Hyper-radial adiadatic expansion for a muonic molecule dtμ

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Abstract

By using the hyper-radius, adiabatic potential energy curves with correct asymptotic energies are obtained for the Coulomb three body problem. The bound state energies of the muonic molecules dtμ with total angular momentum J = 0 calculated adopting the three lowest adiabatic potential energy curves are −318.72 eV and −34.36 eV for vibrational quantum numbers v = 0 and 1, respectively.

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It is well known that the wave function expanded in terms of basis functions which are adiabatic in hyper-radius satisfies correct boundary conditions for a general three body problem. In practical application of such approach, five coordinates other than hyper-radius can be chosen in many ways. Macek[1] and Lin[2] have succesfully used hyper-spherical coordinates to treat atomic three body problems where one particle is heavy and two are light. Recently Matveenko[3] and Matveenko and Abe[4] proposed to use hyper-spheroidal coordinates for more genaral cases. In this letter, we calculate, with sufficient accuracy, the adiabatic potential curves and non-adiabatic coupling terms for the low lying states of dtμ system with total angular momentum J = 0 using hyper-spheroidal coordinates. We also calculate the energies of the bound states with J = 0 by solving the three-state coupled equations

The hyper-radius R for the system of a triton *t*, a deutron *d* and a negative muon μ is defined by

$$M_0 R^2 = M\mathbf{X}^2 + m\mathbf{x}^2, \tag{1}$$

where M and m are reduced masses of systems (*t*, *d*) and (*t*+*d*, μ),

$$1/M = 1/m_t + 1/m_d, \tag{2}$$

$$1/m = 1/(m_t + m_d) + 1/m_\mu, \tag{3}$$

X is the position vector of *d* relative to *t* and **x** is that of μ with respect to the centre of mass of (*t*+*d*) (see Fig. 1). M_0 is an arbitrary mass constant. We choose M_0 = M in the following.

The Hamiltonian for our system is given using the hyper-radius by[1,3]

$$H = -\frac{1}{2M}\frac{1}{R^5}\frac{\partial}{\partial R}R^5\frac{\partial}{\partial R} + h(R;\Omega), \tag{4}$$

where *h* is the adiabatic Hamiltonian operator which includes R as a parameter and Ω represents five dimensionless variables. The eigenfunctions $\Phi_n(R;\Omega)$ and eigenvalues $\varepsilon_n(R)$ of the operator *h* for a given R is obtained by solving the Schroedinger equation

$$[h - \varepsilon_n(R)]\Phi_n(R;\Omega) = 0. \tag{5}$$

In hyper-spheroidal coordinates, Ω is a set of variables (ξ, η, φ, $\hat{\mathbf{X}}$), where

$$\xi = (r_t + r_d)/X, \quad \eta = (r_t - r_d)/X, \tag{6}$$

and φ, the azimuthal angle for x around X axis, are the spheroidal coordinates for x and $\hat{X}$, the unit vector along X. In this coordinate system, h is given explicitly by[3]

$$h = -\frac{\rho^2}{2m}\nabla_r^2 + \frac{\rho}{2MR^2}(J^2 - 2J\cdot l) + V + \frac{\rho q}{MR^2}, \tag{7}$$

where

$$l = -i\mathbf{x}\times\nabla_{\mathbf{x}}, \tag{8}$$

$$\rho = 1 + mx^2/MX^2, \tag{9}$$

$$q = \frac{1}{\rho}\,\mathbf{x}\cdot\nabla_{\mathbf{x}}, \tag{10}$$

$$\nabla_r^2 = \frac{4}{R^2}\left[\frac{1}{(\xi^2-\eta^2)}\left\{\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}\right\} + \frac{1}{(\xi^2-1)(1-\eta^2)}\frac{\partial^2}{\partial\varphi^2}\right], \tag{11}$$

and V the Coulomb interaction between the three particles

$$V = 1/X - 1/r_t - 1/r_d. \tag{12}$$

The following units together with $m_t = 5496.899\ m_e$, $m_d = 3670.481\ m_e$, and $m_\mu = 206.769\ m_e$ (m_e ; electron mass) are used throughout this letter unless otherwise stated.

