Hyperspherical elliptic harmonics and their relation to the Heun equation

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Hyperspherical elliptic (HSE) harmonics are the eigenfunctions of the generalized angular momentum operator obtained by separating variables in HSE coordinates. These functions depend on accessory parameters characterizing the HSE coordinate system and present a more flexible basis on a hypersphere as compared with more familiar hyperspherical polar harmonics. We discuss a special set of HSE harmonics arising in hyperspherical treatments of the three-body problem in the HSE coordinate system introduced in an earlier paper [Tolstikhin *et al.*, Phys. Rev. Lett. **74**, 3573 (1995)]. The separation of variables in these coordinates leads to the Heun equation, which is a generalization of the Gauss hypergeometric equation. We develop an efficient method to solve the corresponding one-dimensional eigenvalue problem and thus construct the HSE harmonics, which opens a way for their application in the studies of various atomic, molecular, and nuclear three-body systems.

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I. INTRODUCTION

The Laplace operator in d-dimensional space expressed in hyperspherical coordinates can be presented in the form

$$\Delta = \frac{1}{R^{d-1}} \frac{\partial}{\partial R} R^{d-1} \frac{\partial}{\partial R} - \frac{\Lambda^2}{R^2}, \tag{1}$$

where R is the hyperradius and Λ^2 is the generalized angular momentum operator squared. Hyperspherical (HS) harmonics are defined as the eigenfunctions of Λ^2 [1],

$$[\Lambda^2 - \lambda(\lambda + d - 2)] Y_\omega(\Omega) = 0, \tag{2}$$

$$\lambda = 0,1,2 \ldots,$$

where Ω is a collective notation for a set of $(d-1)$ hyperangles parametrizing the hypersphere and ω denotes a set of $(d-1)$ quantum numbers uniquely defining λ and $Y_\omega(\Omega)$. HS harmonics play an important role in many applications providing a basis for expanding solutions to various problems in classical and quantum physics. As the most intensively developed direction during the past two decades, and the one closest to our own interests, we mention their applications in the theory of few-body systems [2–5]; see also a recent review article [6] and references therein. HS harmonics are closely related to the rotation group $O(d)$ and can be constructed by the algebraic methods. Another approach to construct these functions is to explicitly express Λ^2 as a differential operator in Ω and solve Eq. (2). In doing so one has to start by choosing a coordinate system in which Eq. (2) allows separation of variables. The coordinate system specifies the set of hyperangles Ω; the quantum numbers ω then acquire a meaning of the numbers of zeros of the solutions to the corresponding separation equations. In this paper we adopt the second approach, therefore we shall not discuss a group-theoretical meaning of ω, but we remark that this set may also include some additional quantum numbers like parity corresponding to discrete subgroups of $O(d)$. For any $d \geqslant 2$, Eq. (2) allows separation of variables in an infinite number of coordinate systems. They can be divided into classes, each class consisting of coordinate systems related to each other by rotations, and the different classes leading to separation equations having different mathematical structure. This can be illustrated by the example $d=3$. It is well-known that the Laplace operator in three-dimensional space allows separation of variables in two (and only two) spherical coordinate systems: these are spherical polar and spherical elliptic (also known as conical [7,8], spheroconal [9,10], spheroelliptic [11], and elliptic [12]) coordinates. Of the two angular separation equations in the spherical polar coordinates the nontrivial one is of the Legendre type, while both angular separation equations in the spherical elliptic coordinates are of the Lamé type. The Legendre equation can be reduced to the hypergeometric equation and solved ''analytically,'' i.e., it is very well studied. This greatly simplifies the work with spherical polar harmonics and explains why in an overwhelming majority of application-oriented treatises dealing with spherical harmonics the spherical polar coordinates are employed. The Lamé equation is much less studied and, although basic discussions of spherical elliptic harmonics can be found in several fundamental mathematical texts [9,10,13], the methods to work with these functions are not sufficiently developed and original papers on this subject still continue to appear [12]. The variety of the different classes of separable coordinate systems on a hypersphere for $d>3$ is larger; see, e.g., Refs. [11,14], where the case $d=4$ is analyzed. However, the situation is similar to that for $d=3$ in the sense that one can distinguish hyperspherical polar (HSP) and hyperspherical elliptic (HSE) coordinate systems leading to the hypergeometric and Lamé or, more generally, Heun separation equations, respectively. For the same reasons as above, all known to us studies dealing with HS harmonics and their applications employ HSP coordinates and consider

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only HSP harmonics; see, e.g., Refs. [1–6]. Meanwhile, HSE harmonics provide much more flexibility in choosing a basis in the best way suiting the needs of a particular physical problem, which in our opinion warrants more detailed study of and closer acquaintance with these functions.

