ molecule.

In the above calculations or anywhere else, validity of the adiabatic approximation and the dipole approximation in the $d\mu$ atom has not been examined; this is due to the difficulty in the three-body calculation appearing in Eq. (1).

B. Nonadiabatic three-body model

We neglect spin dependence in the nucleon-nucleon force. This is because the polarization calculation is very

tedious with spin-dependent forces, but we consider that virtual breakup of deuteron can be well studied with the central potential. The three-body Hamiltonian of the system is written as

$$H=-\frac{\hbar^2}{2M}\nabla_R^2-\frac{\hbar^2}{2m}\nabla_r^2+v_{np}(R)+V_{\mu p}\left(\left|\mathbf{r}-\frac{\mathbf{R}}{2}\right|\right), \tag{10}$$

where $v_{np}(R)$ is the nuclear potential between n and p, and $V_{\mu p}$ is the Coulomb potential between μ and p with the proton charge distribution folded. M and m are the reduced mass associated with the coordinates $\mathbf{R}$ and $\mathbf{r}$, respectively. The Hamiltonian is rewritten as

$$H=H_{np}+H_{\mu p}+V_{\rm int} \tag{11}$$

with

$$H_{np}=-\frac{\hbar^2}{2M}\nabla_R^2+v_{np}(R), \tag{12}$$

$$H_{\mu d}=-\frac{\hbar^2}{2m}\nabla_r^2-\frac{e^2}{r}, \tag{13}$$

$$V_{\rm int}=V_{\mu p}\left(\left|\mathbf{r}-\frac{\mathbf{R}}{2}\right|\right)+\frac{e^2}{r}. \tag{14}$$

We introduce the eigenfunctions of the Hamiltonians H_{np} and $H_{\mu d}$:

$$(H_{np}-E_{NL})\chi_{NL}(\mathbf{R})=0, \tag{15}$$

$$(H_{\mu d}-\varepsilon_{nL})\phi_{nL}(\mathbf{r})=0, \tag{16}$$

where L is the angular momentum of the n-p system and that of the μ-(np) system, and N and n are used to specify the eigenstates both for discrete and continuum states, for the sake of simplicity of expressions. The deuteron ground state is described by $\chi_{00}(\mathbf{R})$. Since v_{np} is considered to be spin independent in this work, we do not explicitly write spin components (spin $=1$) of χ.

We consider a three-body wave function with angular momentum $J=0$, $\Psi_{J=0}(\mathbf{r},\mathbf{R})$, for which the Schrödinger equation is

$$(H-E)\Psi_{J=0}(\mathbf{r},\mathbf{R})=0. \tag{17}$$

In order to solve Eq. (17), we expand $\Psi_{J=0}$ in the eigenfunctions of Eqs. (15) and (16):

$$\Psi_{J=0}(\mathbf{r},\mathbf{R})=\sum_{n,N,L}A_{nNL}[\chi_{NL}(\mathbf{R})\phi_{nL}(\mathbf{r})]_{J=0}. \tag{18}$$

In order to avoid the difficulty of dealing the infinite number of continuous basis functions, we approximate the continuum states, as often done, in the following manner. We first diagonalize the Hamiltonian H_{np} with a finite number of L^2-integrable basis functions and get the same number of discrete-state wave functions which stand for bound and discretized (pseudo-) continuum states. We then regard the finite number of wave functions so-obtained as the χ_{NL} in Eq. (18). We similarly define a finite number of ϕ_{nL}. Use of the Rayleigh-Ritz variational principle for Eq. (17) leads to the matrix equations for A_{nNL}:

$$(E_{nL}+\varepsilon_{nL}-E)A_{nNL}=-\sum_{n',N'}\langle[\phi_{nL}\chi_{NL}]_{J=0}|V_{\rm int}|[\phi_{n'L}\chi_{N'L}]_{J=0}\rangle A_{n'N'L}. \tag{19}$$

Within the second-order perturbation, we have

$$\Delta E_{d\mu}^{\rm pol}=-\sum_{(n,L;N,L)\neq(1,s;0,0)}\frac{|\langle[\phi_{nL}\chi_{NL}]_{J=0}|V_{\rm int}|\phi_{1s}\chi_{00}\rangle|^2}{\varepsilon_{nL}+E_{NL}-(\varepsilon_{1s}+E_{00})}, \tag{20}$$

$$A_{nNL}=\frac{\langle[\phi_{nL}\chi_{NL}]_{J=0}|V_{\rm int}|\phi_{1s}\chi_{00}\rangle}{\varepsilon_{nL}+E_{NL}-(\varepsilon_{1s}+E_{00})}. \tag{21}$$

We examined higher-order effects in $\Delta E_{d\mu}^{\rm pol}$ solving directly Eq. (19) with $L=0$ and 1, and found them to be $\sim 10^{-3}$ meV. We therefore discuss below the case of the second-order perturbation only.

C. Interaction and basis functions

As the nuclear potential $v_{NP}(R)$, we employ the Malfliet-Tjon potential [17] which is often used in the studies of few-nucleon problems:

$$v_{NP}(R)=v_1\frac{e^{-\mu_1 R}}{\mu_1 R}-v_2\frac{e^{-\mu_2 R}}{\mu_2 R}. \tag{22}$$

The potential parameters are taken as $v_1=1438.72$ MeV, $v_2=626.885$ MeV, $\mu_1=3.11$ fm^{-1}, and $\mu_2=1.55$ fm^{-1}. This potential reproduces the deuteron binding energy and low-energy triplet n-p scattering.