$$e = \hbar = m = 1. \tag{13}$$

We have calculated $\varepsilon_n(R)$ and $\phi_n(R;\Omega)$ for the dtμ system with J = 0 by variational method. The form of the trial function adopted is

$$\Phi_n = \sqrt{\rho}\,\Sigma\, b_{in}\zeta_i(R), \tag{14}$$

$$\zeta_i(R) = \xi^{c_i} exp(-\beta_i R\,\xi)\, P_{l_i}(\eta), \tag{15}$$

for small R and

$$\zeta_i(R) = \xi^{c_i} exp(-\beta_i R\,\xi)\,\eta^{l_i} exp(-\gamma_i R\,\eta), \tag{16}$$

for large R. Normalization of ϕ_n is

$$(\Phi_n \Phi_n) = \int \frac{1}{\rho^3} (\xi^2 - \eta^2) |\Phi_n|^2 d\xi\, d\eta\, d\varphi. \tag{17}$$

Using 77 basis functions, we have obtained $\varepsilon_n(R)$ for the lowest three states (n = 1, 2 and 3) with sufficient accuracy in the region R > 0.3. The results for R<0.3 are not very reliable. This inaccuracy is caused partly by the numerical integration carried out over ξ and η. In the region R ≦ 0.3, we have used a trial function consisting of 91 eigenfunctions of squared angular momentum[1,5]

$$\Lambda^2 = -\frac{1}{\sin\alpha\cos\alpha}\frac{\partial}{\partial\alpha}\sin\alpha\cos\alpha\frac{\partial}{\partial\alpha} + \frac{1}{\cos^2\alpha}(-i\mathbf{X}\times\frac{\partial}{\partial\mathbf{X}})^2 + \frac{1}{\sin^2\alpha}(-i\mathbf{x}\times\frac{\partial}{\partial\mathbf{x}})^2, \tag{18}$$

where

$$\alpha = tan^{-1}(\sqrt{M}X / \sqrt{m}x). \tag{19}$$

With this hyper-spherical trial function, accurate results are obtained for R < 0.01. Convergence becomes slower for R > 0.01. This is because (dtμ) system is more like a molecule rather than an atom. In the following, we use hyper-spheroidal results for R > 0.3 and hyper-spherical results for R ≦ 0.3.

The total wave-function ψ is expanded as

$$\psi = R^{-5/2}\Sigma\,\Phi_n(R;\Omega)\ \chi_\mu(R). \tag{20}$$

Then the radial wave-function χ_n satisfies a set of coupled equations

$$[-\frac{1}{2M}\frac{d^2}{dR^2} + V_n(R) - E]\chi_\mu(R) + \Sigma[W_{nm}(R) + 2U_{nm}(R)\frac{d}{dR}]\chi_m(R) = 0, \tag{21}$$

where

$$V_n(R) = \varepsilon_n(R) + \frac{15}{8MR^2} + W_{nn}(R), \tag{22}$$

$$U_{nm}(R) = -\frac{1}{2M}(\Phi_n \frac{\partial}{\partial R}\Phi_m), \tag{23}$$

$$W_{nm}(R) = -\frac{1}{2M}(\Phi_n \frac{\partial^2}{\partial R^2}\Phi_m), \tag{24}$$

and E is the total energy. The coupling matrix elements W_{nm} is devided into symmetric part S_{nm} and antisymmetric part A_{nm},

$$S_{nm}(R) = -\frac{1}{2M}\left(\frac{\partial}{\partial R}\Phi_n \frac{\partial}{\partial R}\Phi_m\right), \tag{25}$$

$$A_{nm}(R) = \frac{d}{dR} U_{nm}(R). \tag{26}$$

In Figs. 2, 3 and 4, the potential energy curves $\varepsilon_n(R)$, off diagonal non-adiabatic coupling terms $U_{nm}(R)$, $A_{12}(R)$ and $S_{12}(R)$ are presented as functions of the hyper-rudius R. The coupling terms U_{nm} are calculated by numerical differentiation of ϕ_n and by using the Hellmann and Feynman theorem. Both results have agreed at least 3 digits in the calculation in the hyper-spheroidal coordinates. W_{nm} are calculated by numerical differentiation. It is confirmed that the numerical calculation well reproduces the following correct asymptotic forms of V_n[6]

