X-ray spectrum due to the deexcitation of a muonic molecule $p\alpha\mu$

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The x-ray spectrum due to the deexcitation of a muonic molecule $p\alpha\mu$ with total angular momentum $J=1$ composed of ^{4}He, ^{1}H (and its isotopes), and a muon is investigated. There is a small second peak in the spectrum of $p\alpha\mu$. The lifetime of the muonic molecules is three times longer than that determined by a previous calculation.

I. INTRODUCTION

The bound state of a muonic molecule $(p\alpha\mu)_{J=1}$ composed of a proton p (or its isotopes deuteron d and triton t), an α particle α, and a negative muon μ with total angular momentum $J=1$ is related to the muon transfer process

$$p\mu+\mathrm{He}\rightarrow[(p\alpha\mu)_{J=1}e]+e\ , \tag{1}$$

$$(p\alpha\mu)_{J=1}\rightarrow\alpha\mu+p+h\nu\ . \tag{2}$$

In order to avoid confusion, we refer to the state $(p\alpha\mu)_{J=1}$ as a bound state in the following, although, strictly, it may be referred to as a resonant state because it is imbedded in the continuum of $\alpha\mu+p$. Above processes are important since the mesic atoms such as $p\mu$ contribute to the muon-catalyzed fusion reaction, whereas the final product $\alpha\mu$ does not. Aristov *et al.*[1] and Kravtsov *et al.*[2] theoretically investigated the bound-state energies of $(p\alpha\mu)_{J=1}$ (and its isotopes) and the formation rate of $(p\alpha\mu)_{J=1}$ in process (1). The bound state $(p\alpha\mu)_{J=1}$ decays into the ground repulsive $\alpha\mu+p$ state with x-ray emission by electric dipole transition (see Fig. 1). The lifetime of $(p\alpha\mu)_{J=1}$ and x-ray spectrum for process (2) were studied by Kravtsov *et al.*[3] by use of the Born-Oppenheimer approximation to the initial bound and final repulsive states. An experiment is now in progress to measure the x-ray spectrum for process (2).[4]

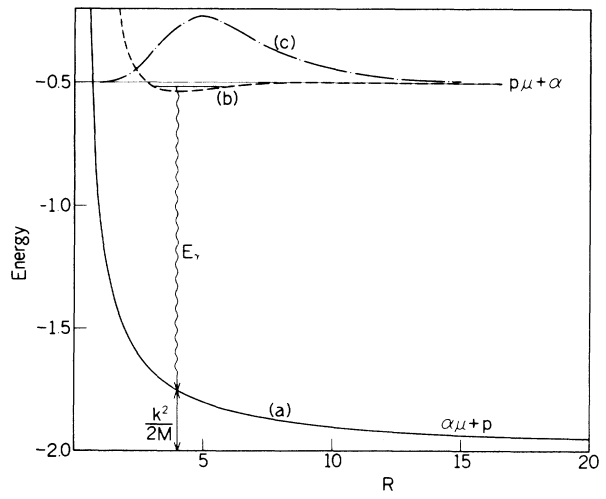

FIG. 1. Schematic diagram for the deexcitation of $(p\alpha\mu)_{J=1}$. The units are defined by Eq. (7). (a) Adiabatic potential energy curve $\varepsilon_0(R)$ for $\alpha\mu+p$, (b) adiabatic potential energy curve for $p\mu+\alpha$, (c) probability density of the bound state $(p\alpha\mu)_{J=1}$ $\rho(\mathbf{R})=\int|\Psi^{JM}(\mathbf{r},\mathbf{R})|^2 d\mathbf{r}\,2\pi\sin\Theta\,d\Theta$. The ordinate for curve (c) is arbitrary.

