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Coriolis Coupling in Exotic Three-Body Coulomb Systems

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Our approach provides high precision spectroscopic calculations and general formalism for the quantum description of three-body Coulomb systems. We seek the exact solutions of the 6D Schrödinger equation. For this we propose a new algorithm for the case of nonzero total angular momentum, taking into account the overall rotation of the system which is affected indirectly by the Coriolis coupling. The robustness, efficiency, and accuracy of the adopted algorithm are studied in detail. We employ Discrete Variable Representation (DVR) and construct a special set of hyperspherical harmonics which provides much more flexibility in choosing the best basis for the needs of this particular physical problem. The method is applied to the computation of the nonrelativistic energy levels of the exotic meta-stable antiprotonic helium.

1. INTRODUCTION

The discovery of long-lived antiprotonic states in helium (Yamazaki, 1993) presented a new type of interesting exotic three-body Coulomb system. This type of exotic systems has become a subject of intense theoretical and experimental studies. The accuracy of calculations is highly motivated by the high precision of the present experiments. The first theoretical predictions, based on rather simple atomic (Yamazaki and Ohtsuki, 1992) provided a qualitative description of the energy level structure but approached the experimental measurements with a dispersion of 1000 ppm. Currently on going work is being carried out at CERN in the experiments ATHENA studying properties of antiprotonic Coulomb systems in traps at low temperatures (Atomic spectroscopy . . . 1997/1998); properties of antiprotonic helium are mainly determined by its extremely large total angular

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momentum ($L \approx 35 - 40$). Elaborate calculations of the energy levels, collisions cross sections, radiative and Auger transition rates are essential for the interpretation of the measurements. Hence, the development of appropriate numerical methods (Morse and Feshbach, 1953) for computing the desired spectroscopic data with sufficient accuracy is necessary for better understanding of the collision processes taking place in the exotic three-body systems. For the theoretical description of three-body problem, the choice of an optimal coordinate system is an essential step as it has important consequences of the possibilities to reduce the dimensionality of the problem and thus ease the numerical computation. Since we now intend to solve the wave function in a space of high dimensionality it is natural to turn to hyperspherical coordinates and hyperspherical harmonics (Avery, 1989), which are the d-dimensional generalization of the 3D spherical coordinates and spherical harmonics (Fano *et al.*, 1999). In hyperspherical coordinate approach (Macek, 1968), the internal wave functions of three-body systems are expanded in terms of complete set of angular functions which can in turn be expanded in terms of complete set of harmonics (eigenfunctions of grand angular momentum operator). There are some complications in constructing the hyperspherical harmonics as these functions are not localized and cannot be simply expressed as a direct product basis in the two hyperangles. In the complete description of the exotic three-body system with nonzero total angular momentum (LittleJohn and Mitchell, 1998, 2000), we show that a simple product of Legendre polynomials is not capable of accurately representing all of the hyperspherical harmonics. Thus, here our efforts have been directed toward developing appropriate numerical techniques to construct more general basis set. We propose a new algorithm for efficient evaluation of the kinetic derivative operators, using hyperspherical coordinate method. In this method our choice of the internal angular coordinates are analytically defined in connection with the spheroidal coordinates. Throughout this paper we calculate the kinetic matrix elements using these special shape coordinates. Our paper is organized as follows: In Section 2 the three-body problem with Coulomb interaction formulated within the adiabatic hyperspherical method is considered. In Section 3 an efficient and stable hyperquantization algorithm extended for the case of nonzero total angular momentum is reported. In Section 4 the necessary actions for the numerical evaluations of the generalized kinetic matrix elements are presented; the 1D approach developed in this section allow us to construct analytically a special set of the hyperspherical harmonics. In Section 5 the exact numerical solutions of the eigenvalue problem are presented with full analysis of hyperspherical harmonics and quantum numbers; here our approach has been thoroughly tested on a parametric eigenvalue problem for an exotic helium system (antiprotonic helium), calculating the nonrelativistic energy levels of the metastable states (Korobov, 1996). In Section 6 conclusions and possible applications are discussed.

2. HYPERSPHERICAL ADIABATIC EIGENVALUE PROBLEM

We introduce the theoretical framework of our approach to three-body Coulomb systems having nonzero total angular momentum. Implementing the hyperspherical approach (Macek, 1968), the Schrödinger equation reads

$$\left(-\frac{1}{2R^5}\frac{\partial}{\partial R}R^5\frac{\partial}{\partial R}+\frac{\Lambda^2}{2R^2}+\frac{C}{R}-E\right)\Psi(R,\Omega)=0. \tag{1}$$

where Λ^2 denotes the Smith generalized angular momentum squared (Smith, 1959, 1962), C is the effective charge and E is the total energy of the system. The collective set of coordinates is denoted by (R, Ω), where R is the hyperradius, a parameter which specifies the overall size of the system and $\Omega \equiv (\Omega_S, \Omega_E)$ represent the five angular coordinates. The two internal shape angles collectively denoted by Ω_S represent separable coordinate system on a hypersphere S in 6D configuration space. The other three angles denoted by Ω_E represent the well-known Euler angles which parameterize the overall rotation of the system. The two shape angles are generalized in the spirit of the spheroidal coordinates. These generalized shape coordinates can be simply defined as the sum and difference of the two Delves angles (Delves, 1958/1959, 1960) (χ_1, χ_2) follows (Tolstikhin *et al.*, 1995a,b):

$$\xi = \chi_1 + \chi_2, \qquad 2\gamma < \xi < 2\pi - 2\gamma, \tag{2}$$

$$\eta = \chi_1 - \chi_2, \qquad -2\gamma < \eta < 2\gamma, \tag{3}$$

where the rotation mass parameter γ connected to the configuration of the particles with the three masses m indexed by l, n, and k, is given by

$$\tan(\gamma_{ln}) = \sqrt{\frac{m_k M}{m_l m_n}}, \quad 0 \le \gamma \le \frac{\pi}{2}, \tag{4}$$

where M denotes the total mass of the system. In the hyperspherical adiabatic approximation (HSA) the solutions of the Schrödinger equation (1) assume a separable form,

$$\Psi(R,\Omega) = \frac{1}{R^{5/2}}\sum_{\nu} F_\nu(R)\Phi_\nu(\Omega;R), \tag{5}$$