The basis functions χ_{NL} and ϕ_{nL} in Eqs. (15) and (16) are described in terms of Gaussian-tail functions:

$$\chi_{NLM}(\mathbf{R})=\sum_{I=1}^{I_{\max}}a_{NI}^{(L)}R^L e^{-(R/R_I)^2}Y_{LM}(\hat{\mathbf{R}}), \tag{23}$$

$$\phi_{nLM}(\mathbf{r})=\sum_{i=1}^{i_{\max}}b_{ni}^{(L)}r^L e^{-(r/r_i)^2}Y_{LM}(\hat{\mathbf{r}}). \tag{24}$$

Here, the range parameters are taken to be geometrical progressions:

$$R_I=R_1 A^{I-1},\quad I=1\sim I_{\max} \tag{25}$$

TABLE I. The parameters used in the calculation for the $p+n+\mu$ system.

	$I_{\max}$	R_1 (fm)	$R_{I_{\max}}$ (fm)	$i_{\max}$	r_1 (fm)	$r_{i_{\max}}$ (fm)
$L=0$	30	0.05	20	30	1.0	2000
$L=1$	30	0.2	40	30	3.0	4000

$$r_i = r_1 a^{i-1}, \quad i = 1 \sim i_{\max} . \tag{26}$$

Usefulness of this type of basis functions was demonstrated in the work of the $dt\mu$ molecule [3] and the three-nucleon bound states [12].

The parameters used in the following calculation are listed in Table I.

Use of the parameters reproduces accurately the ground-state solution of Eq. (15) (cf. Ref. [12]); ε_{nL} is given with an accuracy of the seven significant figures for $n=1-3$ with the use of the parameter sets of Table I.

In the interaction $V_{\mu p}$ between muon and proton, we take into account the finite size of the proton charge density with a Gaussian function with the range of 0.64 fm (as shown later, this effect cannot be ignored in $\Delta E_{d\mu}^{\rm pol}$).

We note that since the wave functions χ's and ϕ's in Eqs. (23) and (24) are described with the Gaussian functions, the calculation of matrix elements which appear in the variational calculations can easily be performed. It is also noted that the dipole approximation for $V_{\rm int}$, Eq. (4), is not taken in our calculation.

D. Numerical results

It was first found that contribution to Eq. (20) from the excited states with $L \neq 1$ is less than 10^{-3} meV. We therefore neglect it and take the case of $L=1$ alone in the following investigations. We obtained

$$\Delta E_{d\mu}^{\rm pol} = -9.9 \text{ meV} \tag{27}$$

by calculating Eq. (20). Contributions of individual terms (n,N) in Eq. (20) are illustrated in Fig. 2 with the magnitude being represented by the area of the circles.

It is clearly seen that dominant contributions come from the excited states with $\varepsilon_{nL=1}-\varepsilon_{1s} \approx E_{NL-1}-E_{00}$ approximately equal to several MeV. This shows breakdown of the adiabatic approximation $\varepsilon_{nL}-\varepsilon_{1s} \ll E_{NL}-E_{00}$, Eq. (3), which was assumed in the previous work of Startsev, Petrun'kin, and Khomkin [13]. In the calculation of Eq. (20), if we neglected the excitation energy of the $(d\mu)$ atom (namely, $\varepsilon_{nL}-\varepsilon_{1s}=0$), we would get $\Delta E_{d\mu}^{\rm pol} = -28.5$ meV, which deviates much from our result of -9.9 meV.

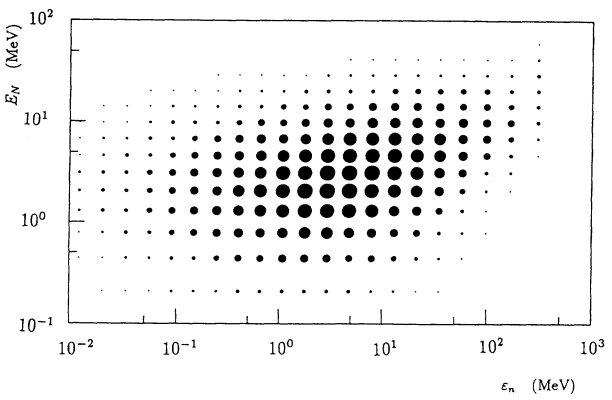

FIG. 2. Contributions to $\Delta E_{d\mu}^{\rm pol} = -9.9$ meV from the individual terms of Eq. (20). The area of the circle is proportional to the magnitude of each contribution (multiplied by -1). The largest circle corresponds to a contribution of -0.19 meV.

Also poor is the dipole approximation for $V_{\rm int}$, Eq. (4), which was adopted in Ref. [13]. Namely, calculation of Eq. (20) with this approximation (but without the adiabatic approximation) results in $\Delta E_{d\mu}^{\rm pol} = -12.7$ meV. Use of these two approximations leads to Eq. (5) for $\Delta E_{d\mu}^{\rm pol}$, but Startsev, Petrun'kin, and Khomkin modified it by taking a cutoff prescription for small r; this gave -9.1 meV, which is close to our result of -9.9 meV. As mentioned before, Bakalov [7] also modified Eq. (5) using the polarization potential (8) instead of (5) so as to fit $\Delta E_{d\mu}^{\rm pol} = -9.1$ meV of Ref. [13].