In this paper we discuss a special set of HSE harmonics arising in hyperspherical treatments of the three-body problem in the HSE coordinates introduced in Ref. [15]. Finding this coordinate system has led to the development of a new powerful method for studying various three-body systems with Coulomb [15–21] and molecular [22–24] interparticle interactions. Further extensions of this approach require developing appropriate analytical and numerical techniques, a task that has motivated the present paper and is partially addressed here. In the following, we shall always keep in mind applications to the three-body problem to be discussed elsewhere. The HSE harmonics considered in this paper are functions of the two HSE coordinates η and ξ, an accessory parameter γ characterizing the HSE coordinate system, and an azimuthal quantum number m having a meaning of the projection of the total angular momentum along a body-fixed axis. For $m=0$, they give a new representation of the HS harmonics for a three-body system with zero total angular momentum, $L=0$; for $m\neq 0$, they constitute a more general set of functions providing a new basis for expanding the internal wave functions of a three-body system with $L\neq 0$ [27]. The paper is organized as follows: Sec. II summarizes basic equations in the HSE coordinates, the corresponding separation eigenvalue problem is analyzed in Sec. III, its solutions are used to construct the HSE harmonics in Sec. IV, and Sec. V concludes.

II. BASIC EQUATIONS

Configuration space of the three-body problem has six dimensions, $d=6$, so the set of hyperspherical angles Ω in this case consists of five variables. This set can be divided into two parts, $\Omega=(\Omega_s,\Omega_o)$, where Ω_s denotes a set of two angles defining the shape of the three-body triangle, its size being determined by hyperradius R, and Ω_o denotes a set of three angles defining the overall orientation of the system in space, e.g., the Euler angles. For states with $L=0$ the wave function does not depend on Ω_o. Then Λ^2 can be considered as a differential operator in two shape angles Ω_s and we denote it by Λ_0^2. A discussion of the different sets of shape angles for the three-body problem can be found in Ref. [22]. The coordinate systems introduced by Delves [25] and Smith and Whitten [26] present two most well-known examples of HSP coordinates in configuration space. Here we put $\Omega_s=(\eta,\xi)$, where η and ξ are HSE coordinates introduced in Ref. [15]. These variables vary in the intervals

$$-2\gamma\leqslant\eta\leqslant 2\gamma, \tag{3a}$$

$$2\gamma\leqslant\xi\leqslant 2\pi-2\gamma, \tag{3b}$$

where γ is a parameter such that

$$0\leqslant\gamma\leqslant\pi/2. \tag{4}$$

In the applications to the three-body problem [15–24] γ is defined by the masses of particles; here we assume that γ may take arbitrary values in the interval (4). The freedom in choosing this parameter reveals the mentioned above flexibility of the HSE coordinate system. In these coordinates the operator Λ_0^2 is given by [15]

$$\Lambda_0^2=\frac{-16}{\cos\eta-\cos\xi}\left[\frac{\partial}{\partial\eta}(\cos\eta-c)\frac{\partial}{\partial\eta}+\frac{\partial}{\partial\xi}(c-\cos\xi)\frac{\partial}{\partial\xi}\right]. \tag{5}$$

Having in mind to extend the present construction to the case $L\neq 0$, we consider a more general operator,

$$\Lambda_m^2=\Lambda_0^2+\frac{4s^2m^2}{\cos\eta-\cos\xi}\left[\frac{1}{\cos\eta-c}+\frac{1}{c-\cos\xi}\right], \tag{6}$$

where

$$c\equiv\cos 2\gamma,\quad s\equiv\sin 2\gamma. \tag{7}$$

The additional term $\propto m^2$ with a non-negative integer m having a meaning of an azimuthal quantum number indeed arises in treating the three-body problem within the symmetric top approximation [16,18], and we include it here without making the analysis more complex.