Here the quantum number ν characterizes an HSA channel function and the angular function $\Phi_\nu(\Omega; R)$ satisfies

$$[H_{\text{ad}}(R) - U_\nu(R)]\Phi_\nu(\Omega;R) = 0; \tag{6}$$

$$H_{\text{ad}}(R) = \frac{\Lambda^2}{2} + RC.$$

The solutions of Eq. (1) in HSA approximations (neglecting all nonadiabatic couplings) can be obtained by coupling many HSA channels in the radial equation

$$\left[-\frac{1}{2}\frac{d^2}{dR^2} + \frac{U_\nu(R) + 15/8}{R^2} - E\right] F_\nu(R) = 0. \tag{7}$$

To obtain an accurate solution for Eq. (6) it is necessary to take into account the peculiarities of the behavior of the function in the region of the most accessible singularities i.e., at $R = 0$. In this limit, the kinetic operator in Eq. (6) prevails and the potential energy operator which is the second term in the adiabatic Hamiltonian H_{ad} vanishes. Accordingly, the 6D hyperspherical harmonics and the eigenvalues $U_\nu(0)$ of Λ^2 are given by (Smith, 1959, 1962)

$$\left[\frac{1}{2}\Lambda^2 - \lambda(\lambda + 4)\right] \Phi_\nu(\Omega) = 0; \quad \lambda = 0, 1, 2, \ldots \tag{8}$$

The main purpose of this paper is to develop an effective numerical method that will allow us to calculate the derivative operators with high accuracy and use them to calculate the matrix elements of Λ^2 in our adopted angular coordinates.

3. METHODOLOGY

The algorithm proposed here allows us to determine the proper basis sets and accordingly investigate the system dynamics in 6D configuration space. Shape-orientation decomposition of the HSA channel function has the form

$$\Phi(\Omega) = \sum_{m=-L}^{L} \Phi_m(\xi, \eta)|m\rangle, \tag{9}$$

with a standard rotational basis defined as

$$|m\rangle \equiv \sqrt{2L+1} D^{L*}_{Mm} \tag{10}$$

$$L \geq 0, \quad -L \leq M \leq L, \quad -L \leq m \leq L \tag{11}$$

where $m \equiv L_z$ is the projection of the total angular momentum on the z-axis, here chosen to coincide with body-fixed (BF) axis going through the two heaviest particles, and M is the L projection in space-fixed (SF) frame. Here we make use of short-hand notation for the evaluation of the diagonal and off diagonal matrix elements Λ^2 in the conventional rotational basis.

$$\langle m|\Lambda^2|m\rangle = \Lambda_0^2 + \mathcal{V}^{\text{r}}, \tag{12a}$$

and

$$\langle m|\Lambda^2|m'\rangle = \mathcal{V}^{\text{c}\pm}; \tag{12b}$$

with rather obvious definitions. The diagonal element denoted by Λ_0^2 accounts for the kinetic motion on the surface of the hypersphere S (separable coordinate system), r stands for rotational, and c for Coriolis (Lin, 1986, 1995, 1999; LittleJohn

and Mitchell, 1998, 2000). Then in the adopted hyperspherical coordinate system (Tolstikhin *et al.*, 1995a,b), the diagonal elements with respect to azimuthal quantum number m read

$$\Lambda_0^2 = \frac{-16}{\cos\eta - \cos\xi}\left[\frac{\partial}{\partial\eta}(\cos\eta - c)\frac{\partial}{\partial\eta} + \frac{\partial}{\partial\xi}(c - \cos\xi)\frac{\partial}{\partial\xi}\right], \tag{13}$$

$$\mathcal{V}^{\mathrm{r}} = \frac{4s^2m^2}{(\cos\eta - c)(c - \cos\xi)} + \frac{L(L+1) - 2m^2}{\sin^2(\chi/2)}. \tag{14}$$

The off-diagonal matrix elements read

$$\mathcal{V}^{\mathrm{c}\pm} = \frac{\sqrt{L(L+1) - m(m\pm 1)}}{\sin^2(\chi/2)}\left[\pm\frac{\partial}{\partial\theta} + (m\pm 1)\cot\theta\right], \tag{15}$$

with the derivative operator of the form

$$\begin{aligned}\frac{\partial}{\partial\theta} = 2\frac{\sqrt{(\cos\eta - c)(c - \cos\xi)}}{\cos\eta - \cos\xi}\Big[&(p^+\cos(\eta/2)\sin(\xi/2)\\ &- p^-\sin(\eta/2)\cos(\xi/2))\frac{\partial}{\partial\eta} + (p^-\cos(\eta/2)\sin(\xi/2)\\ &- p^+\sin(\eta/2)\cos(\xi/2))\frac{\partial}{\partial\xi}\Big].\end{aligned} \tag{16}$$