$$V_1(R) = -2.4190/R^4, \tag{27}$$

$$V_2(R) = 0.0087 - 2.6454/R^4, \tag{28}$$

where 0.0087 is the difference in the binding energies between the dμ and tμ atoms in the 1s-state in our energy units. Energy is measured relative to the ground state of tμ. In the potential curve $\varepsilon_2(R)$, there is a shallow minimum of about 5eV at $R \simeq 7$. This dip almost disappears when the coupling term W_{22} is added to $\varepsilon_2(R)$. It should be noted that U_{12} is zero in the Born-Oppenheimer approximation because of g-u symmetry, while in the hyper-radial adiabatic approximation this coupling term is non-zero. U_{12} is large at $R \simeq 7$, where systems (tμ) + d or (dμ) + t begin to form (dtμ) molecule. It is known[7] that there exists non-adiabatic interaction which behaves as 1/R at large R. In Fig. 3, $R \cdot U_{13} \rightarrow -0.385$, while $R \cdot U_{12}$ and $R \cdot U_{23} \rightarrow 0$ as R goes to infinity.

We have solved eq. (19) and obtained the bound state energies of dtμ molecule with J = 0. Calculations are carried out both variationally and by solving coupled differential equations numerically [6] for one- and two-state cases and variationally for the three-state case. In the variational calculation, $12 \times n$ (n = 1, 2, 3, are numbers of states) basis functions are adopted. The results are shown in Table 1. By the three-state calculation, we have obtained −318.72 eV and −34.36 eV, for vibrational quantum numbers v = 0 and 1, respectively. These values are compared with −319.14 eV and −34.83 eV obtained by full variatioal calculations [8, 9, 10] using more than several hundreds trial functions.

We have obtained, for the first time, the asymptotically correct hyper-radial adiabatic potential energy curves and non-adiabatic coupling terms for the muonic molecule dtμ. A few state calculation for bound states gives satisfactory results. The present results suggest that the hyper-spheroidal method is particularly useful to treat molecular system such as HD^+.

References

[1] J. Macek, J. Phys. B; Atom. Molec. Phys., 1 (1968) 831

[2] C, D. Lin, Phys. Rev., A10 (1974) 1986

[3] A. V. Matveenko, Phys. Lett., 129 (1983) 11
A. V. Matveenko, JETP Lett., 40 (1984) 1329

[4] A. V. Matveenko and Y. Abe, Few-Body Systems, 2 (1987) 127

[5] P. M. Morse and H. Feschbach, Methods in Theoretical Physics (McGraw-Hill Book Company, New York) 1953, pp1730

[6] H. Fukuda, S. Hara and T. Ishihara, to be published

[7] J. Macek, Phys. Rev., A31 (1985) 2162

[8] S. Hara, T. Ishihara and N. Toshima, J. Phys. Soc. Japan, 55 (1986) 3229

S. Hara, T. Ishihara and N. Toshima, Muon Catalyzed Fusion, 1 (1987) 277

[9] L. I. Ponomarev, Atomic Physics, 10 (1987) 197

[10] M. Kamimura, Muon Catalyzed Fusion, 2 (1988) to be published

Figure captions

Fig. 1. Coordinates for three-body system

Fig. 2. Adiabatic potential energy curves $\varepsilon_n(R)$ for dtμ system, as a function of hyper-radius R. Energy and length are in the units given in eq. (13)

Fig. 3. Non-adiabatic coupling terms $U_{nm}(R)$, labeled by (n,m).

Fig. 4. Symmetric part $S_{12}(R)$ and anti-symmetric part $A_{12}(R)$ of non-adiabatic coupling term $W_{12}(R)$.

	v=0	v=1
one-state	−317.75	−31.99
two-state	−317.80	−33.46
three-state	−318.72	−34.36
variation[8,9,10]	−319.14	−34.83

Table 1. Bound state energies(in eV) of the dtμ molecule with J = 0.