HSE harmonics are defined by

$$\left[\frac{1}{2}\Lambda_m^2-U\right]\Phi(\eta,\xi)=0, \tag{8}$$

where the factor 1/2 is introduced for consistency with Refs. [15–24]. This equation allows separation of the variables η and ξ. Seeking its solutions in the form

$$\Phi(\eta,\xi)=f(\eta)g(\xi) \tag{9}$$

one obtains ordinary differential equations defining the functions $f(\eta)$ and $g(\xi)$,

$$\left[8\frac{d}{d\eta}(\cos\eta-c)\frac{d}{d\eta}-\frac{2s^2m^2}{\cos\eta-c}+U(\cos\eta-c)+A\right]f(\eta)=0, \tag{10a}$$

$$\left[8\frac{d}{d\xi}(c-\cos\xi)\frac{d}{d\xi}-\frac{2s^2m^2}{c-\cos\xi}+U(c-\cos\xi)-A\right]g(\xi)=0, \tag{10b}$$

where A is the separation constant. The possibility to separate the variables in Eq. (8) results from the existence of an additional integral of the motion represented by an operator commuting with Λ_m^2 whose eigenvalues are given by A. Indeed, as follows from Eqs. (10), the solutions of Eq. (8) having the form (9) also satisfy

$$[\Upsilon_m-A]\Phi(\eta,\xi)=0, \tag{11}$$

where

$$\Upsilon_m=\frac{-8}{\cos\eta-\cos\xi}\left[(c-\cos\xi)\frac{\partial}{\partial\eta}(\cos\eta-c)\frac{\partial}{\partial\eta}-(\cos\eta-c)\frac{\partial}{\partial\xi}(c-\cos\xi)\frac{\partial}{\partial\xi}\right]+2s^2m^2\left[\frac{1}{\cos\eta-c}-\frac{1}{c-\cos\xi}\right]. \tag{12}$$

Equations (10) must be solved subject to the regularity boundary conditions for $f(\eta)$ and $g(\xi)$ at the end points of the intervals (3), which can be satisfied only for certain values of U and A. Thus each HSE harmonic (9) can be characterized by a pair of eigenvalues U and A or, alternatively, by a pair of HSE quantum numbers n_η and n_ξ giving the numbers of zeros of the functions $f(\eta)$ and $g(\xi)$.

It can be easily seen that Eqs. (10a) and (10b) are actually identical: they amount to the same differential equation considered in different intervals of the independent variable. Equation (10b) can be reduced to Eq. (10a) by substituting $\pi/2-\gamma$, $\eta+\pi$, $-A$, and f for γ, ξ, A, and g, respectively. Thus it is sufficient to analyze Eq. (10a).

III. ANALYSIS OF THE SEPARATION EIGENVALUE PROBLEM IN HYPERSPHERICAL ELLIPTIC COORDINATES

Consider the equation

$$\left[8\frac{d}{d\tau}(\cos\tau-c)\frac{d}{d\tau}-\frac{2s^2m^2}{\cos\tau-c}+U(\cos\tau-c)+A\right]T(\tau)=0, \tag{13a}$$

$$-2\gamma\leqslant\tau\leqslant2\gamma,\quad T(\pm2\gamma)<\infty, \tag{13b}$$

where c and s are related to γ by Eqs. (7). The end points $\tau=\pm2\gamma$ of the interval of τ are regular singular points of Eq. (13a), each with the characteristic exponents $\pm m/2$. The boundary conditions (13b) select the regular solutions at both singularities, i.e., those corresponding to the exponent $+m/2$ if $m\neq0$ and having no logarithmic terms in their expansions near $\tau=\pm2\gamma$ if $m=0$. In this section we shall regard γ, m, and U as external parameters that may take arbitrary values, while A will be treated as a spectral parameter. The boundary conditions (13b) can be satisfied only for a discrete set of the values of A, thus we are dealing with a singular Sturm-Liouville eigenvalue problem. The eigenvalues and eigenfunctions of Eqs. (13) will be denoted by

$$A_n(\gamma,m,U),\quad T_n(\tau;\gamma,m,U),\quad n=0,1,2,\ldots, \tag{14}$$

where n is the number of zeros of $T_n(\tau;\gamma,m,U)$ as a function of τ. The eigenfunctions are orthogonal with unit weight and we normalize them by

$$\int_{-2\gamma}^{2\gamma}T_n(\tau;\gamma,m,U)T_{n'}(\tau;\gamma,m,U)\,d\tau=\delta_{nn'}. \tag{15}$$

Equations (13) remain unchanged upon changing the sign of τ, so the eigenfunctions with even (odd) n are even (odd) functions of τ.