The second θ dependent term is represented as

$$\cot\theta = \frac{d^-\cos(\eta/2)\cos(\xi/2) - d^+\sin(\eta/2)\sin(\xi/2)}{\sqrt{(\cos\eta - c)(c - \cos\xi)}}. \tag{17}$$

Here the dominator involving $\sin^2(\chi/2)$, which is of the repulsive type singularity, is defined as

$$\frac{1}{\sin^2(\chi/2)} = \frac{2}{1 + p^+\cos(\eta/2)\cos(\xi/2) + p^-\sin(\eta/2)\sin(\xi/2)} \tag{18}$$

with

$$\begin{gathered}c = \cos 2\gamma, \quad s = \sin 2\gamma, \quad p^+ = 1 + \frac{2m_3}{m_1 + m_2},\\ p^- = \frac{m_1 - m_2}{m_1 + m_2}, \quad d^\pm = (1\pm c)p^\pm\end{gathered} \tag{19}$$

Our coordinates has the merit of being adapted to simultaneously *two* Coulomb attractive singularities (Tolstikhin *et al.*, 1995a,b). Namely, the dominator involving $(\cos\eta - \cos\xi)$ which are of the coordinate "attractive" type singularities can be fairly treated by this particular hyperspherical coordinate system. In this paper, our algorithm is considered only for discrete symmetry of the problem—parity with respect to inversion of space. For symmetric systems, there is an additional discrete symmetry—parity with respect to permutation of identical particles, which

we shall consider elsewhere. With the inversion parity included, the expansion Eq. (9) becomes

$$\Phi(\Omega) = \sum_{m=\frac{1}{2}(1-\sigma)}^{L} \Phi_m(\eta,\xi)|m\sigma\rangle, \quad \sigma = \pm 1, \tag{20}$$

where σ denotes the normal and anomalous parity, respectively. Here our rotational basis is defined as

$$|\bar{m}\sigma\rangle = \frac{1}{\sqrt{2(1+\delta_{\bar{m}0})}}(|\bar{m}\rangle + \sigma(-1)^{\bar{m}}|-\bar{m}\rangle) \quad \bar{m} \equiv |m| = 0, 1, \ldots \tag{21}$$

$$\langle \bar{m}\sigma \mid \bar{m}'\sigma'\rangle = \delta_{\bar{m}\bar{m}'}\delta_{\sigma\sigma'}. \tag{22}$$

The described algorithm relates to block tridiagonal structure of kinetic matrix (Aquilanti *et al.*, 1986, 1998), which contains the coupling between different channels labeled by m and m'. Solving the HSA eigenvalue problem Eq. (6) for an arbitrary total angular momentum L, we simply deal with full Hamiltonian which is real symmetric and can be split into two blocks of even and odd inversion parity. Within the given parity block, here described for normal parity ($\sigma = 1$), the Hamiltonian is banded along the diagonal and the neighboring m blocks are coupled as follows:

$$\begin{pmatrix} \Lambda^2_{00} & \sqrt{2}\Lambda^2_{01} & 0 & 0 & \cdots & 0 \\ \sqrt{2}\Lambda^2_{10} & \Lambda^2_{11} & \Lambda^2_{12} & 0 & \cdots & 0 \\ 0 & \Lambda^2_{21} & \Lambda^2_{22} & \Lambda^2_{23} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 0 & \Lambda^2_{L-1L-2} & \Lambda^2_{L-1L-1} & \Lambda^2_{L-1L} \\ 0 & \cdots & 0 & 0 & \Lambda^2_{LL-1} & \Lambda^2_{LL} \end{pmatrix} \begin{pmatrix} \Phi_0 \\ \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_{L-1} \\ \Phi_L \end{pmatrix} = 2U \begin{pmatrix} \Phi_0 \\ \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_{L-1} \\ \Phi_L \end{pmatrix} \tag{23}$$

The spareness in the global matrix represents the main advantage of the procedure. The total dimension is given by $N^{\Omega_s} * (L+1)$, where $N^{\Omega_s} = N_1 * N_2$ denotes the dimension of each m block with N_1 and N_2 representing the grid points of the shape coordinates ξ and η, respectively. In pursuit of the most efficient method, we consider the approach based on the discrete variable representation (DVR) and thus by transferring to the DVR we eliminate 2D numerical quadratures associated with the matrix elements; in DVR the potential energy operators are diagonal and the kinetic operators are tensor products. In the limit $\gamma \to 0$ this problem has an analytical solutions (to be discussed in Section 5). This allows direct comparison of the results obtained by our proposed algorithm to the exact solutions. In the following section we develop an efficient method to solve the corresponding ID eigenvalue problem and construct a special set of hyperspherical harmonics.