In the above calculation, the finite size of the proton charge density was taken into account. But, if we neglected the proton size (namely if $V_{\mu p} = -e^2/r_{\mu p}$), we would obtain $\Delta E_{d\mu}^{\rm pol} = -10.1$ meV instead of -9.9 meV mentioned above. As long as we are interested in the accuracy of 0.1 meV, we cannot neglect the proton finite-size effect in $\Delta E_{d\mu}^{\rm pol}$.

We examined dependence of $\Delta E_{d\mu}^{\rm pol}$ on the number of basis functions, $I_{\max}$ and $i_{\max}$, in Eqs. (23) and (24). The value of $\Delta E_{d\mu}^{\rm pol} = -9.9$ meV, which was obtained for $I_{\max}=i_{\max}=30$, did not change for $I_{\max}=i_{\max}=25$ and 20. We tried different sets of $(R_1, R_{I_{\max}})$ and $(r_1, r_{i_{\max}})$ in their reasonable ranges, but results did not change significantly. These tests clarify that the choice of the parameters in Table I is suitable enough for our purpose.

E. Deuteron polarization potential

We calculated the polarization potential $V_{d\mu}^{\rm pol}(r)$ from our second-order solution. Definition of the potential is given by

$$V_{d\mu}^{\rm pol}(r)\phi_{1s}(r) = -\sum_{n,N,L} A_{nNL} \langle [\phi_{nL}(\mathbf{r})\chi_{NL}(\mathbf{R})]_{J=0} | V_{\rm int} | \chi_{00}(\mathbf{R}) \rangle_{\mathbf{R}} , \tag{28}$$

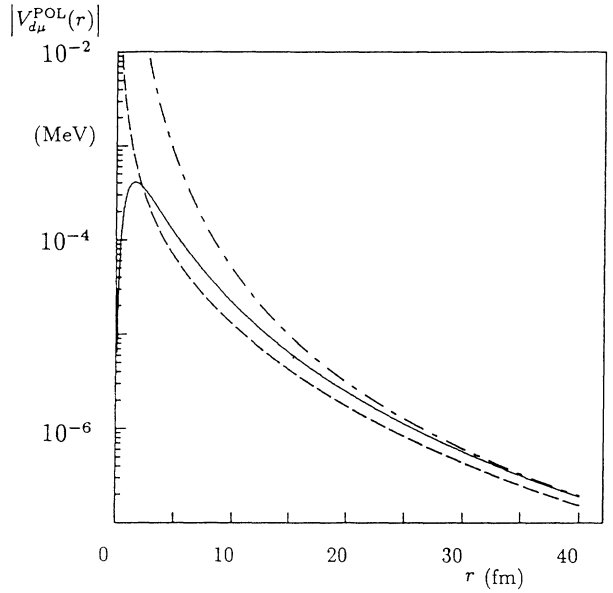

FIG. 3. Deuteron polarization potentials given by our calculation (solid curve), by Bakalov [7] (dashed curve), and by the r^{-4} approximation (dot-dashed curve).

where A_{nNL} is given by Eq. (21). Note that Eqs. (20) and (21) result in Eq. (28). Therefore we can write

$$\Delta E_{d\mu}^{\rm pol} = \langle \phi_{1s}(\mathbf{r}) | V_{d\mu}^{\rm pol}(r) | \phi_{1s}(\mathbf{r}) \rangle \ . \tag{29}$$

Calculated $V_{d\mu}^{\rm pol}(r)$, which gives $\Delta E_{d\mu}^{\rm pol} = -9.9$ meV, is illustrated in Fig. 3 (multiplied by -1) together with Bakalov's approximated potential [7], Eq. (8).

Also illustrated is the r^{-4} potential (the dot-dashed curve) which is given by the dipole and adiabatic approximation [see Eqs. (3)–(7)]; this curve is normalized to our $V_{d\mu}^{\rm pol}$ at $r=40$ fm. Our potential tends to be proportional to r^{-4} for $r \gtrsim 40$ fm (much outside the deuteron tail region), but deviates much from it in the internal region; this clearly shows the breakdown of the dipole and adiabatic approximations. At $r \sim 0$, our potential is proportional to r^2; this is reasonable because $V_{\rm int} \simeq -e^2(\mathbf{r}\cdot\mathbf{R}/R^3)^2$ for $r \ll R$. Bakalov's potential is smaller by $\sim 50\%$ in magnitude than ours for $r \gtrsim 5$ fm, but much larger for $r \lesssim 2$ fm (nearly the deuteron size). This difference in the short-range region is very significant since 50% of the contribution of $V_{d\mu}^{\rm pol}(r)$ to $\Delta E_{d\mu}^{\rm pol}$ comes from the region of $r=10$ fm. We emphasize that this calculation of the deuteron polarization potential is based on the three-body model, and clarifies the error of the literature approximations.

The polarization potential $V_{d\mu}^{\rm pol}(r)$ will be used in Sec. IV in the calculation of deuteron polarization effect in the $dt\mu$ molecule.

