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THE CHARACTER OF METASTABLE STATES OF THE ANTIPROTONIC HELIUM

A.V.Matveenko, H.Fukuda*

A simple semianalytic wave function for «the Atomcule» — metastable state of the antiprotonic helium — is derived using body-fixed hyperspherical coordinates:

$$\Psi^J(R, \xi, \eta, \tilde{\alpha}, \beta, \gamma) = R^J[c_1(R) \sin^J\alpha_a \, e^{-\sqrt{-\varepsilon_n}x_a} P_J(\omega_a) +$$

$$+ c_2(R) \cos^J \alpha_b \, e^{-\sqrt{-\varepsilon_1}x_b} P_J(\omega_b - \theta_b)] B_0^J(\gamma, \beta, \tilde{\alpha}),$$

where $B_0^j(\gamma, \beta, \tilde{\alpha})$ is σ-projection of the rotational motion, α_i and θ_i are the usual two-body-channel hyperspherical angles, $\cos\omega_a = \hat{\omega} \cdot \hat{\mathbf{x}}_a$ defines the angle fixing the position of the inertia tensor principal axis $\hat{\omega}$ in the particle triangle plane with respect to one of its sides x_a (same for ω_b). Formally this expression is the well-known linear combination of two approximately resonant hydrogenic orbitals: the novel position is their angular part that exhibits the common pure rotational (dynamic) component $B_0^j(\gamma, \beta, \tilde{\alpha})$ and the kinematic part coupling together collective (ω_i) and channel (θ_i) angles in a general case. Hyperradius R and ξ, η are internal dynamic variables.

As lower lying states of $\bar{p}He^+$ have the configuration of the ground one, i.e., the product of two hydrogenic orbitals, all they have a rather different character. This determines the longevity of high angular momentum molecular states.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

Характер метастабильных состояний антипротонного гелия

А.В.Матвеенко, Х.Фукуда

Получена простая полуаналитическая волновая функция для метастабильных состояний антипротонного гелия. Используются гиперсферические координаты с осью квантования, направленной вдоль одной из главных осей тензора инерции системы трех частиц. Выбор оси квантования позволяет факторизовать вращательную составляющую волновой функции. Ее оставшаяся часть имеет вид обычной молекулярной орбитали; новым моментом является характерная зависимость атомных орбиталей от так называемых «внутренних углов», которыми в данном случае являются: угол между парой якобиевских векторов, а также угол, задающий положение главной оси тензора инерции.

*School of Administration and Informatics, University of Shizuoka, Yada 52-1, Shizuoka-shi, Shizuoka 422, Japan

Поскольку состояния, лежащие ниже, имеют главным образом конфигурацию основного состояния (произведение атомных орбиталей), автоматически решается вопрос о метастабильности данных состояний (линейной комбинации атомных орбиталей).

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Recently observed laser-induced transitions in antiprotonic helium atoms [1] unambiguously demonstrated that the anomalous longevity of antiprotons results from the formation of high angular momentum states of $\bar{p}\mathrm{He}^+$ [2,3]. The full variational calculation [4] of the corresponding Coulombic three-body problem has practically reproduced the observed transitions. On the other hand, there are many experimental findings that have not been explained theoretically. Among them are phase and density effects, isotopic effect and quenching by foreign gases [1]. Though it is widely believed that the formation of the exotic system is due to an atomic electron replacement by the incoming antiproton, there is neither direct experimental information nor reliable theoretical prediction on the distribution of the captured particles. The most probable principal quantum number of the initially formed state is estimated to be $n = \sqrt{M^*/m_e} \simeq 38$, where M^* is the reduced mass of the captured antiproton and m_e is the electronic mass. The total angular momentum J of this state is expected to be equal to the angular momentum of the corresponding circular orbit, i.e., $J = l = n - 1$. In this communication we shall derive a semianalytic wave function for metastable states of $\bar{p}\mathrm{He}^+$ which has all symmetry properties of the state and its kinematical features exactly incorporated. They define the probability distribution and, as a result, the physical characteristics of the state. Though a pseudosymmetry operator, accounting for the above-mentioned kinematic features of metastable states can be formally created, we just consider them as forming «the character» of the state [5,6]. In a similar context, propensity rules for radiative and non-radiative decay of resonant states of two-electron atoms, also of the positronium negative ion [7], based on the underlying approximate molecular-orbital structure, demonstrate the usefulness of the idea.