4. ALGORITHM AND GENERAL CONSIDERATIONS ON CONVERGENCE

The study of the hyperspherical harmonics for $R = 0$ is considered as one of the most stringent tests for convergence. One can never be certain that convergence is achieved in applications for which R is large unless the harmonics for $R = 0$ can be accurately reproduced. The algorithm adopted for the calculations of kinetic matrix elements is simple and efficient to get the accurate eigenvalues and eigenfunctions. This approach allows us to construct 6D harmonics defined in terms of the two hyperspherical quantum numbers n_η and n_ξ. As follows from the preceding section, extending the algorithm to the case $m \neq 0$, we now deal with the diagonal block matrices Λ_m^2, considering only Eq. (13) and the first term in Eq. (14),

$$\Lambda_m^2 = \Lambda_0^2 + \frac{4s^2m^2}{\cos\eta - \cos\xi}\left[\frac{1}{W(\eta)} + \frac{1}{W(\xi)}\right], \tag{24}$$

with

$$W(\eta) = (\cos\eta - c), \qquad W(\xi) = (c - \cos\xi). \tag{25}$$

The necessary action described above for the numerical evaluations of the generalized kinetic matrix elements in coordinates is useful here to introduce an efficient analytical technique developed for 1D eigenvalue problem as follows: For any m, we seek the solutions in the form

$$\Phi_{n_{\eta,\xi}}(\eta, \xi) = f_1(\eta)\, f_2(\xi) \tag{26}$$

and obtain ordinary differential equations defining the functions $f_1(\eta)$ and $f_2(\xi)$:

$$\left[L^\eta - \frac{2s^2m^2}{W(\eta)} + UW(\eta) + \kappa\right] f_1(\eta) = 0, \tag{27a}$$

$$\left[L^\xi - \frac{2s^2m^2}{W(\xi)} + UW(\xi) - \kappa\right] f_2(\xi) = 0, \tag{27b}$$

where κ denotes the separation constant and the 1D derivative operators are defined as

$$L^\eta \equiv 8\frac{d}{d\eta}W(\eta)\frac{d}{d\eta}, \tag{28a}$$

$$L^\xi \equiv 8\frac{d}{d\xi}W(\xi)\frac{d}{d\xi}, \tag{28b}$$

The equations subject to the regularity boundary conditions and can be satisfied only for certain values of U and κ. They amount to same differential equation considered on the two different intervals (2–3). Thus it is sufficient to consider the

numerical treatment of either one. Here we may introduce Eq. (27) in a simple algebraic form

$$(L + V)\psi(\tau) = \kappa\psi(\tau) \tag{29}$$

$$-2\gamma \leq \tau \leq 2\gamma, \qquad \psi(\pm 2\gamma) < \infty \tag{30}$$

where

$$L = -8\frac{d}{d\tau}(\cos\tau - c)\frac{d}{d\tau} + \frac{2s^2m^2}{\cos\tau - c} \tag{31}$$

$$V = -U(\cos\tau - c) \tag{32}$$

In DVR we define a new variable

$$\tau = 2\gamma x \rightarrow -1 \leq x \leq 1 \tag{33}$$

Then

$$L = -\frac{2}{\gamma^2}\frac{d}{dx}W(x)\frac{d}{dx} + \frac{2s^2m^2}{W(x)}, \tag{34}$$

with

$$W(x) \equiv \cos(2\gamma x) - c \tag{35}$$

with the basis given by

$$\phi_i(x) = \left[\frac{w(x)}{w(x_i)}\right]^{m/2}\pi_i(x), \quad i = 1, \ldots, N \tag{36}$$

$$w(x) \equiv 1 - x^2 \tag{37}$$

Here x_i, w_i, and $\pi_i(x)$ denote Legendre DVR abscissas, weights, and basis functions, respectively. We seek the solution in DVR expansion:

$$\psi(x) = \sum_{i=1}^{N}\psi_i\phi_i(x) \tag{38}$$

thus the equation can be reduced to the following algebraic form:

$$(\mathbf{L} + \mathbf{V})\psi = \kappa\boldsymbol{\rho}\psi \tag{39}$$

where

$$\mathbf{L}_{ij} = \frac{2}{\gamma^2}\int_{-1}^{1}\frac{d\phi_i(x)}{dx}W(x)\frac{d\phi_j(x)}{dx}\,dx + \int_{-1}^{1}\phi_i(x)\frac{2s^2m^2}{W(x)}\phi_j(x)\,dx \tag{40}$$

$$\mathbf{V}_{ij} = \int_{-1}^{1}\phi_i(x)V(x)\phi_j(x)\,dx \tag{41}$$

$$\boldsymbol{\rho}_{ij} = \int_{-1}^{1}\phi_i(x)\phi_j(x)\,dx \tag{42}$$

At first we calculate the kinetic matrix elements in Gaussian–Legendre DVR, here after we shall call it as our first approach. Manipulating the calculations in the Legendre quadrature approximation, the 1D derivative operator is evaluated as

$$\frac{d}{dx}\phi_i(x) = \sum_{k=1}^{N} \tilde{b}_{ik}\phi_k(x) - \frac{mx}{w(x)}\phi_i(x) \tag{43}$$

where

$$\tilde{b}_{ik} = b_{ik}\left[\frac{w(x_k)}{w(x_i)}\right]^{m/2} \tag{44}$$

Then

$$\begin{aligned}\mathbf{L}_{ij} \approx \frac{2}{\gamma^2}\Bigg[\sum_{k=1}^{N}\tilde{b}_{ik}W(x_k)\tilde{b}_{jk} - mx_i\tilde{b}_{ji}\frac{W(x_i)}{w(x_i)} - mx_j\tilde{b}_{ij}\frac{W(x_j)}{w(x_j)} \\ + m^2x_i^2\frac{W(x_i)}{w(x_i)^2}\Bigg] + \delta_{ij}\frac{2m^2s^2}{W(x_i)}\end{aligned} \tag{45}$$

$$\mathbf{V}_{ij} \approx \delta_{ij}V(x_i) \tag{46}$$

$$\boldsymbol{\rho}_{ij} = \delta_{ij} \tag{47}$$

Amounting to the similar treatment of the derivative operator mentioned above, we calculate the Coriolis coupling matrix elements in the Legendre–DVR approximation. Hence the off-diagonal matrix elements, the first and the second term in Eq. (15), are evaluated respectively as