III. TRITON POLARIZATION IN THE $t\mu$ ATOM

A. Triton three-body wave function

Polarization of triton by muon has not been clarified in the literature at all. This is because of the difficulty of obtaining the triton three-body wave function in tractable form so that one can discuss the excitation of triton by muon-proton interaction. Kameyama, Kamimura, and Fukushima [12] developed the coupled-rearrangement-channel method for three-nucleon bound states (t and ^{3}He) and obtained very accurate and tractable wave functions for them. In that work, a realistic nucleon-nucleon force was used, but we consider that such a precise nucleon-nucleon force is not necessary in the calculation of triton polarization by muon. We therefore take the Malfliet-Tjon potential [17], MT-V, in the form of Eq. (22), but the parameters are taken as $v_1 = 1458.05$ MeV, $v_2 = 578.09$ MeV, $\mu_1 = 3.11$ fm^{-1}, and $\mu_2 = 1.55$ fm^{-1}, which are assumed both for n-n and n-p pairs with no spin dependence. Therefore, spin part is neglected in the three-body wave function.

Following the prescription of Ref. [12], we calculate the triton wave function with the above interaction. Three rearrangement channels ($c=1,2,3$) and the Jacobian coordinates are taken as shown in Fig. 4.

We discriminate proton and neutron, and antisymmetrize the two neutrons. The two neutrons are assumed to couple to spin $=0$ and therefore the spatial part is taken to be symmetric between them. The triton wave function with the total angular momentum L is then expanded in the basis functions of coordinates $\mathbf{x}$ and $\mathbf{y}$:

$$\Phi_{LM} = \sum_{c=1}^{3} \sum_{i_c, l_c, i_c', l_c'} A_{i_c l_c i_c' l_c'}^{(c)} [\phi_{i_c l_c}(\mathbf{x}_c) \chi_{i_c' l_c'}(\mathbf{y}_c)]_{LM} \tag{30}$$

with

$$A_{i_1 l_1 i_1' l_1'}^{(1)} = A_{i_2 l_2 i_2' l_2'}^{(2)} \quad \text{for } (i_1 l_1 i_1' l_1') = (i_2 l_2 i_2' l_2') \ , \tag{31}$$

where l and l' are angular momenta associated with $\mathbf{x}$ and $\mathbf{y}$, respectively, and i and i' are numbers which specify the spatial dependence of the basis functions.

The Hamiltonian for triton, H_t, is given in the form

$$H_t = -\frac{\hbar^2}{2m}\nabla_x^2 - \frac{\hbar^2}{2M}\nabla_y^2 + v(x_1) + v(x_2) + v(x_3) \ . \tag{32}$$

The Schrödinger equation for this system is

$$(H_t - E_L)\Phi_{LM} = 0 \ . \tag{33}$$

The basis functions ϕ_{il} and $\chi_{i'l'}$ are defined by

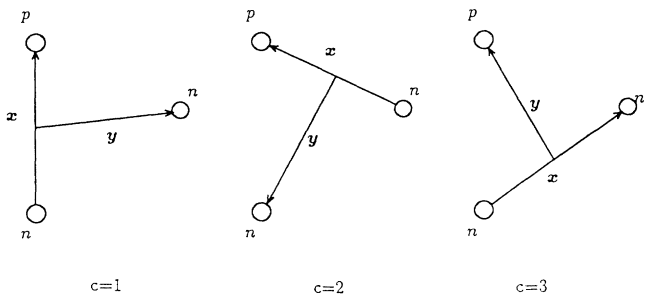

FIG. 4. Three rearrangement channels and Jacobian coordinates of the $p+n+n$ system.

$$\phi_{ilm}(\mathbf{x})=x^l e^{-(x/x_i)^2} Y_{lm}(\hat{\mathbf{x}}) \tag{34}$$

and

$$\chi_{i'l'm'}(\mathbf{y})=y^{l'} e^{-(y/y_{i'})^2} Y_{l'm'}(\hat{\mathbf{y}}) \tag{35}$$

and the radial parameters are taken to be geometrical progressions,

$$x_i=x_1 a_x^{i-1}, \quad i=1 \text{ to } i_{\max} \tag{36}$$

and

$$y_{i'}=y_1 a_y^{i'-1}, \quad i'=1 \text{ to } i'_{\max} . \tag{37}$$

As done in Ref. [12], the eigenenergy and the expansion coefficients of Eq. (31) are to be determined by the Rayleigh-Ritz variational principle.

As far as the Malfliet-Tjon potential is used, we found that the ground state is well described by the $l=l'=0$ components alone for the three rearrangement channels. Energy of the ground state is obtained as $E_0=-8.2423$ MeV, which agrees with the value in the literature obtained with the same interaction; the observed energy is -8.482 MeV. The Gaussian radial parameters employed are listed in Table II(a); the number of the total basis functions is 200.

As for the $L=1^-$ excited states, we took the case with $(l,l')=(0,1)$ for all three channels and $(l,l')=(1,0)$ for channels 1 and 2. The radial parameters used are shown in Table II(b); the number of the total basis functions is 360. We thus obtained 360 energies, $E_{NL=1}$, above the breakup threshold which stand for the energies of discretized continuum states, $\Phi_{NL=1}$. We have examined several other choices of the parameter sets, but found no significant change in the final result shown below.

