# Hyperradial adiabatic treatment of $d \mu+t$ collisions at low energies 

H. Fukuda* and T. Ishihara<br>Institute of Applied Physics, University of Tsukuba, Ibaraki 305, Japan

S. Hara

Institute of Physics, University of Tsukuba, Ibaraki 305, Japan
(Received 5 July 1989)


#### Abstract

Using the hyperradial adiabatic expansion method, $d \mu+t$ collisions at thermal energies are studied in a two-state approximation. Analytic expressions for the lowest two hyperradial adiabatic potentials and their nonadiabatic correction terms are derived to order $1 / R^{4}$ for large values of hyperradius $R$.


## I. INTRODUCTION

The hyperradial adiabatic expansion method ${ }^{1}$ has been applied to atomic three-body systems such as the doubly excited states of $\mathrm{H}^{-}$and $\mathrm{He} .{ }^{2-4}$ For molecular systems, it has an advantage over the conventional BornOppenheimer ( $\mathbf{B O}$ ) representation, since it has no constant spurious couplings. In fact, hyperradial calculations have given better results for energies of the $\mathrm{HD}^{+}$ ion $^{5-7}$ and $(d t \mu)^{+}$(Refs. 8 and 9) than the BO representation using the same number of expansion terms. The hyperradial expansion is also expected to be useful for collision processes. At present, however, there is no practical application except for the simple $e+\mathrm{H}$ elastic collision. ${ }^{10}$

The object of this paper is to examine the applicability of the hyperradial method to the collision processes, using as an example the $d \mu+t$ system at thermal energies. This process is important in the muon-catalyzed-fusion research. In Sec. II the method is summarized briefly. Results are given in Sec. III. In Appendix A analytic forms of the two lowest hyperradial adiabatic potentials and their nonadiabatic correction terms are given explicitly to order $1 / R^{4}$ for large values of hyperradius $R$. These formulas will be useful for future applications.

## II. FORMULATION

For a three-body system composed of a deuteron $d$, a triton $t$, and a negative muon $\mu$, we define Jacobi coordinates $\left(\mathbf{R}_{d}, \mathbf{r}_{d}\right)$ and $\left(\mathbf{R}_{t}, \mathbf{r}_{t}\right)$ as shown in Fig. 1, and reduced masses as

$$
\begin{align*}
& \frac{1}{M_{d}}=\frac{1}{m_{d}+m_{\mu}}+\frac{1}{m_{t}}, \quad \frac{1}{\mu_{d}}=\frac{1}{m_{\mu}}+\frac{1}{m_{d}}  \tag{1a}\\
& \frac{1}{M_{t}}=\frac{1}{m_{t}+m_{\mu}}+\frac{1}{m_{d}}, \quad \frac{1}{\mu_{t}}=\frac{1}{m_{\mu}}+\frac{1}{m_{t}} \tag{1b}
\end{align*}
$$

where $m_{d}, m_{t}$, and $m_{\mu}$ are the masses of $d, t$, and $\mu$, respectively. The hyperradius $R$ is defined by

$$
\begin{equation*}
\mu R^{2}=M_{d} R_{d}^{2}+\mu_{d} r_{d}^{2}=M_{t} R_{t}^{2}+\mu_{t} r_{t}^{2} \tag{2}
\end{equation*}
$$

where the arbitrary mass parameter $\mu$ is chosen to be

$$
\begin{equation*}
\frac{1}{\mu}=\frac{1}{m_{t}}+\frac{1}{m_{d}} \tag{3}
\end{equation*}
$$

In the following, we use the units $\hbar=e=m=1$ with

$$
\begin{equation*}
\frac{1}{m}=\frac{1}{m_{\mu}}+\frac{1}{m_{d}+m_{t}} \tag{4}
\end{equation*}
$$

The total Hamiltonian after separating the center-of-mass motion is written by ${ }^{5}$

$$
\begin{equation*}
H=-\frac{1}{2 \mu} \frac{1}{R^{5}} \frac{d}{d R} R^{5} \frac{d}{d R}+h(\Omega ; R) \tag{5}
\end{equation*}
$$

The adiabatic Hamiltonian $h(\Omega ; R)$ contains $R$ as a parameter. Five angular variables are represented by $\Omega$ collectively.