Let $\mathbf{X}$ and $\mathbf{x}$ be Jacobi vectors for the three-body system $\bar{p} + e + \alpha$ (see the Figure). It is a standard molecular configuration but contrary to the usual case the mass of the «valence» particle is the biggest. The hyperradius R and the corresponding reduced masses M and μ are given by

$$MR^2 = MX^2 + \mu x^2$$

$$\frac{1}{M} = \frac{1}{m_{\bar{p}}} + \frac{1}{m_e}, \quad \frac{1}{\mu} = \frac{1}{m_\alpha} + \frac{1}{m_{\bar{p}} + m_e}. \tag{1}$$

The total centre of mass Hamiltonian of the problem then reads

$$H = -\frac{1}{2M}\frac{1}{R^5}\frac{\partial}{\partial R}R^5\frac{\partial}{\partial R} + \frac{\Lambda^2}{2MR^2}, \tag{2}$$

depending on the set of six coordinates $\{R, \hat{o}\}$, where $\hat{o}$ serves for five hyperspherical angles. The most commonly used space-fixed choice of variables $\hat{o}$ is $\{\alpha_c, \hat{\mathbf{x}}, \hat{\mathbf{X}}\}$ with $\hat{\mathbf{x}}$ and $\hat{\mathbf{X}}$ defining the polar angles of the corresponding vectors and

$$\alpha_c = \arctan\left(\frac{\sqrt{M}X}{\sqrt{\mu}x}\right). \tag{3}$$

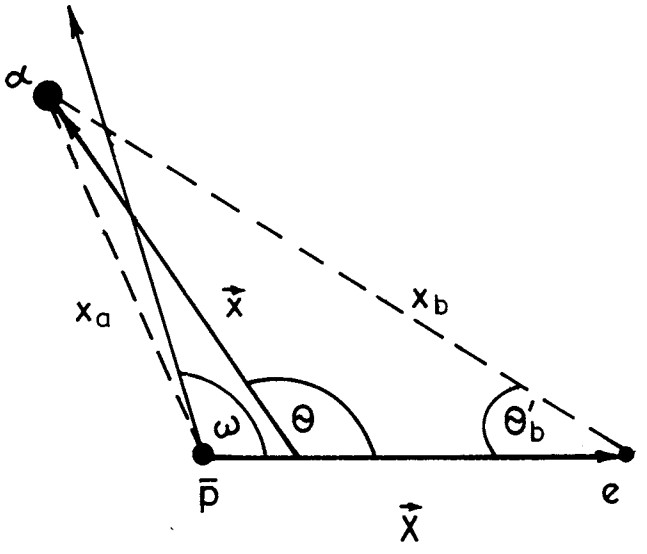

Figure. Three-body molecular Jacobi coordinates **X** and **x** (*c*-set), with α-particle playing the role of the valence particle, form the reference configuration [$\tan(2\omega) = \mu x^2 \sin(2\theta)/(MX^2 + \mu x^2 \cos(2\theta))$]. As α-particle and $\bar{p}$ are much more heavier than electron, the actual position of **x** and the inertial tensor principal axis cannot be pictured properly, they practically coincide with x_a and $\omega \approx \theta_a'$. Two additional Jacobi-vector sets (*a* and *b*) are not pictured. They are defined as in our paper [8]

In this case

$$\Lambda^2 = -\frac{1}{\sin^2 2\alpha_c}\frac{\partial}{\partial\alpha_c}\sin^2 2\alpha_c \frac{\partial}{\partial\alpha_c} + \frac{\mathbf{l}^2}{\cos^2\alpha_c} + \frac{\mathbf{L}^2}{\sin^2\alpha_c}, \tag{4}$$

where **l** and **L** are the angular momenta corresponding to **x** and **X**. As is well known there are three different sets of Jacobi vectors for a three-body problem so the underscript notifies the set chosen.

The hyperspherical harmonics (HH) are defined as the solutions of the angular part of the Schrödinger equation

$$[\Lambda^2 - K(K+4)]\mathbf{Y}_K(\hat{o}) = 0, \tag{5}$$

with K being the quantum number of the so-called grand angular momentum. As only normal parity states, i.e., those for which the quantum number of the total parity $p = (-)^J$, will be considered in the communication, we can omit the superscript in the corresponding context.