The role of Eq. (13a) in the construction of the HSE harmonics is similar to that of the Legendre equation in the theory of three-dimensional spherical polar harmonics or of the corresponding separation equation in the theory of spheroidal wave functions. This analogy is not accidental since Eq. (13a) is a generalization of the spheroidal equation, which in turn is a generalization of the Legendre equation, as will be shown shortly. The Legendre equation can be reduced to the hypergeometric equation and, as a consequence, is very well studied; see, e.g., Chap. 8 in Ref. [28]. The spheroidal equation is not reducible to the hypergeometric equation, which essentially complicates its analysis, however, it also has been intensively studied due to its importance for many physical applications and a number of practically useful results have been obtained and are available in the literature; see, e.g., Chap. 21 in Refs. [28] and [29]. Equation (13a) has even more involved mathematical structure and we do not know a treatise to be referred to in this respect. The purpose of this section is to derive some results relevant to the present paper. Here we show that Eq. (13a) can be reduced to the so-called Heun equation, construct an efficient analytical representation for the solutions of Eqs. (13), and discuss a special class of polynomial solutions defining the HSE harmonics.

Let us introduce a new variable x and a new function $\varphi(x)$,

$$x=\sin^2(\tau/2), \tag{16a}$$

$$(x-a)^{m/2}\varphi(x)=T(\tau), \tag{16b}$$

where $a\equiv\sin^2\gamma\leqslant1$. Then $\varphi(x)$ satisfies

$$\left[\frac{d^2}{dx^2}+\left(\frac{1-\epsilon_0}{x}+\frac{1-\epsilon_1}{x-1}+\frac{1-\epsilon_a}{x-a}\right)\frac{d}{dx}+\frac{px+q}{x(x-1)(x-a)}\right]\varphi(x)=0, \tag{17}$$

which is a form of the Heun equation [10,13]. The Heun equation directly generalizes the Gauss hypergeometric equation by having one more finite regular singular point. The different types of spectral problems that can be formulated on the basis of this equation generate several new types of eigenvalue schemes, which could find numerous applications in physics, however, the Heun equation is still much less studied than its hypergeometric relative; reviews of some recent achievements in this direction can be found in Ref. [30]. Equation (17) has characteristic exponents 0 and ϵ_0 at $x=0$, 0 and ϵ_1 at $x=1$, 0 and ϵ_a at $x=a$, and $\epsilon_\pm$ at $x=\infty$; the parameter p is defined by the exponents, $p\equiv\epsilon_-\epsilon_+$, and q is a spectral parameter. The cases when some of the exponent differences are equal to 1/2 occupy a special position since the Heun equation then allows a broader group of transformations. The case when the exponent differences at all three finite singular points are equal to 1/2 is known as

the Lamé equation; this equation arises when variables in the three-dimensional Laplace operator are separated in ellipsoidal coordinates [9,10,13]. In our case the parameters in Eq. (17) are related to those in Eq. (13a) by

$$\epsilon_0=\frac{1}{2},\quad \epsilon_1=\frac{1}{2},\quad \epsilon_a=-m,\quad \epsilon_\pm=\frac{1}{2}(m+1\pm\sqrt{1+U/2}), \tag{18a}$$

$$p=\epsilon_-\epsilon_+=\frac{1}{8}[2m(m+2)-U], \tag{18b}$$

$$q=\frac{1}{16}[A+2aU-4m(1+m-am)]. \tag{18c}$$

Thus two of the exponent differences are equal to 1/2, which is known as the Wangerin equation [8]. A detailed classification of the different particular cases of the Heun equation and its confluent forms is given in Ref. [31]. As follows from Eqs. (13b) and (16a), the new variable varies in the interval $0\leqslant x\leqslant a$, i.e., between two singular points of Eq. (17). The boundary conditions for Eq. (17) can be obtained from Eqs. (13) and (16) and consist of the following: (i) the solutions of Eq. (17) must be regular at $x=a$, and (ii) even (odd) solutions of Eqs. (13) are represented by the solutions of Eq. (17) corresponding to the exponent 0 (1/2) at $x=0$.