In this paper, process (2) is reformulated. The x-ray spectra and the lifetime of $(p\alpha\mu)_{J=1}$ and its isotopes are calculated using the exact wave function for the initial bound state. The obtained spectrum for $(p\alpha\mu)_{J=1}$ has a small second peak at the emitted photon energy $E_\gamma=8.02$ keV. Intensities of x-ray spectra are three times smaller and thus the lifetime three times longer than those of a previous calculation.[3]

II. THEORY

The total wave function for $(p\alpha\mu)_{J=1}$ and its isotopes can be written in the following form:

$$\Psi^{JM}=\sum_m \Phi^{Jm}(\xi,\eta,R)\left[\frac{2J+1}{8\pi^2}\right]^{1/2} D^{J*}_{Mm}(\Phi,\Theta,\varphi)\ . \tag{3}$$

Here M and m are components of the total angular momentum J along a space fixed z axis and along internuclear distance vector $\mathbf{R}$, respectively, D^{J*}_{Mm} is the rotation matrix,[5] and $R=|\mathbf{R}|$. A set of variables $\mathbf{r}(\xi,\eta,\varphi)$ represents spheroidal coordinates for the muon; Θ and Φ are the polar and azimuthal angles for the vector $\mathbf{R}$ in the space-fixed coordinates. The position vector of the muon relative to the midpoint of p and α is represented by $\mathbf{r}$.

We adopt Eq. (3) for the wave function of the initial bound state and the Born-Oppenheimer (BO) approximation for the ground repulsive state. Thus the wave function for the final state, in which the momentum for the

relative motion of p and α is k, is given by

$$\Psi_{\rm BO}^{JM}=\Phi_{1\sigma}(\xi,\eta;R)\frac{X_J(kR)}{R}\left[\frac{2J+1}{8\pi^2}\right]^{1/2}D_{M0}^{J*}(\Phi,\Theta,\varphi)\ . \tag{4}$$

The ground-state 1σ orbital for $p\alpha\mu$ $\Phi_{1\sigma}(\xi,\eta;R)$ is determined by the following equation:

$$\left[-\frac{1}{2m}\nabla_r^2+\frac{2}{R}-\frac{2}{r_{\alpha\mu}}-\frac{1}{r_{p\mu}}-\varepsilon_0(R)\right]\Phi_{1\sigma}(\xi,\eta;R)=0\ , \tag{5}$$

where $r_{\alpha\mu}$ and $r_{p\mu}$ are distances between α and μ and p and μ, respectively, $\epsilon_0(R)$ the adiabatic potential energy for $\alpha\mu+p$, and

$$1/m=1/M_\alpha+1/m_\mu\ . \tag{6}$$

Here M_α and m_μ are masses of α and μ, respectively. This choice of m gives correct dissociation limit for $\alpha\mu+p$ in the BO approximation. Unless otherwise stated, the following units are used throughout this paper:

$$e=\hbar=m=1\ . \tag{7}$$

The radial function $X_J(kR)$ satisfies the following equation:

$$\left[-\frac{1}{2M}\left[\frac{d^2}{dR^2}-\frac{J(J+1)}{R^2}\right]+\varepsilon_0(R)-\frac{1}{2M}k^2\right]X_J(kR)=0\ , \tag{8}$$

with boundary conditions,

$$X_J(0)=0\ . \tag{9}$$

$$X_J(kR)\rightarrow\sin\left[kR-\frac{J\pi}{2}-\frac{M}{k}\ln(2kR)+\delta_J\right]\ , \tag{10}$$

where δ_J is the phase shift including the Coulomb phase. In Eq. (8),

$$1/M=1/M_p+1/M_\alpha\ , \tag{11}$$

and M_p is the proton mass. The momentum k for the relative motion is determined by

$$E_{p\alpha\mu}-\varepsilon_0(\infty)=E_\gamma+\frac{k^2}{2M}\ , \tag{12}$$

where $E_{p\alpha\mu}$ is the bound-state energy.