Hyperradial adiabatic basis functions $F_{j}(\Omega ; R)$ and adiabatic potentials $U_{j}(R)$ are defined by eigenfunctions and eigenvalues of $h$,

$$
\begin{equation*}
\left[h-U_{j}(R)\right] F_{j}(\Omega ; R)=0 \tag{6}
\end{equation*}
$$

For each total angular momentum ( $J, M$ ) and total parity $p$, the total wave function is expanded as

$$
\begin{equation*}
\Psi^{(J, M, p)}=R^{-5 / 2} \sum_{j} \chi_{j}(R) F_{j}(\Omega ; R) \tag{7}
\end{equation*}
$$



FIG. 1. Jacobi coordinates $\left(\mathbf{R}_{d}, \mathbf{r}_{d}\right)$ and $\left(\mathbf{R}_{t}, \mathbf{r}_{t}\right)$.

Substituting Eq. (7) into the Schrödinger equation, we obtain a set of coupled equations for $\chi_{j}(R)$. However, as has been discussed by Macek, ${ }^{11}$ it is difficult to solve these equations in general because of the long-range couplings.

In the following, we consider the collision system $d \mu+t$ at thermal energies and take into account only two open channels,

$$
\begin{equation*}
(d \mu)_{1 S}+t \rightarrow(d \mu)_{1 S}+t \tag{8a}
\end{equation*}
$$

and

$$
\begin{equation*}
(d \mu)_{1 S}+t \rightarrow(t \mu)_{1 S}+d \tag{8b}
\end{equation*}
$$

In this two-state approximation, there appears no longrange coupling. The radial functions $\chi_{J}(R)$ satisfy the following coupled equations:

$$
\begin{align*}
& \left(-\frac{1}{2 \mu} \frac{d^{2}}{d R^{2}}+V_{d}(R)-E\right) \chi_{d}(R) \\
& \quad-\frac{1}{2 \mu}\left[W_{d, t}(R)+2 P(R) \frac{d}{d R}\right] \chi_{t}(R)=0  \tag{9a}\\
& \left(-\frac{1}{2 \mu} \frac{d^{2}}{d R^{2}}+V_{t}(R)-E\right) \chi_{t}(R) \\
& \quad-\frac{1}{2 \mu}\left[W_{t, d}(R)-2 P(R) \frac{d}{d R}\right] \chi_{d}(R)=0 \tag{9b}
\end{align*}
$$

where $E$ is the center-of-mass total energy, and subscripts $d$ and $t$ represent the channel ( 8 a ) and ( 8 b ), respectively. The effective potentials $V_{j}(R)(j=d, t)$ and the coupling terms $P(R)$ and $W_{j, j^{\prime}}(R)$ are defined by

$$
\begin{align*}
& V_{j}(R)=U_{j}(R)+\frac{15}{8 \mu R^{2}}-\frac{1}{2 \mu} W_{j, j}(R),  \tag{10}\\
& P(R)=\left\langle F_{d} \left\lvert\, \frac{d}{d R} F_{t}\right.\right\rangle  \tag{11}\\
& W_{j, j^{\prime}}(R)=\left\langle F_{j} \left\lvert\, \frac{d^{2}}{d R^{2}} F_{j^{\prime}}\right.\right\rangle, \tag{12}
\end{align*}
$$

where basis functions are normalized as $\left\langle F_{j} \mid F_{j}\right\rangle=1$. The angular bracket represents integration over angular variables $\Omega$.

As $R \rightarrow \infty$, the effective potentials $V_{j}(R)$ behave as

$$
\begin{equation*}
V_{j}(R) \rightarrow \varepsilon_{j, 1}+\frac{J(J+1)}{2 \mu R^{2}}+\frac{\beta_{j}}{R^{4}}, \tag{13}
\end{equation*}
$$

where $\varepsilon_{j, n}$ is the energy of the muonic atom ( $j \mu$ ),

$$
\begin{equation*}
\varepsilon_{j, n}=-\frac{\mu_{j}}{2 n^{2}} \tag{14}
\end{equation*}
$$

and the coefficient $\beta_{j}$ is given by

$$
\begin{equation*}
\beta_{j}=-\frac{9}{4} \frac{M_{j}^{2}}{\mu^{2} \mu_{j}^{3}}\left[1-\frac{2 \mu_{j}^{2}}{3 M_{j}^{2}}\left[J(J+1)+\frac{1}{8}\right]\right) \tag{15}
\end{equation*}
$$