B. Triton polarization

The total Hamiltonian for the $t+\mu$ system is given by

$$H=H_t+H_{t\mu}+V_{\text{int}} \tag{38}$$

with

$$H_{t\mu}=-\frac{\hbar^2}{2m}\nabla_r^2-\frac{e^2}{r} , \tag{39}$$

$$V_{\text{int}}=V_{p\mu}+\frac{e^2}{r} , \tag{40}$$

where $\mathbf{r}$ is the muon position vector with respect to the c.m. of triton, and $V_{p\mu}$ is the Coulomb potential between proton and muon with the proton charge distribution folded. Basis functions for muon orbits are given by the solution of the equation

$$(H_{t\mu}-\varepsilon_{nl})\phi_{nlm}(\mathbf{r})=0 . \tag{41}$$

Similar to the case of the $d\mu$ atom in Sec. II, ϕ_{nl} is expanded in terms of Gaussian basis functions [cf. Eq. (24)]:

$$\phi_{nlm}(\mathbf{r})=\sum_i C_{ni} r^l e^{-(r/r_i)^2} Y_{lm}(\hat{\mathbf{r}}) \tag{42}$$

with

$$r_i=r_1 a_r^{i-1}, \quad i=1 \text{ to } i_{\max} . \tag{43}$$

The Gaussian range parameters employed for $l=0$ and 1 are listed in Table III.

The triton polarization energy is calculated within second-order perturbation theory in the same manner as in Sec. II. The energy is given by the expression

$$\Delta E_{t\mu}^{\text{pol}}=-\sum_{n,N}\frac{|\langle[\phi_{nl=1}\Phi_{NL=1}]_{00}|V_{\text{int}}|\phi_{1s}\Phi_{00}\rangle|^2}{E_{NL=1}+\varepsilon_{nl=1}-E_{00}-\varepsilon_{1s}} . \tag{44}$$

Since we take Gaussian basis functions, all the integrations appearing in Eq. (44) can be performed analytically, although the results are not shown here explicitly.

The calculation results

$$\Delta E_{t\mu}^{\text{pol}}=-1.1 \text{ meV} . \tag{45}$$

This is 1 order of magnitude smaller than the deuteron polarization effect, $\Delta E_{d\mu}^{\text{pol}}=-9.9$ meV, which is reasonable because triton is much harder to excite than deuteron is; note their binding energies, -2.22 MeV for d and -8.48 MeV for t.

Contributions of individual terms in Eq. (44) with (n,N) for muon and triton excitations are illustrated in Fig. 5.

This is to be compared with the same illustration (Fig.

TABLE II. The parameters used in the calculation for the $p+n+n$ system: Gaussian radial parameters for (a) $L=0^+$ and (b) $L=1^-$.

c	l	l'	$i_{\max}$	x_1 (fm)	$x_{i_{\max}}$ (fm)	$i'_{\max}$	y_1 (fm)	$y'_{i'_{\max}}$ (fm)
				(a) $L=0$				
1+2	0	0	10	0.1	12.0	10	0.5	8.0
3	0	0	10	0.1	12.0	10	0.5	8.0
				(b) $L=1$				
1+2	0	1	12	0.3	16.0	10	0.6	12.0
3	0	1	12	0.3	16.0	10	0.6	12.0
1+2	1	0	12	0.3	16.0	10	0.6	12.0

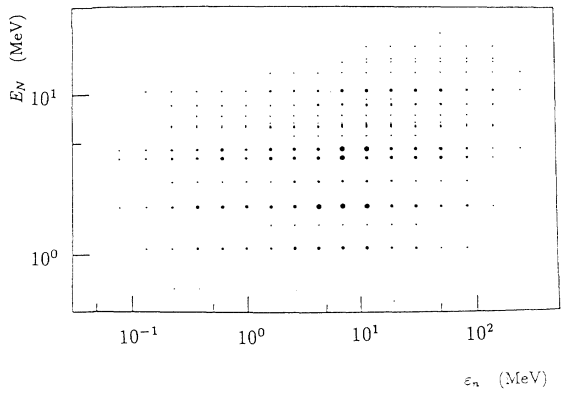

FIG. 5. Contributions to $\Delta E_{t\mu}^{\rm pol} = -1.1$ meV from the individual terms of Eq. (44). The area of the circle is proportional to the magnitude of each contribution (multiplied by -1). The largest circle corresponds to a contribution of -0.02 meV.

2) for the $d\mu$ atom. We find that dominant contributions come from the state (n,N) with $\varepsilon_{nL=1}-\varepsilon_{1s} \approx 1 \sim 50$ MeV and $E_{NL=1}-E_{00} \approx 10 \sim 20$ MeV. This shows breakdown of the adiabatic approximation $\varepsilon_{nL=1}-\varepsilon_{1s} \ll E_{NL=1}-E_{00}$. If we assumed this in the calculation of Eq. (44), then we would have $\Delta E_{t\mu}^{\rm pol} = -2.9$ meV, which is much different from the correct value -1.1 meV.