The recently derived parametrization of the body-frame HH [8] will be intensively used in our derivation. It reads

$$\mathbf{Y}^{JpM_J}_{KlL(c)}(\xi, \eta, \gamma, \beta, \tilde{\alpha}) = \sum_{m'=0(1)}^{J} y^{Jp}_{KlLm'(c)}(\xi, \eta) B^{JpM_J}_{m'}(\gamma, \beta, \tilde{\alpha}), \tag{6}$$

where

$$y^{Jp}_{KlLm'(c)}(\xi, \eta) = f_{KlL}(\alpha_c) \sum_{m}^{J} P^m_l(\theta) d^{Jp}_{m,m'}(\omega) U^{Jpl}_{mL}, \tag{7}$$

$$B^{JpM_J}_m(\gamma, \beta, \tilde{\alpha}) = \frac{(-i)^m}{4\pi} \sqrt{\frac{2J+1}{1+\delta_{0m}}} [D^J_{-m,-M_J}(\gamma, \beta, \tilde{\alpha}) + p(-)^J D^J_{m,-M_J}(\gamma, \beta, \tilde{\alpha})] \tag{8}$$

with the coefficients forming the Clang-Fano orthogonal matrix [9]

$$U^{Jpl}_{mL} = p(-)^{J+l+m} \sqrt{2-\delta_{0m}} (l, J, -m, m \,|\, L, 0). \tag{9}$$

$P^m_l(\theta)$ are the normalized associated Legendre polynomials of cos θ and the parity projected combination of the Rose d-functions [10] is of the form

$$d^{Jp}_{m,m'}(\omega) = \frac{1}{\sqrt{(1+\delta_{0m})(1+\delta_{0m'}}} [d^J_{m,m'}(\omega) + p(-)^{J+m'} d^J_{m,-m'}(\omega)] . \tag{10}$$

As is indicated in (7) all three auxiliary variables α_c, cos θ, ω should be expressed in terms of common dynamic variables $\{\xi, \eta\}$, say, hyperspheroidal coordinates [8]. The parameter ω defines the angle between the vector **X** and the principal axis of the three-body inertia-tensor (Figure). The $\{\gamma, \beta, \tilde{\alpha}\}$-set is given by the Euler rotation bringing the space-fixed frame into the inertia-tensor frame. Following [11] we shall choose among solutions (6) the HH which do not have internal (configurational) excitation by putting

$$K = J = l + L. \tag{11}$$

Under this condition we have

$$f_{KlL}(\alpha_c) = \cos^l \alpha_c \sin^L \alpha_c \tag{12}$$

thus finishing the specification of the three-body angular basis (6).

By introducing the partial-wave expansion of HH into the eigenvalue equation (5) and integrating over $\{\gamma, \beta, \tilde{\alpha}\}$-variables we arrive at the system of $J+1$ Schrödinger equations for vector-column HH (7) with the components $m' = 0, 1, ..., J$ defining the projection of the total angular momentum onto the body-fixed z-axis.

Now we are ready to construct the wave-function for $\bar{p}\mathrm{He}^+$ metastable states. They should be molecular orbitals formed by two approximately degenerate atomic orbitals: $(\alpha + e)$-hydrogenic state depending on radial variable x_b, with principal quantum number $n_b = 1$, and $(\alpha + \bar{p})$-hydrogenic state depending on $\mathbf{x}_a$ with $n_a = J + 1$, angular momentum $L_{\mathbf{x}_a} = J$.

Firstly, we note that due to specific mass relations for the particles constituting $\bar{p}\mathrm{He}^+$ we have $\omega \simeq \theta_a'$ (Fig.), and the quantization axis practically coincides with the corresponding side of the particle triangle. Thus, as the electron is occupying the ls-state the total angular momentum J is mainly due to the pair angular motion given by $L_{\mathbf{x}_a}$ and,

as a result, only ($m' = 0$)-component of the wave-function survives. Accordingly, the molecular orbital of the metastable state can be written in the form

$$\varphi(R, \xi, \eta, \tilde{\alpha}, \beta, \gamma) = B_0^J(\gamma, \beta, \tilde{\alpha}) R^J [\tilde{c}_1(R) f_{J0J}(\alpha_a) d_{0,0}^{Jp}(\omega_a) U_{0J}^{Jp0} e^{-\sqrt{-\varepsilon_n} x_a} +$$

$$+ \tilde{c}_2(R) f_{JJ0}(\alpha_b) \sum_J \sum_m P_J^m(\theta_b) d_{m,0}^{Jp}(\omega_b) U_{m0}^{JpJ} e^{-\sqrt{-\varepsilon_1} x_b}], \tag{13}$$

where we have used the functional form (7) twice with

$$\tan \alpha_a = \frac{\sqrt{\mu_a} x_a}{\sqrt{M_a} X_a}, \quad \cos \theta_a = \hat{\mathbf{x}}_a \cdot \hat{\mathbf{X}}_a, \quad \omega_a = \theta_a' - \omega \text{ (Fig.)}, \tag{14}$$