$$\begin{aligned}\left(\mathcal{V}_1^{c\pm}\right)_{mi_1i_2,m\pm1j_1j_2} = \pm2\frac{\sqrt{L(L+1)-m(m\pm1)}}{F_0(i_i,\,i_2)}\sqrt{\frac{W_1(i_1)W_2(i_2)}{W(i_1,\,i_2)W(j_1,\,j_2)}} \\ \times\Bigg(\frac{1}{\gamma_1}F_1(i_1,\,i_2)\delta_{i_2j_2}\Bigg(b_{j_1i_1}\left[\frac{w_1(i_1)}{w_{1(j_1)}}\right]^{\frac{m\pm1}{2}} - (m\pm1) \\ \times\frac{x_{1_{i_1}}}{w_1(i_1)}\delta_{i_1j_1}\Bigg) + \frac{1}{\gamma_2}F_2(i_1,\,i_2)\delta_{i_1j_1}\Bigg(b_{j_2i_2}\left[\frac{w_2(i_2)}{w_2(j_2)}\right]^{\frac{m\pm1}{2}} \\ - (m\pm1)\frac{x_{2i_2}}{w_2(i_2)}\delta_{i_2j_2}\Bigg)\Bigg),\end{aligned} \tag{48}$$

$$\left(\mathcal{V}_2^{c\pm}\right)_{mi_1i_2,m\pm1j_1j_2} = 2(m\pm1)\frac{\sqrt{L(L+1)-m(m\pm1)}}{F_0(i_1,\,i_2)}\frac{F_3(i_1,\,i_2)}{\sqrt{W_1(i_1)W_2(i_2)}}\delta_{i_1j_1}\delta_{i_2j_2}. \tag{49}$$

where the coefficients F_i are defined as,

$$F_0(x_1, x_2) = 1 + p^+ \cos(\eta/2)\cos(\xi/2) + p^- \sin(\eta/2)\sin(\xi/2), \tag{50}$$

$$F_1(x_1, x_2) = p^+ \cos(\eta/2)\sin(\xi/2) - p^- \sin(\eta/2)\cos(\xi/2), \tag{51}$$

$$F_2(x_1, x_2) = p^- \cos(\eta/2)\sin(\xi/2) - p^+ \sin(\eta/2)\cos(\xi/2), \tag{52}$$

$$F_3(x_1, x_2) = d^- \cos(\eta/2)\cos(\xi/2) - d^+ \sin(\eta/2)\sin(\xi/2). \tag{53}$$

The second term of Eq. (14) is diagonal in DVR and thus can be easily calculated. The inclusion of this term which is of repulsive-type singularity with the off-diagonal terms in the calculations of the generalized angular momentum Λ^2 completes our numerical treatment. Here our adopted algorithm in the first approach simplifies the calculations of the Coriolis coupling terms as shown above. However testing our methodology by investigating the accurate harmonics we found that this approach failed to get all the accurate harmonics for $m \neq 0$. Namely, there were some false roots occuring in the low-lying part of the spectrum. These eigenvalues did not converge and could be distinguished by the fact that their corresponding eigenfunctions oscillate too rapidly; though the other eigenvalues rapidly converge and come out accurately. We found that the problem mainly lies in our choice of the suitable set of polynomials that best represent the eigenfunction of the generalized angular momentum operator Λ^2 in a space of high dimensionality. Hence we have adopted a new basis functions, and accordingly we have modified our algorithm (see appendix) for the derivative operators so that the integral $\mathbf{L}$ to be calculated essentially in the Gauss–Jacobi quadrature as follows: The derivative operator in Eq. (43) becomes

$$w(x)\frac{d}{dx}\phi_i(x) = \left[\frac{w(x)}{w(x_i)}\right]^{m/2} \sum_{n=1}^{N} T_{ni}[A_n\varphi_{n-1}(x) - B_n\varphi_{n+1}(x)], \tag{54}$$

Accordingly, the 1D kinetic matrix elements are efficiently evaluated as

$$\mathbf{L}_{ij} = \frac{1}{[w(x_i)w(x_j)]^{m/2}} \sum_{n=1}^{N}\sum_{k=1}^{N} T_{ni}\,T_{kj}\,\tilde{\mathbf{L}}_{nk}, \tag{55}$$

where

$$\tilde{\mathbf{L}}_{nk} = \int_{-1}^{1} \left(\frac{2}{\gamma^2}[A_n\varphi_{n-1}(x) - B_n\varphi_{n+1}(x)]\frac{W(x)}{w(x)}[A_k\varphi_{k-1}(x) - B_k\varphi_{k+1}(x)] \right.$$
$$\left. + 2m^2 s^2 \varphi_n(x)\frac{w(x)}{W(x)}\varphi_k(x) \right) [w(x)]^{m-1}\,dx; \tag{56}$$

with

$$A_n = \frac{(n-m)(n-1)}{\sqrt{4(n-1)^2 - 1}}, \qquad B_n = \frac{(n+m-1)\,n}{\sqrt{4n^2-1}}. \tag{57}$$

The best convergence is achieved with Gegenbauer polynomials (Avery, 1989) with $\alpha = \beta = m - 1$. Similarly we have modified the algorithm for the off-diagonal terms as well so that almost the integrals of all the singular terms of Λ^2 are evaluated in the same quadrature. The accuracy of this approach have been tested with full analysis on a special set of hyperspherical harmonics (to be discussed in Section 5).