Consider an equivalence transformation of Eq. (17) to be used in the following. Let us introduce a new function,

$$\tilde{\varphi}(x)=\frac{\varphi(x)}{x^{\alpha_0}(x-1)^{\alpha_1}}. \tag{19}$$

It can be shown that for α_i equal to 0 or ϵ_i, $i=0,1$, $\tilde{\varphi}(x)$ satisfies an equation of the same form as Eq. (17) with the same values of a and ϵ_a and the other parameters replaced by

$$\tilde{\epsilon}_0=\epsilon_0-2\alpha_0,\quad \tilde{\epsilon}_1=\epsilon_1-2\alpha_1, \tag{20a}$$

$$\begin{aligned}\tilde{p}&=p+\alpha_0(2-\epsilon_1-\epsilon_a)+\alpha_1(2-\epsilon_0-\epsilon_a)+2\alpha_0\alpha_1\\&=p+(m+3/2)(\alpha_0+\alpha_1)+2\alpha_0\alpha_1,\end{aligned} \tag{20b}$$

$$\begin{aligned}\tilde{q}&=q-\alpha_0(1-\epsilon_a)-a[\alpha_0(1-\epsilon_1)+\alpha_1(1-\epsilon_0)+2\alpha_0\alpha_1]\\&=q-\alpha_0(1+m)-a[(\alpha_0+\alpha_1)/2+2\alpha_0\alpha_1].\end{aligned} \tag{20c}$$

We shall distinguish four classes of the solutions of Eq. (17) according to the following four possibilities in choosing the exponents α_0 and α_1 in Eq. (19), where $\tilde{\varphi}(x)$ is assumed to have only non-negative integer powers in the expansions near $x=0$ and $x=1$: (I) $\alpha_0=\alpha_1=0$, (II) $\alpha_0=0$ and $\alpha_1=1/2$, (III) $\alpha_0=1/2$ and $\alpha_1=0$, and (IV) $\alpha_0=\alpha_1=1/2$. Classes I and II represent even solutions of Eqs. (13), and classes III and IV represent odd ones.

The solutions of Eq. (17) can be sought as an expansion in terms of a suitable set of functions complete in the interval $x\in[0,a]$. Let us first consider the solutions regular at $x=a$ and corresponding to the exponent 0 at $x=0$, i.e., representing even solutions of Eqs. (13). We have analyzed several choices of the basis functions and found that the fastest convergence is achieved with the Jacobi polynomials,

$$\varphi(x)=\sum_{k=0}^{\infty}\varphi_k P_k^{(-\epsilon_a,-\epsilon_0)}(2x/a-1). \tag{21}$$

Substituting this expansion into Eq. (17), one obtains a three-term recursion relation defining the coefficients φ_k,

$$(B_0+q)\varphi_0+C_0\varphi_1=0, \tag{22a}$$

$$A_k\varphi_{k-1}+(B_k+q)\varphi_k+C_k\varphi_{k+1}=0,\quad k=1,2,\ldots, \tag{22b}$$

where

$$A_k=a[p+(k-1)(k+\delta-\epsilon_1)]\frac{k(k+\delta-1)}{(2k+\delta-2)(2k+\delta-1)}, \tag{23a}$$

$$\begin{aligned}B_k=\frac{a}{2}\left[p+(\epsilon_a-\epsilon_0)\frac{k(k+\delta)(\delta-2\epsilon_1+1)+p(\delta-1)}{(2k+\delta-1)(2k+\delta+1)}\right]\\+(a/2-1)k(k+\delta),\end{aligned} \tag{23b}$$

$$C_k=a[p+(k+\epsilon_1)(k+\delta+1)]\frac{(k-\epsilon_0+1)(k-\epsilon_a+1)}{(2k+\delta+1)(2k+\delta+2)}, \tag{23c}$$

and $\delta\equiv 1-\epsilon_0-\epsilon_a$. Let $\Delta_k(q)$ denote the determinant of the upper-left $k\times k$ block of the tridiagonal matrix multiplying the vector of coefficients φ_k in Eqs. (22). Then the values of q for which Eqs. (22) are satisfied can be found from the characteristic equation

$$\Delta_K(q)=0 \tag{24}$$

for a sufficiently large K. The characteristic polynomial $\Delta_K(q)$ can be computed for any trial value of q from the recurrence

$$\Delta_0(q)=1, \tag{25a}$$

$$\Delta_1(q)=B_0+q, \tag{25b}$$

$$\Delta_{k+1}(q)=(B_k+q)\Delta_k(q)-A_kC_{k-1}\Delta_{k-1}(q),\quad k=1,2,\ldots \tag{25c}$$