and where the reduced masses μ_a and M_a correspond to Jacobi vectors $\mathbf{x}_a$ and $\mathbf{X}_a$, respectively; similar notation holds for the Jacobi pair $\mathbf{x}_b$ and $\mathbf{X}_b$. Naturally, ε_n and ε_1 are the energies of the corresponding orbitals or variational parameters close to their values. The particular form (13) demonstrates the flexibility of the parametrization of HH in the form (7): starting from the space-fixed frame we were able to factorize γ, β, $\tilde{\alpha}$-Euler rotation as

$$\hat{D}^{Jp}(\gamma, \beta, \tilde{\alpha}) = \hat{D}^{Jp}(0, \omega_a, 0) \hat{D}^{Jp}(\phi_a, \hat{\mathbf{x}}_a) \tag{15}$$

for the antiprotonic orbital and as

$$\hat{D}^{Jp}(\gamma, \beta, \tilde{\alpha}) = \hat{D}^{Jp}(0, \omega_b, 0) \hat{D}^{Jp}(\phi_b, \hat{\mathbf{x}}_b) \tag{16}$$

for the electronic state, where $\hat{D}^{Jp}(0, \omega, 0)$ is the parity-preserving rotation in the triangle plane and $\phi_{a(b)}$ is the azimuthal angle of the corresponding vectors.

The general expression for $y_{KlLm'}^J$ (7) can be further simplified for both $y_{J0J0(a)}^J$ and $y_{JJ00(b)}^J$ if we make use of the following expressions

$$U_{m0}^{JpJ} = p(-)^{J+m} \sqrt{2 - \delta_{0m}} \frac{1}{\sqrt{2J+1}}$$

$$P_J^m(\theta) = (-)^m \frac{\sqrt{(2J+1)(1+\delta_{0m})}}{2} d_{0m}^{Jp}(\theta) \tag{17}$$

and apply the group property of $\mathbf{d}^{Jp}$-matrices [11]

$$d_{mm'}^{Jp}(\alpha + \beta) = \sum_{\mu=0}^{J} d_{m\mu}^{Jp}(\alpha) d_{\mu m'}^{Jp}(\beta). \tag{18}$$

The simplified form of (13) will then be

$$\psi(\text{Atomcule}) = [c_1(R) x_a^J e^{-\sqrt{-\varepsilon_n} x_a} P_J(\omega_a) +$$

$$+ c_2(R) X_b^J e^{-\sqrt{-\varepsilon_1} x_b} P_J(\omega_b - \theta_b)] B_0^J(\gamma, \beta, \tilde{\alpha}). \tag{19}$$

Here the $\sin^J \alpha$ factor supplied by the scalar part (12) of the HH (7) has been used to account exactly for the pair-interaction singularity. Though $\omega_a \simeq 0$ and $\omega_b \simeq \theta_b$ hold, the

Legendre polynomials $P_j(\omega_a)$ and $P_j(\omega_b - \theta_b)$ provide the correlation due to electron-antiproton interaction and play the crucial kinematic role incorporating the two-body relative motion into the three-body wave function.

«The character» of the long-lived antiprotonic states is emphasized by the primitive form of their wave function (19). Accordingly, these states comprise a specific series of resonant states with its own «ground state». As the probability distribution for the states (19) is of some particular configuration one might expect the overlap integral between them and non-molecular states to be small. The approximate solution (19) is keeping equal to zero the projection of the total angular momentum onto the body-fixed z-axis. One more approximate quantum number specifying «the character» of the metastable state will appear if we introduce the hyperradial-adiabatic approximation [12,13]: it will be the vibrational quantum number describing the excitation mode in the corresponding adiabatic potential.

To finish the paper we answer the question: «What metastable antiprotonic states are: atomic or molecular states?» They are definitely molecular states as they exist due to the peculiar correlation between the electron and antiproton motion and they are long-lived just because of their molecular form (19). On the other hand, crude energetic characteristics of the metastable states can be calculated in a kinematically more primitive approaches: keeping either α-particle (atomic picture) or both, α-particle and antiproton (Born-Oppenheimer adiabatic description), fixed.

The title of the recent paper by J.M.Rost and D.Wintgen [7] is: «Positronium Negative Ion: Molecule or Atom?» Using hyperspherical adiabatic approach they demonstrate the molecular mode in the resonance spectrum of $(e + e + e^+)$-system that is, of course, not so much evident for the ground state of the system.

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