5. RESULTS AND DISCUSSION

In the preceding section we have outlined the algorithm combined with the efficient numerical technique to treat up to 6D problem. Here we analytically investigate a special set of 6D hyperspherical harmonics constructed in the limit $\gamma \to 0$. As has been already noticed, Eqs. (27) amount to the same 1D separation equation Eq. (29) considered in the intervals $[-2\gamma, 2\gamma]$ and $[2\gamma, 2\pi - 2\gamma]$, respectively. Assuming $\gamma \to 0$ and U as a parameter with an arbitrary value $\neq 0$, Eq. (29) coincides with a spheroidal separation equation (Abramowitz and Stegun, 1972) as it takes the form

$$\left[\frac{d}{dx}w(X)\frac{d}{dx} - \frac{m^2}{w(x)} + \frac{1}{2}\gamma^2 U w(x) + \frac{1}{4}\kappa\right]\psi(x) = 0, \tag{58}$$

with $U = 0$, Eq. (58) can be easily solved analytically as it is here reduced to a simple Legendre equation (Abramowitz and Stegun, 1972). Hence following the approach described above, we can analytically solve the HSA Eq. (8), treating Eqs. (27) separately with κ as an eigenvalue and U as a spectral parameter and the two shape quantum numbers n_η and n_ξ as the numbers of zeros of the corresponding eigenfunctions $f_1(\eta)$ and $f_2(\xi)$, we obtain the following eigenvalues:

$$\kappa_n = 4\lambda(\lambda + 2), \quad \lambda = n + m, \quad n = 0, 1, 2 \ldots \tag{59}$$

The corresponding eigenfunctions are expanded in Gegenbauer polynomials $P^{(\alpha,\beta)}\,|_{\alpha=\beta=m}$ as previously defined in Section 4. Finally with $\lambda = 2(n + m)$ the HSA Eq. (8) has the form

$$\left[\Lambda_m^2 - 2(n+m)((n+m)+2)\right]\Phi(\xi, \eta) = 0, \qquad n = n_\eta + n_\xi, \tag{60}$$

$$\left\langle \Phi_{n_\eta n_\xi} \;\middle|\; \Phi_{n_{\eta'} n_{\xi'}} \right\rangle = \delta_{n_\eta n'_\eta}\delta_{n_\xi n'_\xi}. \tag{61}$$

The solutions form a complete basis set with $W(\eta, \xi) = \frac{\pi^2}{4s}(W(\eta) + W(\xi))$ as previously defined in Eq. (25). Different partitions of λ yield hyperspherical harmonics with two alternative nodal lines, reflecting alternative sharing of kinetic energy. The harmonics with similar values of λ are degenerate as shown in Fig. (1). The highly convergent eigenvalues of the global matrix Eq. (23) obtained for odd $L = 1$, $\lambda = 0.3\pi$, and with normal parity considered in the current approach follow as 0,6,16,30, . . . (even values) with the correspnding degeneracy 1,3,5, . . . (odd values). Having succeeded in constructing a special set of harmonics, now we further test our methodology with the calculations of the hyperspherical adiabatic