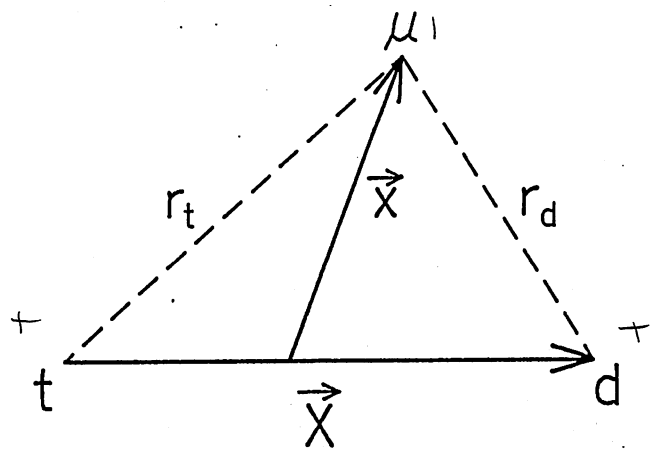

Fig.

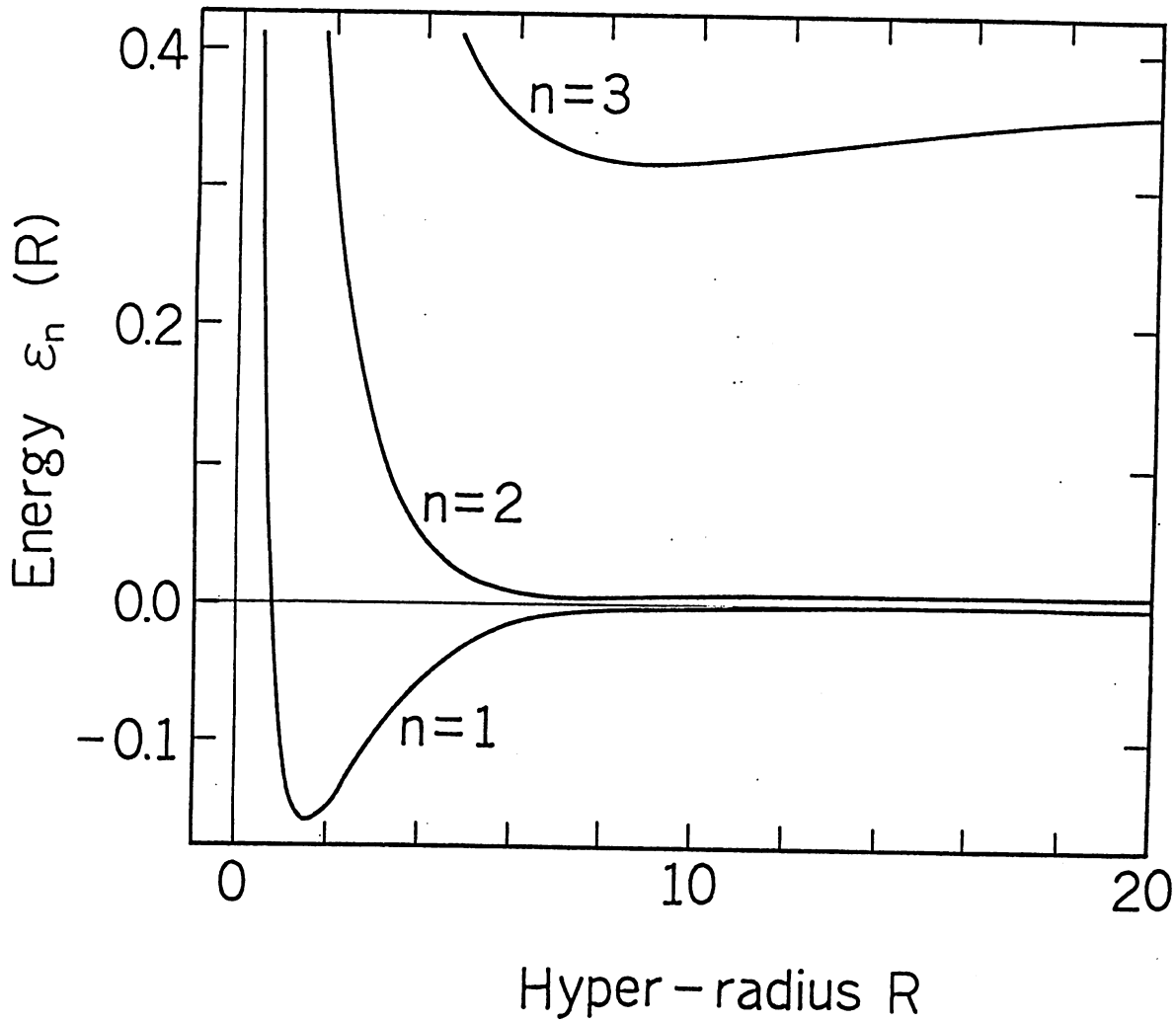

Fig. 2

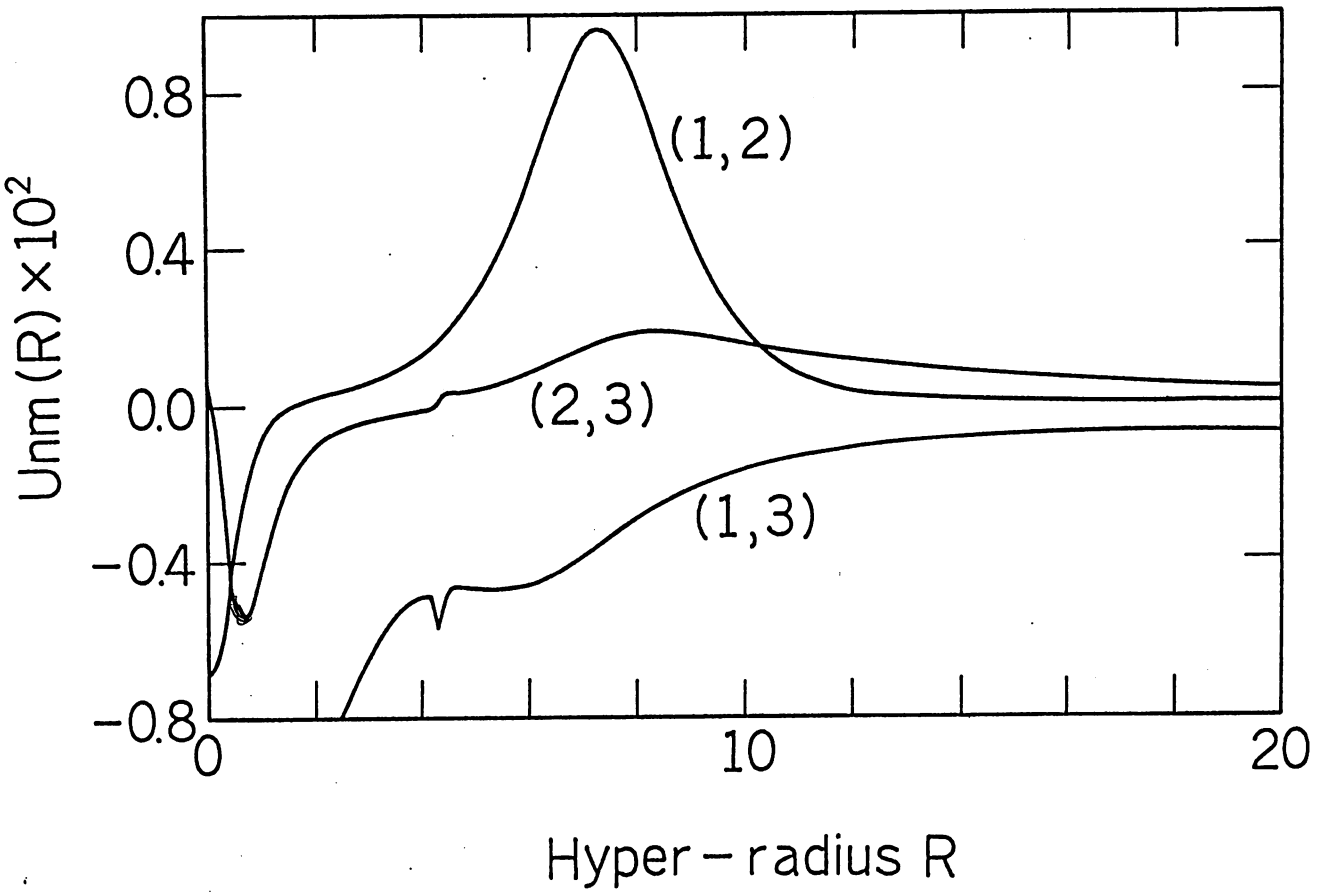