These formulas are derived in Appendix A. The coupling terms vanish exponentially as $R \rightarrow \infty$ because of the spa-
tial separation between basis functions $F_{d}(\Omega ; R)$ and $F_{t}(\Omega ; R)$. Considering the asymptotic form of the effective potential (13) and the short-range nature of the coupling terms, the radial wave functions satisfy the following boundary conditions as $R \rightarrow \infty$ :

$$
\begin{align*}
& \chi_{j}(R) \rightarrow \delta_{j, d} \\
& \frac{1}{K_{j}} \sin \left[K_{j} R-\frac{J \pi}{2}\right] \\
&+ {\left[\frac{\mu_{j}}{\mu_{d}}\right]^{1 / 4}\left[\frac{M_{d}}{\mu}\right)^{1 / 2} f_{j, d}^{(J)} }  \tag{16}\\
&\left.\times \exp \left[i \left\lvert\, K_{j} R-\frac{J \pi}{2}\right.\right]\right]
\end{align*}
$$

where $K_{j}=\sqrt{2 \mu\left(E-\varepsilon_{j, 1}\right)}$. Since

$$
\begin{equation*}
R \rightarrow\left(\frac{M_{j}}{\mu}\right)^{1 / 2} R_{j}+O\left(\frac{1}{R_{j}}\right) \text { as } \quad R_{j} \rightarrow \infty \tag{17}
\end{equation*}
$$

the total wave function satisfies the physical boundary conditions for $R_{j} \rightarrow \infty$,

$$
\begin{align*}
& \Psi^{(J, M, p)} \rightarrow \mathrm{const} \times \frac{1}{R_{j}}\left\{\frac{\delta_{j, d}}{k_{j}} \sin \left[k_{j} R_{j}-\frac{J \pi}{2}\right]\right. \\
&+\left.f_{j, d}^{(J)} \exp \left[i\left(k_{j} R_{j}-\frac{J \pi}{2}\right]\right]\right\} \\
& \times R_{1,0}^{(j)}\left(r_{j}\right) Y_{J, M}\left(\hat{\mathbf{R}}_{j}\right), \tag{18}
\end{align*}
$$

where $R_{n, l}^{(j)}\left(r_{j}\right)$ is the normalized radial function of a muonic atom $(j \mu), Y_{J, M}\left(\widehat{\mathbf{R}}_{j}\right)$ the spherical harmonics, and $k_{j}=\sqrt{2 M_{j}\left(E-\varepsilon_{j, 1}\right)}$ the asymptotic relative momentum in channel $j$. We have used Eq. (A6) in deriving Eq. (18). The integrated cross sections for processes (8a) and (8b) are given by

$$
\begin{equation*}
\sigma_{j, d}=4 \pi \frac{k_{j} M_{d}}{k_{d} M_{j}} \sum_{J=0}^{\infty}(2 J+1)\left|f_{j, d}^{(J)}\right|^{2} \tag{19}
\end{equation*}
$$

## III. RESULTS AND DISCUSSION

We have carried out numerical calculations for the process (8) with $J=0$. Two regular solutions of the coupled equation (9) are obtained by solving it starting out with the following generalized power-series expansions for small $R$; for the first regular solution,

$$
\begin{align*}
& \chi_{d}(R)=R^{9 / 2}\left(1+d_{1,0}^{(1)} R+\cdots\right)  \tag{20a}\\
& \chi_{t}(R)=R^{9 / 2}\left(t_{1,0}^{(1)} R+t_{2,0}^{(1)} R^{2}+\cdots\right) \tag{20b}
\end{align*}
$$

For the second regular solution,

$$
\begin{align*}
& \chi_{d}(R)=R^{5 / 2}\left(d_{1,0}^{(2)} R+d_{2,1}^{(2)} R^{2} \ln R+\cdots\right)  \tag{21a}\\
& \chi_{t}(R)=R^{5 / 2}\left(1+t_{1,0}^{(2)} R+\cdots\right) \tag{21b}
\end{align*}
$$

The explicit form of Eqs. (20) and (21) are given in Appendix B. A linear combination of these two regular solutions yields the radial functions which satisfy the scattering boundary conditions (16).

We have adopted the Runge-Kutta-Gill method to solve Eq. (9) numerically. The adiabatic potentials $V_{j}(R)$ and coupling terms $P(R)$ and $W_{j, j^{\prime}}(R)$ are calculated numerically in our previous paper ${ }^{8}$ for $0<R \leq 25$ by a variational method using spheroidal coordinates for angular variables $\Omega$. Numerical results for $V_{j}(R)$ are well reproduced by the asymptotic form Eq. (13) for $R \geq 20$. Therefore for $R \geq 25$ we use Eq. (13) for $V_{j}(R)$ and set $P(R)$ and $W_{j, j^{\prime}}(R)$ equal to zero. It is confirmed that the use of this simplification for $R \geq 22.5$ does not change the final results.