The transition probability per unit time and unit energy, that is, the energy spectrum of x-ray is given by

$$\frac{d\lambda}{dE}=\tfrac{4}{3}(\alpha E_\gamma)^3\left[\frac{2M}{\pi k}\right]\sum_{M_i}\sum_{J_fM_f}\frac{1}{2J_i+1}|\langle\Psi_{\rm BO}^{J_fM_f}|\mathbf{d}|\Psi^{J_iM_i}\rangle|^2, \tag{13}$$

where the angular bracket denotes volume integral over $\mathbf{R}$ and $\mathbf{r}$, α is the fine-structure constant, and $\mathbf{d}$ the dipole moment of $p\alpha\mu$ with respect to the center of mass of the system,

$$\mathbf{d}=-\left[1+\frac{2m_\mu}{M_{\rm tot}}\right]\mathbf{r}-\frac{1}{M_{\rm tot}}(-3M_p+M_\alpha-m_\mu)\mathbf{R}\ , \tag{14}$$

where

$$M_{\rm tot}=M_p+M_\alpha+m_\mu\ . \tag{15}$$

In Eq. (13), three components of $\mathbf{d}$ give the same contribution. The space-fixed z component of $\mathbf{d}$ can be written in the form

$$d_z=\sum_\lambda D_{0\lambda}^{1*}(\Phi,\Theta,\varphi)g_\lambda(\xi,\eta,R)\ , \tag{16}$$

where g_λ are functions of ξ, η, and R. Substitution of Eqs. (3), (4), and (16) into (13) gives

$$\frac{d\lambda}{dE}=\frac{8M}{3\pi k}(\alpha E_\gamma)^3\sum_{J_f}\left|\sum_m C(J_i1J_f;m,-m)A(J_f,m)\right|^2\ , \tag{17}$$

where

$$A(J_f,m)=\left[\int R\,dR\right]X_{J_f}(kR)(\Phi_{1\sigma}|g_{-m}|\Phi^{J_im})\ . \tag{18}$$

In Eq. (18), the last set parentheses denotes the integral over ξ and η.

III. RESULTS

We have calculated the bound-state energies of $p\alpha\mu$ (and its isotopes) $E_{p\alpha\mu}$ and wave function $\Psi^{J_iM_i}$ with $J_i=1$, $M_i=0$ by a variational method[6,7] using a 300-term trial function. In Table I, $E_{p\alpha\mu}$ values are compared with those obtained by using the BO approximation.[1,2] For the final state, $\Phi_{1\sigma}(\xi,\eta;R)$ and $\varepsilon_0(R)$ are calculated by the method proposed by Bates and Carson.[8] Equation (8) for $J=J_f=0$ and 2 were solved numerically to obtain the radial wave function $X_J(kR)$. We have adopted the following mass constants: $M_\alpha=7294.295m_e$, $M_p=1836.151m_e$, deuteron mass $M_d=3670.481m_e$, triton mass $M_t=5496.899m_e$, and $m_\mu=206.769m_e$, where m_e is the electron mass.

TABLE I. Energies and lifetimes of $(p\alpha\mu)_{J=1}$ and its isotopes. (a) present; (b) Refs. 1 and 3; (c) Ref. 2.

Muonic molecule	Energy (eV)	Lifetime (sec)
$p\alpha\mu$		
(a)	−50.02	5.20×10^{-12}
(b)	−41.6	1.8×10^{-12}
(c)	−43.7	
$d\alpha\mu$		
(a)	−57.84	5.90×10^{-12}
(b)	−55.9	1.9×10^{-12}
(c)	−57.5	
$t\alpha\mu$		
(a)	−63.53	6.03×10^{-12}
(b)	−62.9	2.1×10^{-12}
(c)	−63.9	