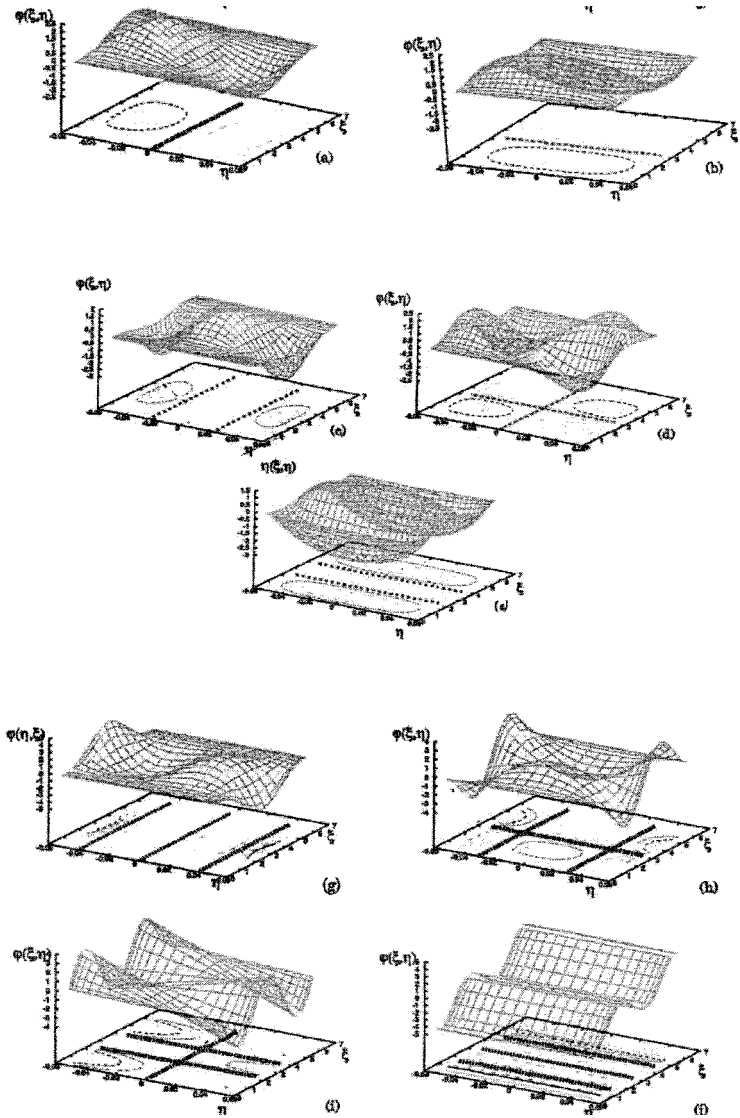

Fig. 1. Hyperspherical harmonics with alternative nodal structures: two degenerate harmonics for $\lambda = 2$ ($n = 1$, $m = 1$): (a) $n_\xi = 0$, $n_\eta = 1$ and (b) $n_\xi = 1$, $n_\eta = 0$, in each the solid dotted line denotes one node. Three degenerate harmonics for $\lambda = 3$ ($n = 2$, $m = 1$): (c) $n_\xi = 0$, $n_\eta = 2$, (d) $n_\xi = 1$, $n_\eta = 1$, and (e) $n_\xi = 2$, $n_\eta = 0$, in each the two solid dotted lines denote two nodes. Four degenerate harmonics for $\lambda = 4$ ($n = 3$, $m = 1$): (g) $n_\xi = 0$, $n_\eta = 3$, (h) $n_\xi = 1$, $n_\eta = 2$, (i) $n_\xi = 2$, $n_\eta = 1$, and (j) $n_\xi = 3$, $n_\eta = 0$, in each the solid dotted lines denote three nodes.

states, which in turn contain more information on the structure, rotations, and all the internal modes. Here we describe the main use of the adiabatic eigenvalues E and eigenvectors for calculating the bound state energies for an exotic system, that is, antiprotonic helium (PHe^+). We deal with a two-center Coulomb problem, for which the off-diagonal matrix elements, connecting states of different azimuthal quantum number m, are proportional to a small parameter that is, m_e/M, where m_e is a mass of lightest particle (electron) and M is a sum of masses of the two heaviest particles (helium nucleus and antiproton). Depending on the mass ratio m_e/M and the required accuracy of the nonrelativistic calculation we can determine the number of m components which is sufficient to be included in the coupling. In the case of antiprotonic helium system the mass ratio order of magnitude is about 10^{-4}. From this we can notice that the inclusion of one m component in the expansion, Eq. (20) yields four digits improvement in the numerical results. In other words, incorporating the Coriolis coupling with $m = 0{,}1$ we have succeeded in bringing the total nonrelativistic energies to the precision of one part to 10^8 (Korobov *et al.*, 1992, 1996), where here we solve Eq. (1) taking into account all the nonadiabatic coupling terms: $(\Phi_\mu|\delta/\delta R|\Phi_\nu)$, $(\Phi_\mu|\delta^2/\delta R^2|\Phi_\nu)$ and the appropriate boundary conditions at $R \to 0$ and $R \to \infty$. The rapid convergence in the expansion with respect to m is demonstrated through the visualization of the hyperspherical adiabatic curves (see Fig. (2)), for the total angular

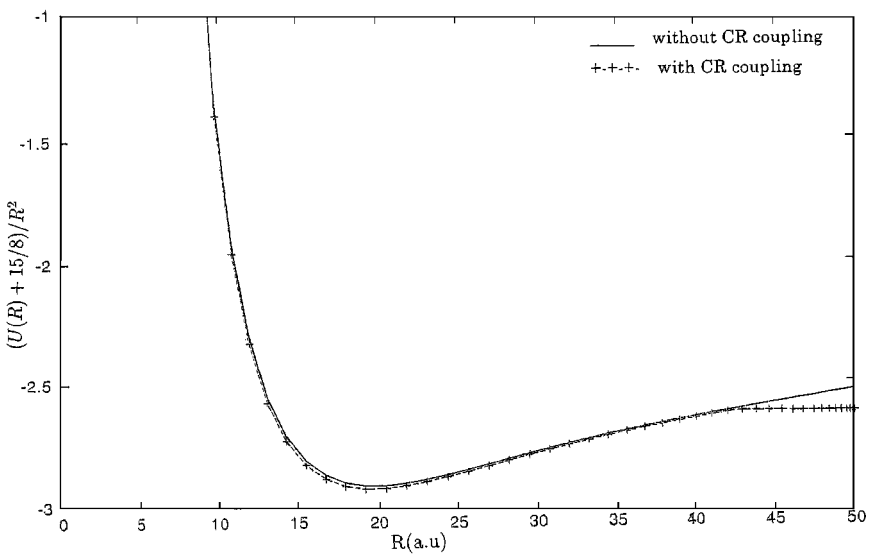

Fig. 2. Adiabatic potential curves for antiprotonic helium with total angular momentum $L = 36$; $m_{\bar{p}} = 1836.1527$, $m_{He^{2+}} = 7294.2996$. The lowest adiabatic curve indicates improved asymptotic convergence after incorporating the coriolis (CR) coupling with $m = 0{,}1$.