The rate of convergence of expansion (21) can be characterized by the roots r_1 and r_2 of the quadratic equation $A+Br+Cr^2=0$, where A, B, and C are the limiting values of A_k, B_k, and C_k at $k\to\infty$. In general, convergence is faster the larger the ratio $|r_2/r_1|$. As can be seen from Eqs. (23), in our case

$$A=ak^2/4,\quad B=(a-2)k^2/2,\quad C=ak^2/4, \tag{26}$$

hence

$$r_1=\tan^2(\gamma/2),\quad r_2=\cot^2(\gamma/2). \tag{27}$$

Thus convergence should be fast for small γ, but may become worse as γ approaches $\pi/2$. The high rate of convergence of expansion (21) for γ not very close to $\pi/2$ and for arbitrary values of the other parameters has been confirmed by our calculations. The difficulty with the case $\gamma\to\pi/2$ can be explained as follows. A general solution of Eq. (17) behaves $\sim\sqrt{1-x}$ at $x\to 1$, but $a\to 1$ as $\gamma\to\pi/2$, and in order to reproduce this square-root behavior, expansion (21) requires more and more terms. To find an efficient expansion for the case $\gamma\to\pi/2$ remains an open problem. Using Eqs. (16) and (18), functions (21) and the roots of Eq. (24) can be transformed to the solutions of Eqs. (13). In this way one can construct the even solutions of Eqs. (13). The odd solutions can be obtained by the same procedure applied after the equivalence transformation (19) with $\alpha_0=1/2$ and $\alpha_1=0$.

The described algorithm is based on the well-known properties of tridiagonal matrixes and is rather standard [32]; for example, a similar method is used for constructing spheroidal wave functions [28,29]. However, let us discuss briefly one circumstance that plays a decisive role in making this algorithm simple in use and really efficient in practical calculations, but which is not usually paid due attention. This concerns the method of how the roots of Eq. (24) are sought. In the general case, there is no other option but to seek the roots iteratively by starting from some independently obtained estimate of the initial interval $q_n^-\leqslant q_n\leqslant q_n^+$, bracketing the desired eigenvalue q_n, and then refining this interval, e.g., using the bisection method. There are two situations where such iterations unambiguously converge to q_n: (a) the initial interval $[q_n^-,q_n^+]$ does not contain other eigenvalues but q_n, which is the case, e.g., if initial intervals for different n do not overlap; then one just has to locate the point where $\Delta_K(q)$ changes sign; (b) the set $\Delta_k(q)$, $k=0,1,\ldots K$, forms a Sturmian sequence [32], then to find a zero of $\Delta_K(q)$ one has to follow the variation of the number of sign changes in this sequence as a function of q; in this case iterations converge to the desired eigenvalue independently of how many other roots of Eq. (24) fall in the initial interval $[q_n^-,q_n^+]$. If neither of these conditions is fulfilled then the algorithm still can be used, of course, but it becomes less definite and requires additional numerical tricks. In our case it can be shown that the eigenvalues of Eqs. (13) satisfy

$$A_n^-\leqslant A_n(\gamma,m,U)\leqslant A_n^+, \tag{28a}$$

where

$$A_n^-=\frac{2s}{\gamma}\epsilon_n-\max[0,U(1-c)], \tag{28b}$$

$$A_n^+=\frac{2(1-c)}{\gamma^2}\epsilon_n-\min[0,U(1-c)], \tag{28c}$$

and

$$\epsilon_n=(n+m\sqrt{\gamma\cot\gamma})(n+m\sqrt{\gamma\cot\gamma}+1). \tag{28d}$$

Together with Eqs. (18) and (20) this provides an estimate for the initial interval $[q_n^-,q_n^+]$. However, there is no guarantee that for each n this interval contains only one eigenvalue, and this is certainly not the case for $\gamma\to\pi/2$. Equations (25) define a Sturmian sequence if $A_kC_{k-1}\geqslant 0$ for all $k=1,2,\ldots K$. As can be seen from Eqs. (18), (20), and (23), in our case this condition depends on the parameters U and m and is not generally satisfied. However, a more detailed analysis shows that A_kC_{k-1} may become negative only for one value of $k\geqslant 1$, and this may happen *either* for even *or* for odd solutions of Eqs. (13). Thus solutions of one parity can always be constructed by the method (b) described above, and since even and odd eigenvalues alternate with each other, this yields nonoverlapping initial brackets for computing solutions of the other parity by the method (a).