In Table I our results for the elastic (8a) and the $\mu$ transfer ( 8 b ) processes at center-of-mass incident energies $E_{i}=E-\varepsilon_{d, 1}=10^{-3}$ and $10^{-2} \mathrm{eV}$ are compared with those of perturbed stationary state (PSS) method ${ }^{12}$ and of the distorted atomic orbital (DAO) method. ${ }^{12}$ Both PSS and DAO results are in the two-state approximation. In the DAO method, basis functions for each channel $j$ are defined by eigenfunctions of the total Hamiltonian with the relative Jacobi coordinate $R_{j}$ fixed. Thus they satisfy the exact boundary conditions for both channels and, therefore, there appears no spurious coupling. In the PSS method, ${ }^{12}$ the reduced mass of the adiabatic Hamiltonian is defined as that of a $d \mu$ atom. Therefore the dissociation energy of the incident channel is given correctly.

For the $\mu$-transfer process, the DAO results are in good agreement with the variational calculations ${ }^{13}$ and with the experimental results ${ }^{14}$ deduced from the muon-catalyzed-fusion data. On the other hand, the PSS cross sections are much smaller than the DAO cross sections. This discrepancy is attributed to the poor description of the final channel wave function in the PSS method. ${ }^{12}$ In the present formalism, the basis functions satisfy the correct boundary conditions as $R \rightarrow \infty$. However, there exist long-range couplings of order $1 / R$ with the states neglected in our two-state approximation. Because of these couplings, improvement over the PSS results is not quite sufficient. For further improvement, more states are necessary in the expansion.

For the elastic process, there are no experimental results to compare with. The present results agree very well with the DAO results. The PSS results are also in good agreement with these two, because the incident channel wave function is not very bad for such low energies.

TABLE I. Elastic and $\mu$-transfer cross sections (in units of $10^{-20} \mathrm{~cm}^{2}$ ) for $d \mu+t$ collisions. $E_{t}$ is the center-of-mass incident energy.

| $E_{i}(\mathrm{eV})$ | Method | Elastic ( $\sigma_{d, d}$ ) | Transfer ( $\sigma_{t, d}$ ) |
| :---: | :---: | :---: | :---: |
| $10^{-3}$ | Present | 1.7 | 9.1 |
|  | DAO ${ }^{\text {a }}$ | 2.0 | 16.0 |
|  | PSS ${ }^{\text {a }}$ | 2.2 | 3.9 |
| $10^{-2}$ | Present | 2.3 | 2.9 |
|  | DAO ${ }^{\text {a }}$ | 2.3 | 4.9 |
|  | PSS ${ }^{\text {a }}$ | 2.8 | 1.2 |

${ }^{\mathrm{a}}$ Reference 12.

## APPENDIX A

In this appendix, we present the expansion coefficients as $R \rightarrow \infty$ for the lowest two adiabatic potentials $U_{j}(R)$ and their diagonal nonadiabatic correction terms $W_{j, j}(R)$ to order $1 / R^{4}$. This expansion is a generalization of Macek's work for two-electron atoms, ${ }^{2}$ and can be applied to three-body systems of arbitrary mass ratio.

We choose the five angular variables as $\Omega=\left(\alpha, \widehat{\mathbf{r}}_{d}, \widehat{\mathbf{R}}_{d}\right)$, where

$$
\begin{equation*}
\tan \alpha=\left(\frac{\mu_{d}}{M_{d}}\right)^{1 / 2} \frac{r_{d}}{R_{d}} \tag{A1}
\end{equation*}
$$

Then, the adiabatic Hamiltonian $h$ is written by ${ }^{5}$

$$
\begin{align*}
h=\frac{1}{2 \mu R^{2}}[- & \frac{1}{\sin \alpha \cos \alpha} \frac{d^{2}}{d \alpha^{2}} \sin \alpha \cos \alpha+\frac{(\mathrm{J}-l)^{2}}{\cos ^{2} \alpha} \\
& \left.+\frac{l^{2}}{\sin ^{2} \alpha}-4\right]-\frac{Z_{d}}{r_{d}}-\frac{Z_{t}}{r_{t}}+\frac{Z_{d} Z_{t}}{R_{d t}} \tag{A2}
\end{align*}
$$

where $l=-i \mathrm{r}_{d} \times \nabla_{r_{d}}$ and $R_{d t}$ is a distance between $d$ and $t$. Considering a general Coulomb three-body system, we denote the charges of $d$ and $t$ by $Z_{d}$ and $Z_{t}$, respectively. As $R \rightarrow \infty$, the adiabatic functions are concentrated in a narrow region near $\alpha=0$ which is the valley of the Coulomb potential. This corresponds to $d \mu+t$ channel because of the definition (A1). Throughout this appendix, we consider this channel only. Expression for the other channel, $t \mu+d$, is given by interchanging the subscripts $d$ and $t$.