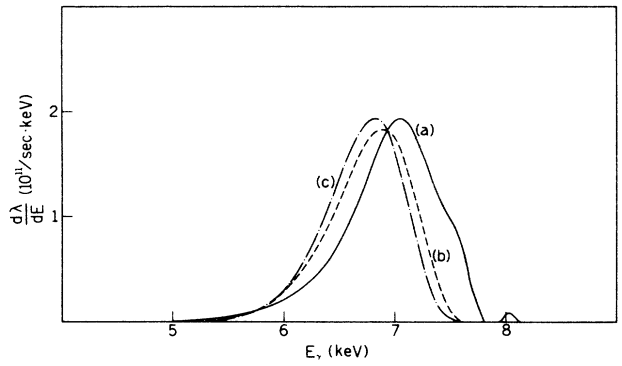

FIG. 2. X-ray spectra due to the deexcitation. (a) $p\alpha\mu \rightarrow \alpha\mu + p$, (b) $d\alpha\mu \rightarrow \alpha\mu + d$, (c) $t\alpha\mu \rightarrow \alpha\mu + t$.

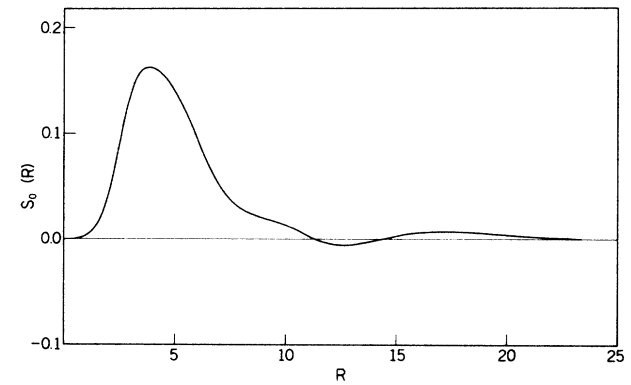

FIG. 3. $S_0(R)$ for $(p\alpha\mu)_{J=1}$, see Eq. (20). The units are defined by Eq. (7).

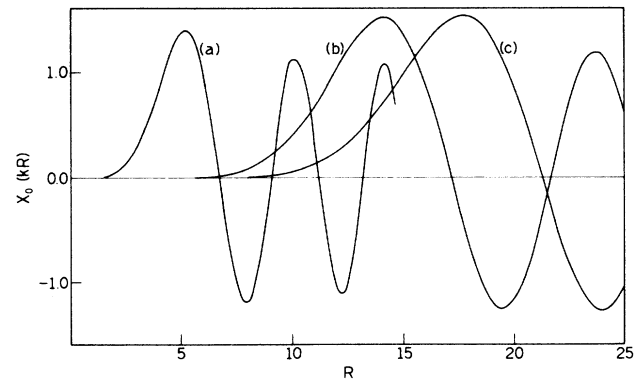

FIG. 4. Normalized continuum wave function $X_0(kR)$ for $\alpha\mu + p$. The units are defined by Eq. (7). (a) $k = 1.91$, $E_\gamma = 7.0$ keV, (b) $k = 1.11$, $E_\gamma = 7.9$ keV, (c) $k = 0.99$, $E_\gamma = 8.0$ keV.

As can be seen from Table I, bound-state energies for $d\alpha\mu$ and $t\alpha\mu$ calculated by the BO approximation are close to those by the present variational method. Thus the wave functions for $d\alpha\mu$ and $t\alpha\mu$ obtained by the BO approximation will not differ very much from ours, which includes nonadiabatic effects. For $p\alpha\mu$, however, the bound-state energy by the BO approximation is rather different from that by the variational method. Ratio of muon mass to the reduced mass of $p+\alpha$ is not very small. The ratio $\frac{1}{7}$ is compared with $\frac{1}{12}$ and $\frac{1}{15}$ of the ratio of muon mass to the reduced masses of $d+\alpha$ and $t+\alpha$, respectively. This implies that the BO approximation is not very good for the $p\alpha\mu$ system. Thus the energy and wave function of $p\alpha\mu$ obtained by the BO approximation is not as good as those of $d\alpha\mu$ and $t\alpha\mu$.