We now discuss a special class of polynomial solutions of the Heun equation (17). The possibility for the existence of such solutions can be seen from Eqs. (25). Indeed, let $A_kC_{k-1}=0$ for some particular k, then the roots of equation $\Delta_k(q)=0$ are also roots of Eq. (24) for any $K\geqslant k$. In this case Eqs. (22) have $(k+1)$ solutions for which $\varphi_{k+1}=\varphi_{k+2}=\ldots=0$, hence Eq. (17) has $(k+1)$ solutions given by polynomials of degree k. Using the equivalence transformation (19), we obtain four classes of the polynomial solutions of Eq. (17) corresponding to the discussed above four possibilities in choosing α_0 and α_1. These solutions exist for

$$U=2(N+m)(N+m+2),\quad N=0,1,2,\ldots, \tag{29a}$$

and have the form

$$\begin{aligned}\varphi^{\mathrm{I}}(x)&=\mathcal{P}_{N/2}(x),\text{—}N/2+1\text{ solutions},\\ \varphi^{\mathrm{IV}}(x)&=\sqrt{x(x-1)}\,\mathcal{P}_{N/2-1}(x),\text{—}N/2\text{ solutions},\end{aligned} \tag{29b}$$

for even N, and

TABLE I. The polynomial solutions (30) of Eqs. (13) obtained for U given by Eq. (29a) for three lowest values of N. The eigenfunctions are not normalized. $d\equiv\sqrt{4(m+1)(m+2)+c^2}$.

N	n	$A_n^{(N)}(\gamma,m)$	$(\cos\tau-c)^{-m/2}T_n^{(N)}(\tau;\gamma,m)$
0	0	$4cm(m+1)$	1
1	0	$4(m+1)[c(m+1)-1]$	$\cos(\tau/2)$
1	1	$4(m+1)[c(m+1)+1]$	$\sin(\tau/2)$
2	0	$4[c(m+1)(m+2)+c-d]$	$2(m+2)\cos\tau-c+d$
2	1	$4c(m+1)(m+2)$	$\sin\tau$
2	2	$4[c(m+1)(m+2)+c+d]$	$2(m+2)\cos\tau-c-d$

$$\varphi^{\mathrm{II}}(x)=\sqrt{x-1}\,\mathcal{P}_{(N-1)/2}(x),\text{—}(N+1)/2 \text{ solutions}, \tag{29c}$$

$$\varphi^{\mathrm{III}}(x)=\sqrt{x}\,\mathcal{P}_{(N-1)/2}(x),\text{—}(N+1)/2 \text{ solutions},$$

for odd N, where $\mathcal{P}_k(x)$ denotes a polynomial in x of precise degree k. Thus in both cases we obtain $N+1$ solutions. The eigenvalues and eigenfunctions of Eqs. (13) corresponding to the polynomial solutions of Eq. (17) will be denoted by

$$A_n^{(N)}(\gamma,m), \quad T_n^{(N)}(\tau;\gamma,m), \quad n=0,1,\ldots,N. \tag{30}$$

These functions for three lowest values of N are given in Table I.

Finally, let us discuss Eqs. (13) in the limit $\gamma\to 0$. In this case it is convenient to introduce a new variable,

$$t=\tau/(2\gamma), \quad -1\leqslant t\leqslant 1. \tag{31}$$

Assuming that $\gamma^2 m^2\to 0$ and $\gamma^2 U\to\tilde{U}\neq 0$ as $\gamma\to 0$, Eq. (13a) takes the form

$$\left[\frac{d}{dt}(1-t^2)\frac{d}{dt}-\frac{m^2}{1-t^2}+\frac{1}{2}\tilde{U}(1-t^2)+\frac{1}{4}A\right]\psi(t)=0. \tag{32}$$

Apart from a trivial change of notation, this coincides with the spheroidal equation, see [28,29]. If $\gamma^2 U\to 0$ as $\gamma\to 0$, then one obtains

$$\left[\frac{d}{dt}(1-t^2)\frac{d}{dt}-\frac{m^2}{1-t^2}+\frac{1}{4}A\right]\psi(t)=0. \tag{33}$$