Following Macek, ${ }^{2}$ we rewrite the adiabatic Hamiltonian $h$ by using, instead of $\alpha$,

$$
\begin{equation*}
\rho=\left(\frac{\mu}{\mu_{d}}\right)^{1 / 2} R \alpha \tag{A3}
\end{equation*}
$$

as an independent variable and expand it in inverse powers of $R$,

$$
\begin{equation*}
h=h^{(0)}+\frac{1}{R}\left(\frac{M_{d}}{\mu}\right)^{1 / 2}\left(Z_{d}-1\right) Z_{t}+\frac{1}{R^{2}} h^{(-2)}+\cdots \tag{A4}
\end{equation*}
$$

where

$$
h^{(0)}=\frac{1}{\sin \alpha \cos \alpha}\left(-\frac{1}{2 \mu_{d}} \frac{d^{2}}{d \rho^{2}}+\frac{l^{2}}{2 \mu_{d} \rho^{2}}-\frac{Z_{d}}{\rho}\right)
$$

$\times \sin \alpha \cos \alpha$.
(A5)
We consider an eigenvalue problem for the Hamiltonian $h^{(0)}$ in the limit of large $R$. The boundary conditions are taken at the point $\rho=(\pi / 2) \sqrt{\mu / \mu_{d}} R \rightarrow \infty$. Since the operator $h^{(0)}$ is hydrogenic except for the factor $\sin \alpha \cos \alpha$ and its inverse, the eigenvalue is given by Eq. (14) and the normalized eigenfunction for a given $(J, M, p)$ is given by

$$
\begin{align*}
\psi_{n, l, m}(\Omega ; R)= & \left(\frac{\mu R^{2}}{\mu_{d}}\right)^{1 / 4} \frac{1}{\sin \alpha \cos \alpha} \rho R_{n, l}^{(d)}(\rho) \bar{P}_{l, m} \\
& \times(\cos \theta) \mathcal{D}_{m}^{(J, M, p)}(\varphi, \Theta, \Phi) \tag{A6}
\end{align*}
$$

where $\bar{P}_{l, m}(\cos \theta)$ is the normalized associated Legendre polynomial and $\theta$ is an angle between $\widehat{\mathbf{r}}_{d}$ and $\widehat{\mathbf{R}}_{d}$. The angular part of the eigenfunction (A6) is defined by Wigner's $D$ function, ${ }^{15} D_{m, M}^{J}(\varphi, \Theta, \Phi)$, as

$$
\begin{align*}
\mathcal{D}_{m}^{(J, M, p)}(\varphi, \Theta, \Phi)= & \frac{1}{4 \pi}\left[\frac{2 J+1}{1+\delta_{0, m}}\right]^{1 / 2} \\
& \times\left[D_{-m,-M}^{J}(\varphi, \Theta, \Phi)\right. \\
& \left.\quad+p(-1)^{J+m} D_{m,-M}^{J}(\varphi, \Theta, \Phi)\right] \tag{A7}
\end{align*}
$$

where $(\Theta, \Phi)=\hat{\mathbf{R}}_{d}$ and $\varphi$ is azimuthal angle of $\mathbf{r}_{d}$ around $\mathbf{R}_{d}$.

The asymptotic expansion of the adiabatic potentials and basis functions are obtained by treating higher-order terms of expansion (A4) as a perturbation. They are given explicitly by