The triton polarization potential induced by muon, $V_{t\mu}^{\rm pol}(r)$, is calculated in the same manner as in Sec. II for the deuteron polarization potential. The result is shown in Fig. 6 (multiplied by -1) together with the r^{-4} dependent behavior which is given under the dipole and adiabatic approximations; this figure is to be compared with Fig. 3 for the deuteron polarization potential. It is reasonable that $V_{t\mu}^{\rm pol}$ is an order of magnitude smaller

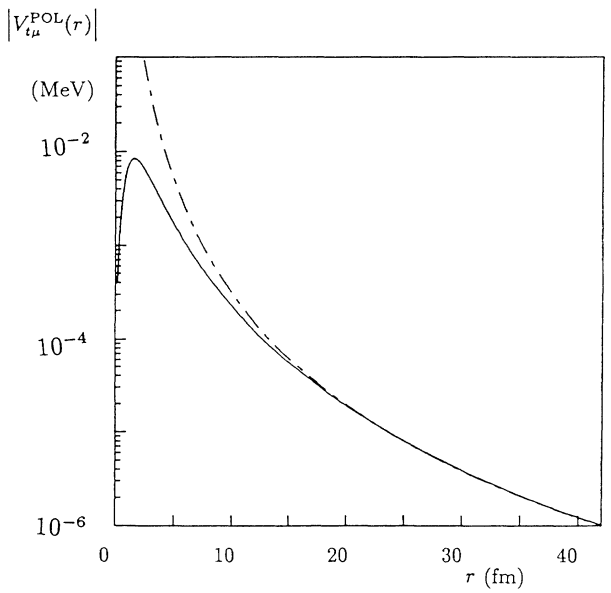

FIG. 6. Triton polarization potentials given by our calculation (solid curve) and by the r^{-4} approximation (dot-dashed curve).

TABLE III. Gaussian range parameters for $l=0$ and 1 of the $t\mu$ system.

	$n_{\rm max}$	r_1 (fm)	$r_{n_{\rm max}}$ (fm)
$l=0$	30	1.25	1800
$l=1$	30	2.0	3000

than $V_{d\mu}^{\rm pol}$. Similar to the deuteron case, we see that $V_{t\mu}^{\rm pol}(r)$ deviates very much from the r^{-4} dependence in the short-range region ($r \lesssim 10$ fm). However, the degree of the deviation is smaller than in the case of deuteron; this is due to the difficulty of excitation of triton compared with deuteron.

The polarization potential $V_{t\mu}^{\rm pol}(r)$ will be used in Sec. IV in the calculation of the triton polarization effect in the $dt\mu$ molecule.

IV. DEUTERON AND TRITON POLARIZATION EFFECTS IN THE $dt\mu$ MOLECULE

In this section we calculate the correction to the energy, ε_{11}, of the $J=v=1$ state of the $dt\mu$ molecule induced by these effects of deuteron and triton polarization.

The deuteron polarization energy in the $(dt\mu)_{11}$ molecule, $\Delta\varepsilon_{11}^{\rm pol}(d)$, is calculated with the first-order perturbation by

$$\Delta\varepsilon_{11}^{{\rm pol},d\mu}(dt\mu) = \langle \Psi_{J=v=1}(dt\mu) | V_{d\mu}^{\rm pol} | \Psi_{J=v=1}(dt\mu) \rangle \ , \tag{46}$$

and the triton polarization correction is given by

$$\Delta\varepsilon_{11}^{{\rm pol},t\mu}(dt\mu) = \langle \Psi_{J=v=1}(dt\mu) | V_{t\mu}^{\rm pol} | \Psi_{J=v=1}(dt\mu) \rangle \ . \tag{47}$$

The sum of the corrections should be measured with respect to the $(t\mu)_{1s}$-d threshold energy which is also corrected by $\Delta E_{t\mu}^{\rm pol} = -1.1$ meV for the $(t\mu)_{1s}$ atom; namely, the total correction, $\Delta\varepsilon_{11}^{\rm pol}(dt\mu)$, due to the nuclear polarization is given by

$$\Delta\varepsilon_{11}^{\rm pol}(dt\mu) = \Delta\varepsilon_{11}^{{\rm pol},d\mu}(dt\mu) + \Delta\varepsilon_{11}^{{\rm pol},t\mu}(dt\mu) - \Delta E_{t\mu}^{\rm pol} \ . \tag{48}$$

In order to perform the integrations in Eqs. (46), we first transform the density $|\Psi_{J=v=1}(dt\mu)|^2$ onto the Jacobi coordinates of the $(d\mu)$-t channel; namely, onto the coordinates $\mathbf{r}_2$ and $\mathbf{R}_2$ of Fig. 7. Then, we make the integration over $\mathbf{R}_2$ on which the potential $V_{d\mu}^{\rm pol}(r_2)$ is independent. We reach the expression

$$\Delta\varepsilon_{11}^{{\rm pol},d\mu}(dt\mu) = \int \rho_{11}(r_2) V_{d\mu}^{\rm pol}(r_2) d\mathbf{r}_2 \tag{49}$$

with

$$\rho_{11}(r_2) = \int |\Psi_{J=v=1}(dt\mu)|^2 d\mathbf{R}_2 \ . \tag{50}$$

Similar procedure is also made for $\Delta\varepsilon_{11}^{{\rm pol},t\mu}(dt\mu)$; we have