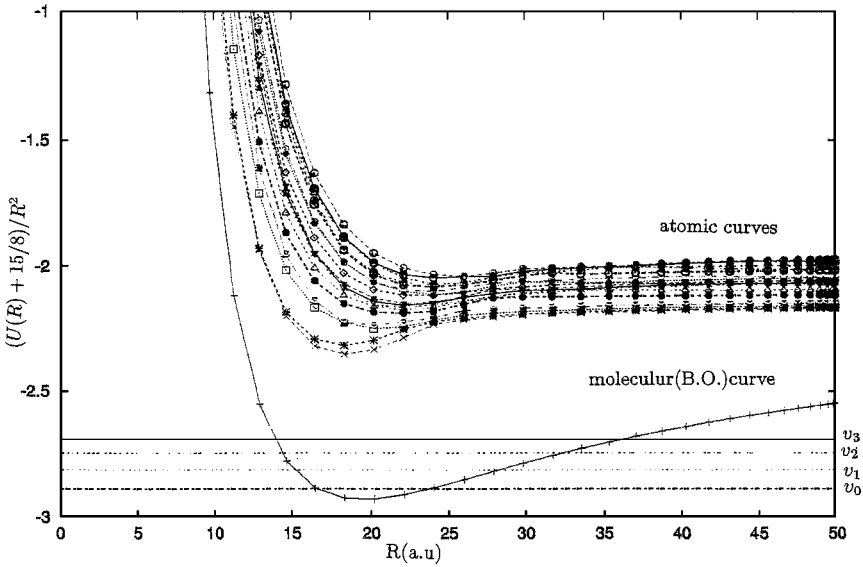

Fig. 3. Atomic (highest) and Born–Oppenheimer molecular (lowest) adiabatic potential curves for antiprotonic helium with total angular momentum $L = 36$. The lines denoted by ν indicate the lowest four energy levels.

momentum $L = 36$. The calculations confirmed the dual nature of the antiprotonic helium atoms as exotic systems exhibiting features of both atoms and molecules. This can be clearly shown in the atomic and molecular adiabatic curves in Fig. (3). The lowest nonrelativistic values show excellent agreement with the results of the calculations of other variational methods (Korobov *et al.*, 1992, 1996), though obtained belatedly. Hence our proposed algorithm now proved to meet the challenging precision required of the experimental verification for the exotic system $\bar{\mathrm{P}}\mathrm{He}^+$. The present approach can also be extended for the calculations of the autoionization Auger widths (Korobov and Shimamura, 1997), to be discussed elsewhere.

6. CONCLUSION

In this paper an efficient algorithm which utilizes DVR is extended for the hyperspherical treatments of the three-body problem having nonzero total angular momentum. Our new approach constitutes a major improvement over the standard techniques for the calculations of kinetic matrix elements. It generates high accuracy of computation, implementing the off-diagonal terms the precision is improved by four order of magnitude. For this purpose we have developed an efficient method to solve the 1D eigenvalue problem and constructed the corresponding special set of hyperspherical harmonics. The calculations done for the metastable

states of the exotic helium $\bar{p}He^+$. Spectral characteristics and properties of the exotic atoms within the present approach can be extracted. The present approach is also readily generalizable for other exotic three-body Coulomb systems with an arbitrary total angular momentum. Our future efforts are directed toward further achievements with more applications in the hyperspherical treatments of various three-body Coulomb systems.

APPENDIX

A N-point DVR–Legendre basis is defined by

$$\pi_i(x) = \sum_{n=1}^{N} T_{ni}\varphi_n(x), \quad i = 1, \ldots N \tag{A1}$$

$$T_{ni} = \sqrt{\omega_i}\varphi_n(x) \tag{A2}$$

$$\varphi_n(x) = \tilde{P}_{n-1}(x) \tag{A3}$$

where $\tilde{P}_n(x)$, $n = 0, 1, \ldots N-1$, are normalized Legendre polynomials, and x_i, ω_i, $i = 1, 2, \ldots N$, are abscissas and weights of the N-point Gauss–Legendre quadrature. Properties of $\varphi_n(x)$:

$$\left[\frac{d}{dx}(1-x^2)\frac{d}{dx} + (n-1)n\right]\varphi_n(x) = 0 \tag{A4}$$

$$x\varphi_n(x) = \frac{(n-1)}{\sqrt{4(n-1)^2-1}}\varphi_{n-1}(x) + \frac{n}{\sqrt{4n^2-1}}\varphi_{n+1}(x) \tag{A5}$$

$$(1-x^2)\frac{d\varphi_n(x)}{dx} = \frac{n(n-1)}{\sqrt{4(n-1)^2-1}}\varphi_{n-1}(x) - \frac{n(n-1)}{\sqrt{4n^2-1}}\varphi_{n+1}(x) \tag{A6}$$

Properties of $\pi_i(x)$:

$$\pi_i(x_j) = \frac{1}{\sqrt{\omega_i}}\delta_{ij} \tag{A7}$$

$$\int_{-1}^{1} \pi_i(x)\pi_j(x)\,dx = \delta_{ij}, \tag{A8}$$

$$\int_{-1}^{1} \pi_i(x)F(x)\pi_j(x)\,dx \approx F(x_i)\delta_{ij} \tag{A9}$$

$$\frac{d\pi_i(x)}{dx} = \sum_{k=1}^{N} b_{ik}\pi_k(x) \tag{A10}$$

where

$$b_{ik} = \sum_{n,m=1}^{N} T_{ni}a_{nm}T_{mk} \tag{A11}$$

and

$$a_{nm} = \begin{cases} \sqrt{(2n-1)(2m-1)} & \text{if } m = n-1, n-3, \ldots \geq 1, \\ 0 & \text{otherwise.} \end{cases} \tag{A12}$$

$$\int_{-1}^{1} \frac{d\pi_i(x)}{dx} F(x)\pi_j(x)\,dx \approx b_{ij} F(x_j) \tag{A13}$$

$$\int_{-1}^{1} \frac{d\pi_i(x)}{dx} F(x) \frac{d\pi_j(x)}{dx}\,dx \approx \sum_{k=1}^{N} b_{ik} F(x_k) b_{jk} \tag{A14}$$

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