$$
\begin{align*}
h^{(-2)}= & \frac{1}{2 \mu}\left[(\mathbf{J}-l)^{2}+\frac{l^{2}}{3}-4-\frac{\rho}{3 a}\right] \\
& -\frac{Z_{t} M_{d} \rho}{\mu}\left(\xi+Z_{d} \eta\right) \cos \theta  \tag{A8}\\
h^{(-3)}= & {\left[\frac{M_{d}}{\mu}\right]^{3 / 2} Z_{t} \rho^{2} } \\
& \times\left[\frac{\mu_{d}}{M_{d}} \frac{Z_{d}-1}{2}-\left(\xi^{2}-Z_{d} \eta^{2}\right) P_{2}(\cos \theta)\right]  \tag{A9}\\
h^{(-4)}= & \frac{\mu_{d} \rho^{2}}{2 \mu^{2}}\left[(\mathbf{J}-l)^{2}+\frac{l^{2}}{15}-\frac{7 \rho}{180 a}\right] \\
& -\frac{Z_{t} M_{d}^{2} \rho^{3}}{\mu^{2}}\left[\frac{5 \mu_{d}}{6 M_{d}}\left(\xi+Z_{d} \eta\right) \cos \theta\right. \\
& \left.+\left(\xi^{3}+Z_{d} \eta^{3}\right) P_{3}(\cos \theta)\right] \tag{A10}
\end{align*}
$$

where $P_{n}(\cos \theta)$ is the Legendre polynomial, $\xi=m_{d} /\left(m_{d}+m_{\mu}\right), \quad \eta=m_{\mu} /\left(m_{d}+m_{\mu}\right), \quad$ and $a=1 /\left(Z_{d} \mu_{d}\right)$. For the lowest adiabatic state with normal parity $p=(-1)^{J}$, the basis function and the adiabatic potential are expanded as

$$
\begin{align*}
F_{d}(\Omega ; R)= & \psi_{1,0,0}(\Omega ; R) \\
& +\frac{1}{R^{2}} \sum_{n \neq 1} \sum_{l} \frac{\psi_{n, l, 0}\left\langle\psi_{n, l, 0}\right| h^{(-2)}\left|\psi_{1,0,0}\right\rangle}{\varepsilon_{d, 1}-\varepsilon_{d, n}}+\cdots, \tag{A11}
\end{align*}
$$

$U_{d}(R)=\varepsilon_{d, 1}+\left(\frac{M_{d}}{\mu}\right)^{1 / 2} \frac{Z_{t}\left(Z_{d}-1\right)}{R}+\frac{1}{R^{2}} U_{d}^{(-2)}+\cdots$.

The angular bracket is the integration over angular variables $\Omega$ with the volume element

$$
\begin{equation*}
d \Omega=\sin ^{2} \alpha \cos ^{2} \alpha d \alpha d \hat{\mathbf{r}}_{d} d \hat{\mathbf{R}}_{d} \tag{A13}
\end{equation*}
$$

The second- and the third-order coefficients of $U_{d}(R)$ are given simply by

$$
\begin{equation*}
U_{d}^{(-2)}=\left\langle\psi_{1,0,0}\right| h^{(-2)}\left|\psi_{1,0,0}\right\rangle=\frac{J(J+1)}{2 \mu}-\frac{9}{4 \mu}, \tag{A14}
\end{equation*}
$$

$$
\begin{align*}
U_{d}^{(-3)} & =\left\langle\psi_{1,0,0}\right| h^{(-3)}\left|\psi_{1,0,0}\right\rangle \\
& =\frac{3 a}{2 \mu}\left[\frac{M_{d}}{\mu_{d}}\right]^{1 / 2} \frac{Z_{t}\left(Z_{d}-1\right)}{Z_{d}} \tag{A15}
\end{align*}
$$

We define

$$
\begin{equation*}
\widetilde{\alpha}=\sum_{n \neq 1} \sum_{l} \frac{\left.\left|\left\langle\psi_{1,0,0}\right| \rho \cos \theta\right| \psi_{n, l, 0}\right\rangle\left.\right|^{2}}{\varepsilon_{d, 1}-\varepsilon_{d, n}} \tag{A16}
\end{equation*}
$$

and

$$
\begin{equation*}
\widetilde{\psi}=\sum_{n \neq 1} \frac{\psi_{n, 0,0}\left\langle\psi_{n, 0,0}\right| \rho\left|\psi_{1,0,0}\right\rangle}{\varepsilon_{d, 1}-\varepsilon_{d, n}} \tag{A17}
\end{equation*}
$$

to write the fourth-order coefficient as

$$
\begin{align*}
U_{d}^{(-4)}= & \left\langle\psi_{1,0,0}\right| h^{(-4)}\left|\psi_{1,0,0}\right\rangle \\
& +\left\langle\psi_{1,0,0}\right| \frac{\rho}{36 \mu^{2} a^{2}}|\widetilde{\psi}\rangle \\
& \left.+\widetilde{\alpha} \left\lvert\, \frac{Z_{t} M_{d}}{\mu}\left(\xi+Z_{d} \eta\right)\right.\right)^{2} . \tag{A18}
\end{align*}
$$