The x-ray spectra are shown in Fig. 2. The overall shapes of $d\alpha\mu$ and $t\alpha\mu$ spectra are similar to those obtained by Kravtsov *et al.*[3] On the other hand, the spectrum of $p\alpha\mu$ is different. As was discussed by Kravtsov *et al.*,[3] the shape of the spectrum is mainly determined by the initial-state wave function. Therefore, the discrepancy of the $p\alpha\mu$ spectrum is attributed to the inaccuracy of the $p\alpha\mu$ wave function in the BO approximation.

The absolute value of $d\lambda/dE$ is about three times smaller in the present calculation for all isotopes. For example, we have obtained the maximum value for $p\alpha\mu$, $1.93\times10^{11}\,\mathrm{sec}^{-1}\,\mathrm{keV}^{-1}$ at $E_\gamma \approx 7.04$ keV, whereas Kravtsov *et al.*, obtained $5.3\times10^{11}\,\mathrm{sec}^{-1}\,\mathrm{keV}^{-1}$ at $E_\gamma \approx 7.0$ keV. The reason of this discrepancy is not clear. It may be due to the effect of interference between $J_f = 0$ and 2 existing in their formalism. The lifetime τ of the resonant states,

$$\tau = 1 \Big/ \int \left[\frac{d\lambda}{dE}\right] dE \ , \tag{19}$$

is also given in Table I. The values are about three times larger than those of previous calculations.[3]

In our $p\alpha\mu$ spectrum, there is a small second peak at $E_\gamma \approx 8$ keV, with peak height about $\frac{1}{22}$ of the main peak and with half width about 0.1 keV. To understand the cause of the second peak, we have plotted

$$S_0(R) = \left[\Phi_{1\sigma}(\xi,\eta;R)\left|\frac{R}{2}\xi\eta\right|\Phi^{J_i 0}(\xi,\eta,R)\right] , \tag{20}$$

for $p\alpha\mu$ as a function of R in Fig. 3. The integrand $R\xi\eta/2$ is proportional to $g_0(\xi,\eta,R)$ of Eqs. (16) and (18) when $(-3M_p + M_\alpha - m_\mu)\mathbf{R}/M_{\mathrm{tot}}$ is neglected in Eq. (14). As can be seen from this figure, $S_0(R)$ remains nonzero even at $R \approx 20$. This is because the bound state is a weakly bound state. Figure 4 shows $X_{J_f}(kR)$ for $J_f = 0$ with $k = 1.91$, 1.11, and 0.99. These values of k correspond to $E_\gamma = 7.0$, 7.9 and 8.0 keV, respectively. At $k \approx 1.9$, overlap between $S_0(R)$ and $X_0(kR)$ is largest. At $k = 1.11$, $X_0(kR)$ is small in the region where $S_0(R)$ is large and

oscillation of $X_0(kR)$ cancels overlap between $S_0(R)$ and $X_0(kR)$ at $10 \leq R$. At $k=0.99$, there is no cancellation in the region $10 \leq R \leq 20$. This nonzero overlap produces the small second peak at $E_\gamma \approx 8$ keV. For other isotopes, $S_0(R)$ is small in $10 \leq R \leq 20$ and there is no second peak which is visible in Fig. 2.

Note added in proof. Recently, the lifetime of the muonic molecule $(d^3\mathrm{He}\mu)$ has attracted much attention in connection with the fusion process $d+{}^3\mathrm{He} \rightarrow p+\alpha$. We have calculated the bound-state energy and the lifetime of $(d^3\mathrm{He}\mu)$. For $J=0$ and 1, the bound-state energies relative to the ground state of $d\mu$ atom are -70.74 and -47.90 eV, the lifetimes are 5.71×10^{-12} and 6.44×10^{-12} sec, respectively. We are grateful to Dr. M. Kamimura for useful discussion on this problem.

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