$$\Delta\varepsilon_{11}^{{\rm pol},t\mu}(dt\mu) = \int \rho_{11}(r_1) V_{t\mu}^{\rm pol}(r_1) d\mathbf{r}_1 \tag{51}$$

with

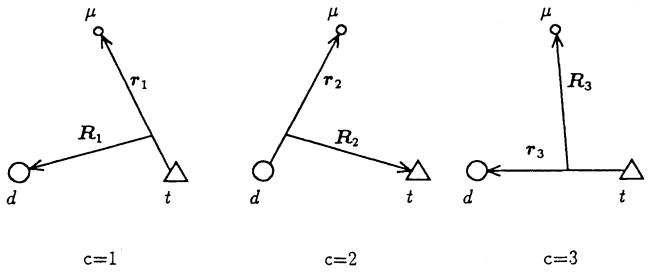

FIG. 7. Three rearrangement channels of the $dt\mu$ system and their Jacobian coordinates.

$$\rho_{11}(r_1)=\int |\Psi_{J=v=1}(dt\mu)|^2 d\mathbf{R}_1 \ . \tag{52}$$

The density functions $\rho_{11}(r_1)$ and $\rho_{11}(r_2)$ were explicitly given in Ref. [8]. Using them, we calculated Eqs. (49) and (51) and obtained

$$\Delta\varepsilon_{11}^{\rm pol}(dt\mu)=-1.7 \text{ meV} \ . \tag{53}$$

It is interesting that the following approximate estimation is very accurate and useful to understand this result. In the short-range region up to about 50 fm, the ratio of the density function ρ_{11} to the $1s$ density of the respective muonic atom in free space is nearly constant: namely,

$$\rho_{11}(r_1)/\rho_{1s}^{t\mu}(r_1)\simeq 0.80 \quad (r_1 \lesssim 50 \text{ fm}) \ , \tag{54}$$

$$\rho_{11}(r_2)/\rho_{1s}^{d\mu}(r_2)\simeq 0.20 \quad (r_2 \lesssim 50 \text{ fm}) \ . \tag{55}$$

Furthermore, as seen in Figs. 3 and 6, $V_{t\mu}^{\rm pol}(r_1)$ and $V_{d\mu}^{\rm pol}(r_2)$ are negligibly small for $r \gtrsim 50$ fm. We can then estimate $\Delta\varepsilon_{11}^{\rm pol}(dt\mu)$ with the relation

$$\begin{aligned}\Delta\varepsilon_{11}^{\rm pol}(dt\mu)&\simeq 0.80\Delta E_{t\mu}^{\rm pol}+0.20\Delta E_{d\mu}^{\rm pol}-\Delta E_{t\mu}^{\rm pol}\\ &=0.20\Delta E_{d\mu}^{\rm pol}-0.20\Delta E_{t\mu}^{\rm pol}\\ &=0.20\times(-9.9 \text{ meV})-0.20\times(-1.1 \text{ meV})\\ &=-1.7 \text{ meV} \ .\end{aligned} \tag{56}$$

This is the same as the value of Eq. (53) which is obtained by accurate integrations of Eqs. (49) and (51).

In the literature, the nuclear polarization effect in the $(dt\mu)_{11}$ molecule was calculated only by Bakalov [7]. He estimated the deuteron polarization correction but not the triton one. In his calculation he took an approximate deuteron polarization potential which is based on the dipole approximation for the muon interaction and the adiabatic approximation for the muon excitation energy. The $(dt\mu)_{11}$ wave function he employed is the one given by Ref. [16], but it is less accurate than the wave function we took here from Ref. [3]. As discussed in Secs. II and III, the two approximations are rather poor. Bakalov gave $\Delta\varepsilon_{11}^{{\rm pol},d\mu}(dt\mu)=-2.2$ meV, which agrees well with our result of $\Delta\varepsilon_{11}^{{\rm pol},d\mu}(dt\mu)=0.20\times(-9.9 \text{ meV})=-2.0$ meV. We understand from the above discussion, however, that this agreement is rather fortuitous.

V. SUMMARY

One of the keys to the muon-catalyzed d-t fusion is the formation of the muonic molecule $(dt\mu)$ in a very loosely bound state with $J=v=1$, and the formation rate is known to depend sharply on the energy of the state, ε_{11}. Three-body calculation of the energy with the nonrelativistic pure Coulombic potentials gave [3] as $\varepsilon_{11}=-660.3$ meV. Since accuracy of the energy was required for at least 0.1–1 meV, various corrections to ε_{11} needed to be estimated carefully. Many authors investigated them, but the deuteron polarization in the $(dt\mu)$ molecule was calculated only in a crude approximation [7], and no calculation has been done for the triton polarization.

In this paper we have developed a three- (four-) body-model calculation for the d-μ (t-μ) system and applied it to the precise calculation of nuclear polarization effects in the $(d\mu)$ and $(t\mu)$ atoms and in the $(dt\mu)$ molecule. We calculated the wave functions of deuteron and triton ground states ($J=0$) and those of continuum-discretized excited states (so-called pseudostates) with $J=1$. The energy of deuteron and triton polarization, $\Delta E_{d\mu}^{\rm pol}$ and $\Delta E_{t\mu}^{\rm pol}$, respectively, were calculated within the second-order perturbation theory.