Here the quantity $\widetilde{\alpha}$ is related to the dipole polarizability of a hydrogenic atom ${ }^{16}$ and is given by $\widetilde{\alpha}=-\frac{9}{4} \mu_{d} a^{4}$. By solving the inhomogeneous differential equation,

$$
\begin{equation*}
\left(h^{(0)}-\varepsilon_{d, 1}\right) \tilde{\psi}=(3 a / 2-\rho) \psi_{1,0,0} \tag{A19}
\end{equation*}
$$

the function $\tilde{\psi}$ is obtained in a closed form as $\widetilde{\psi}=\psi_{1,0,0}\left(3 a^{2}-\rho^{2}\right) \mu_{d} a / 2$. Substituting these expressions for $\widetilde{\alpha}$ and $\widetilde{\psi}$ into Eq. (A18) and carrying out integrations, we obtain

$$
\begin{align*}
U_{d}^{(-4)}=-\frac{9}{4} \frac{\mu_{d} a^{2}}{\mu^{2}} & \left\{a^{2}\left(Z_{t} M_{d}\right)^{2}\left(\xi+Z_{t} \eta\right)^{2}\right. \\
& \left.-\frac{2}{3}\left[J(J+1)-\frac{1}{8}\right]\right\} \tag{A20}
\end{align*}
$$

The diagonal nonadiabatic correction terms are obtained by substituting Eq. (A11) into Eq. (12),

$$
\begin{equation*}
W_{d, d}(R)=\frac{1}{R^{2}} W_{d, d}^{(-2)}+\frac{1}{R^{4}} W_{d, d}^{(-4)}+\cdots \tag{A21}
\end{equation*}
$$

where

$$
\begin{equation*}
W_{d, d}^{(-2)}=\left\langle\psi_{1,0,0} \left\lvert\, R^{2} \frac{d^{2}}{d R^{2}} \psi_{1,0,0}\right.\right\rangle=-\frac{3}{4}, \tag{A22}
\end{equation*}
$$

$$
\begin{align*}
W_{d, d}^{(-4)}= & -\frac{1}{6 \mu a}\left\langle\tilde{\psi} \left\lvert\, R^{2} \frac{d^{2}}{d R^{2}} \psi_{1,0,0}\right.\right\rangle \\
& -\frac{1}{6 \mu a}\left\langle\psi_{1,0,0} \left\lvert\, R^{4} \frac{d^{2}}{d R^{2}} \frac{1}{R^{2}} \tilde{\psi}\right.\right\rangle=-\frac{3 \mu_{d} a^{2}}{4 \mu} . \tag{A23}
\end{align*}
$$

In this appendix, we have assumed implicitly the three-body system composed of distinguishable particles. Nevertheless, the results obtained can be applied to the system containing two identical particles such as twoelectron atoms. In this case, the adiabatic potential and the diagonal nonadiabatic correction term have the same asymptotic expansions for both symmetric and antisymmetric states. Further, the restriction to normal parity $p=(-1)^{J}$ is not necessary for present analysis. The expansion for the lowest two states with abnormal parity $p=-(-1)^{J}$ will be obtained similarly.

## APPENDIX B

In this appendix, we give the explicit form of the generalized power series (20) and (21). Following Klar, ${ }^{17}$ we assume the expansions for the radial functions;

$$
\begin{align*}
& \chi_{d}(R)=R^{\lambda} \sum_{n=0}^{\infty} \sum_{m=0}^{[n / 2]} d_{n, m} R^{n}(\ln R)^{m},  \tag{B1a}\\
& \chi_{t}(R)=R^{\lambda} \sum_{n=0}^{\infty} \sum_{m=0}^{[n / 2]} t_{n, m} R^{n}(\ln R)^{m}, \tag{B1b}
\end{align*}
$$