Fig. 3

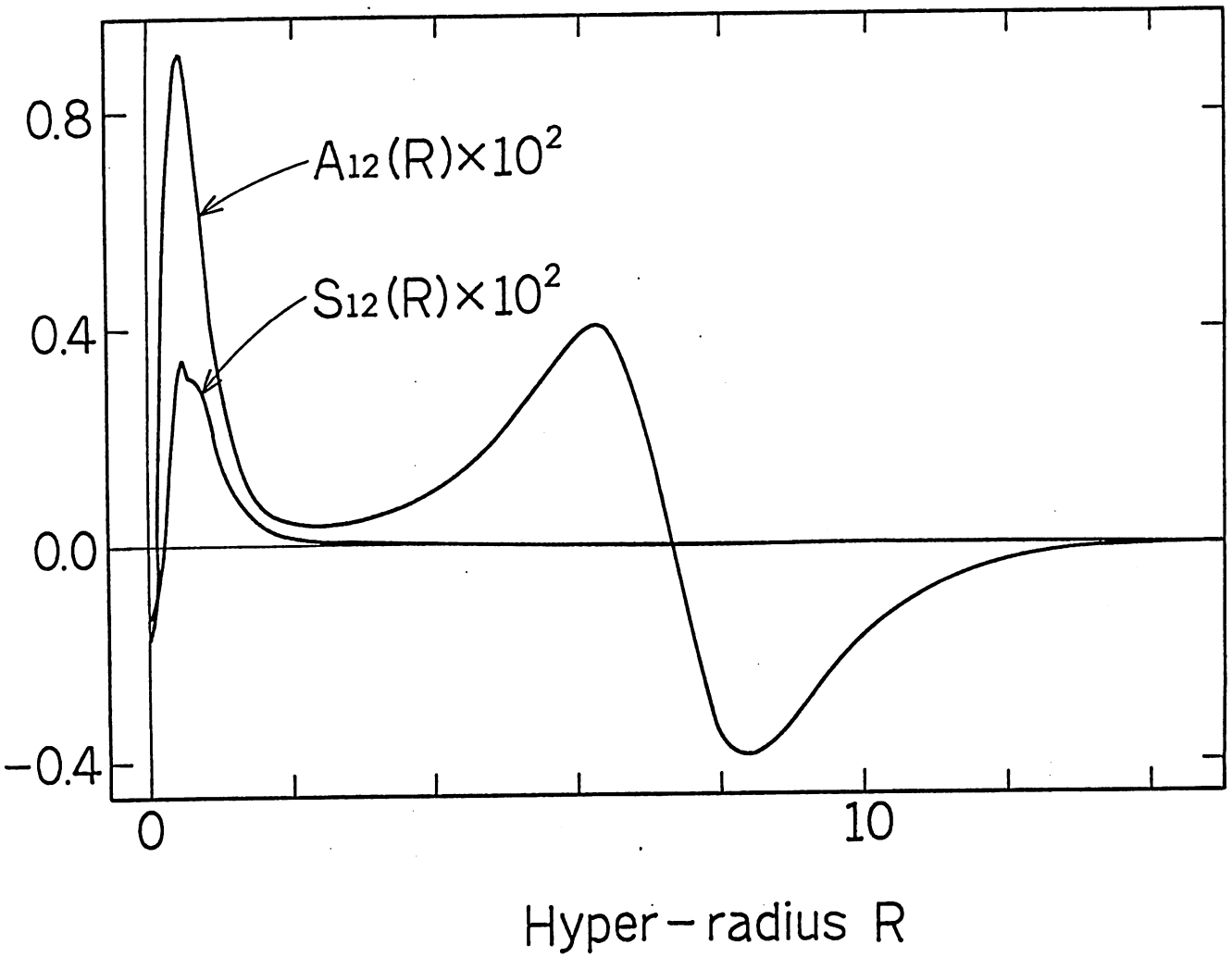

Fig. 4