As for the deuteron polarization, we obtained $\Delta E_{d\mu}^{\rm pol}=-9.9$ meV, and found (Fig. 2) that dominant contributions to it come from the virtual excitation of deuteron internal motion and muon orbital motion both into their $J=1$ continuum states whose excitation energy is several MeV for each. This clearly shows the breakdown of the adiabatic approximation which was employed in the literature calculations; use of the adiabatic approximation (without the dipole approximation) would give $\Delta E_{d\mu}^{\rm pol}=-28.5$ meV. We also found that the dipole approximation is not good; use of the approximation (without the adiabatic approximation) would result in $\Delta E_{d\mu}^{\rm pol}=-12.7$ meV. Using both approximations simultaneously, Startsev, Petrun'kin, and Khomkin [13] gave $\Delta E_{d\mu}^{\rm pol}=-9.1$ meV, but this agreement with our result of -9.9 meV is understood as accidental. We derived the deuteron polarization potential, $V_{d\mu}^{\rm pol}(r)$, induced by the muon-proton interaction in the $d\mu$ atom. It was found (Fig. 3) that the r^{-4}-type potential derived from the dipole and the adiabatic approximations deviates much from our result in the internal region.

We calculated the triton polarization by muon in the $t\mu$ atom, for the first time, within the same manner as for the deuteron polarization, and obtained the polarization energy of $\Delta E_{t\mu}^{\rm pol}=-1.1$ meV. This is an order of magnitude smaller than the deuteron polarization effect but it is reasonable because of the large difference in the binding energies of d and t. Similar to the deuteron case, we found that the adiabatic approximation does not work (Fig. 6) and use of it would give $\Delta E_{t\mu}^{\rm pol}=-2.9$ meV. The triton polarization potential induced by muon, $V_{t\mu}^{\rm pol}(r)$, deviates significantly from the r^{-4} dependence but approaches the r^{-4} behavior much faster than $V_{d\mu}^{\rm pol}(r)$ does; this is reasonable because the effect of the triton excitation is much weaker than that of the deuteron excitation.

With the use of the polarization potentials $V_{d\mu}^{\rm pol}(r)$ and

$V_{t\mu}^{\rm pol}(r)$, we finally calculated the correction to the energy ε_{11} of the $J=v=1$ state of the $dt\mu$ molecule due to the nuclear polarization and obtained it as $\Delta\varepsilon_{11}^{\rm pol}(dt\mu)=-1.7$ meV, to which contribution of the deuteron polarization is -2.0 meV. The nuclear polarization in the $dt\mu$ molecule should significantly affect the resonant formation of the molecule.

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[1] W. H. Breunlich, P. Kammel, J. Cohen, and M. Leon, Annu. Rev. Nucl. Part. Sci. **39**, 311 (1989).
[2] E. A. Vesman, Pis'ma Zh. Eksp. Teor. Fiz. **5**, 113 (1967) [JETP Lett. **5**, 91 (1967)].
[3] M. Kamimura, Phys. Rev. A **38**, 621 (1988).
[4] M. Kamimura, Muon Catal. Fusion **3**, 335 (1988).
[5] V. I. Korobov, I. V. Pusynin, and S. I. Vinitsky, Phys. Lett. B **196**, 272 (1987).
[6] K. Szalewicz, H. J. Monkhorst, W. Kolos, and A. Scrinzi, Phys. Rev. A **36**, 5494 (1987).
[7] D. D. Bakalov, Muon Catal. Fusion **3**, 321 (1988).
[8] K. S. Myint, Y. Akaishi, H. Tanaka, M. Kamimura, and H. Narumi, Z. Phys. A **334**, 423 (1989).
[9] G. Aissing, D. D. Bakalov, and H. J. Monkhorst, Phys. Rev. A **42**, 116 (1990).
[10] L. I. Ponomarev, Muon Catal. Fusion **3**, 629 (1988).
[11] G. Aissing and H. J. Monkhorst, Phys. Rev. A **42**, 3789 (1990); A. Scrinzi and K. Szalewicz, *ibid.* **39**, 4983 (1989).
[12] H. Kameyama, M. Kamimura, and Y. Fukushima, Phys. Rev. C **40**, 976 (1989); M. Kamimura and H. Kameyama, Nucl. Phys. A **508**, 17c (1990).
[13] S. A. Startsev, V. A. Petrun'kin, and A. L. Khomkin, Yad. Fiz. **23**, 1233 (1976) [Sov. J. Nucl. Phys. **23**, 656 (1976)].
[14] N. F. Ramsey, B. J. Malenka, and U. E. Kruse, Phys. Rev. **91**, 1162 (1953).
[15] D. A. Kirzhnits and F. M. Pen'kov, Zh. Eksp. Teor. Fiz. **85**, 80 (1983) [Sov. Phys. JETP **58**, 46 (1983)].
[16] S. I. Vinitsky, V. S. Melezhik, L. I. Ponomarev, I. V. Puzynin, T. P. Puzynina, L. N. Somov, and N. F. Truskova, Zh. Eksp. Teor. Fiz. **79**, 698 (1980) [Sov. Phys. JETP **52**, 353 (1980)].
[17] R. A. Malfliet and J. A. Tjon, Nucl. Phys. A **127**, 161 (1969).