where $\left(d_{0,0}, t_{0,0}\right) \neq(0,0)$ and the square brackets represent integer part. In order to determine $\lambda, d_{n, m}$, and $t_{n, m}$, we expand in powers of $R$ the effective potentials and the coupling terms in Eq. (9). As $R \rightarrow 0$, the basis functions tend to hyperspherical harmonics ${ }^{18}$ which are the eigenfunctions of the adiabatic Hamiltonian $h$
without Coulomb interactions, i.e., the first term of Eq. (A2). By treating the Coulomb interaction as a perturbation, we obtain the following expansions for effective potentials, Eq. (10) and coupling terms, Eqs. (11) and (12), where $j, j$ are either $d$ or $t$;
$V_{j}(R) \rightarrow \frac{l_{j}\left(l_{j}+1\right)}{2 \mu R^{2}}+\frac{C_{j}}{2 \mu R}+v_{j}^{(0)}+v_{j}^{(1)} R+\cdots$,
$P(R) \rightarrow p^{(0)}+p^{(1)} R+\cdots$,
$W_{j, j^{\prime}}(R) \rightarrow w_{j, j^{\prime}}^{(0)}+w_{j, j^{\prime}}^{(1)} R+\cdots$,
with $l_{d}=\frac{7}{2}$ and $l_{t}=\frac{3}{2}$. Substituting these expansions and Eq. (B1) into the radial equation (9) and equating the same terms of generalized powers, we obtain the following two regular solutions. For the first regular solution,

$$
\begin{align*}
& \lambda=l_{d}+1=\frac{9}{2},  \tag{B5}\\
& d_{0,0}=1, t_{0,0}=0,  \tag{B6}\\
& d_{1,0}=\frac{C_{d}}{9}, t_{1,0}=\frac{3}{7} p^{(0)},  \tag{B7}\\
& t_{2,1}=0, \\
& t_{2,0}=\frac{1}{32}\left(\frac{3}{7} C_{t} p^{(0)}+\frac{11}{9} C_{d} p^{(0)}-w_{t, d}^{(0)}-9 p^{(1)}\right) . \tag{B8}
\end{align*}
$$

For the second regular solution,

$$
\begin{align*}
& \lambda=l_{t}+1=\frac{5}{2},  \tag{B9}\\
& d_{0,0}=0, \quad t_{0,0}=1,  \tag{B10}\\
& d_{1,0}=\frac{5}{7} p^{(0)}, \quad t_{1,0}=\frac{C_{t}}{5},  \tag{B11}\\
& d_{2,1}=\frac{1}{8}\left(\frac{5}{7} C_{d} p^{(0)}-\frac{7}{5} C_{t} p^{(0)}-w_{d, t}^{(0)}-5 p^{(1)}\right),  \tag{B12}\\
& d_{2,0}=0 .
\end{align*}
$$

*Present address: Atomic Processes Laboratory, Institute of Physical and Chemical Research (RIKEN), Wako-shi Saitama 351-01, Japan.
${ }^{1}$ U. Fano, Phys. Rev. A 24, 2402 (1981).
${ }^{2}$ J. Macek, J. Phys. B 1, 831 (1968).
${ }^{3}$ C. D. Lin, Phys. Rev. A 29, 1019 (1984).
${ }^{4}$ H. Fukuda, N. Koyama, and M. Matsuzawa, J. Phys. B 20, 2959 (1987).
${ }^{5}$ J. Macek and K. A. Jerjian, Phys. Rev. A 33, 233 (1986); K. A. Jerjian and J. Macek, Phys. Rev. A 36, 2667 (1987).
${ }^{6}$ S. Hara, H. Fukuda, and T. Ishihara, Phys. Rev. A 39, 35 (1989).
${ }^{7}$ R. E. Moss and I. A. Sadler, Mol. Phys. 66, 591 (1989).
${ }^{8}$ S. Hara, H. Fukuda, T. Ishihara, and A. V. Matveenko, Phys. Lett. A 130, 22 (1988).
${ }^{9}$ S. I. Vinitskii et al., Zh. Eksp. Teor. Fiz. 79, 698 (1980) [Sov. Phys.-JETP 52, 353 (1980)].
${ }^{10}$ C. D. Lin, Phys. Rev. A 12, 493 (1975).
${ }^{11}$ J. Macek, Phys. Rev. A 31, 2162 (1985).
${ }^{12}$ K. Kobayashi, T. Ishihara, and N. Toshima, Muon Catalyzed Fusion 2, 191 (1988).
${ }^{13}$ M. Kamimura, Muon Catalyzed Fusion 3, 335 (1988).
${ }^{14}$ D. V. Balin et al., Muon Catalyzed Fusion 2, 163 (1988).
${ }^{15}$ M. E. Rose, Elementary Theory of Angular Momentum (John Wiley and Sons, New York, 1957), p. 52.
${ }^{16}$ L. D. Landau and E. M. Lifshitz, Quantum Mechanics (Pergamon, Oxford, 1977), p. 269.
${ }^{17}$ H. Klar, J. Phys. A 18, 1561 (1985).
${ }^{18}$ P. M. Morse and H. Feshbach, Methods of Theoretical Physics (McGraw-Hill, New York, 1953), p. 1730.