This is the Legendre equation, see Ref. [28]. From this for the solutions of Eqs. (13) one obtains

$$A_n(\gamma,m,U)\big|_{\gamma\to 0}=4(n+m)(n+m+1), \tag{34a}$$

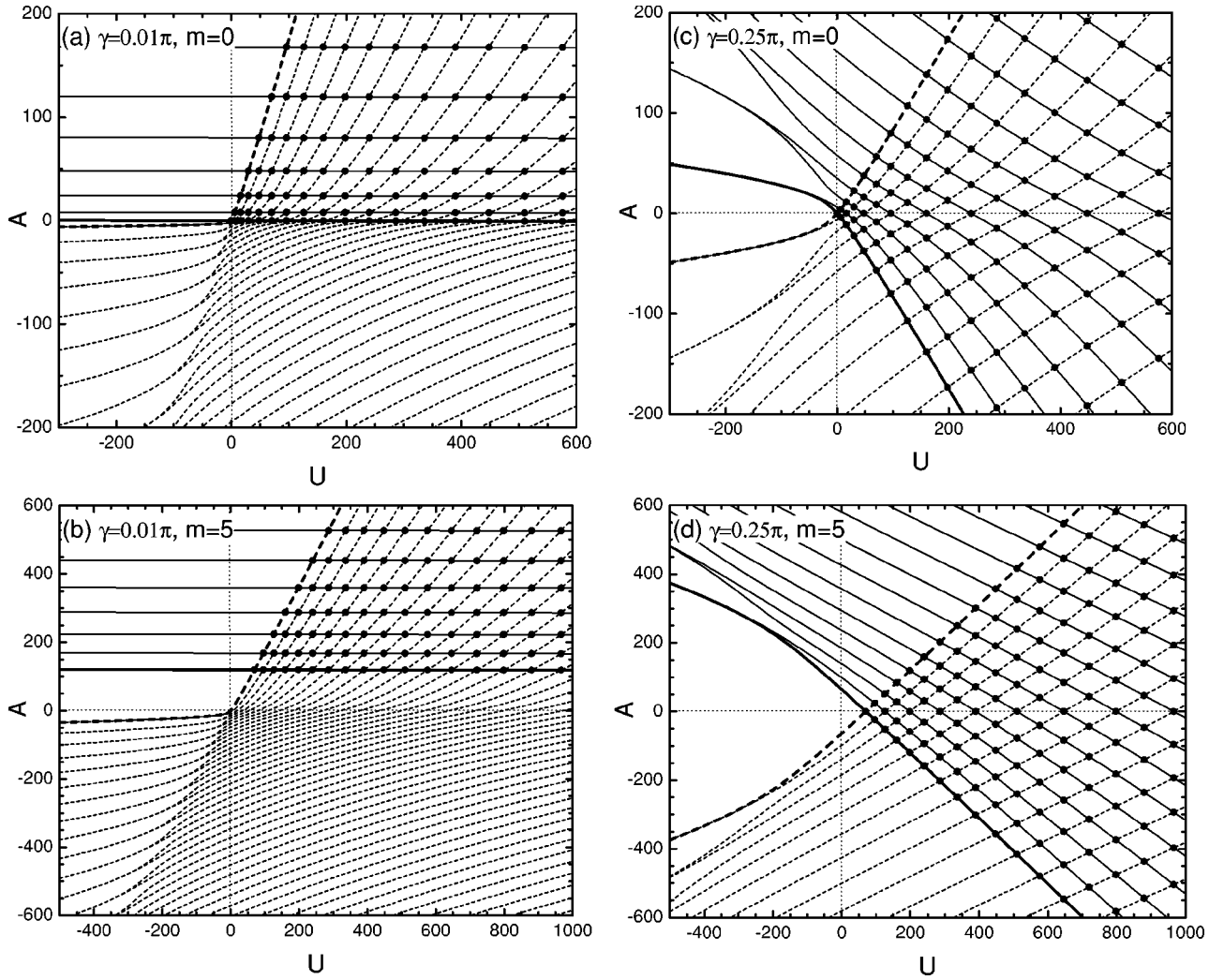

FIG. 1. Solid lines—the eigenvalues of Eq. (10a) given by $A_{n_\eta}(\gamma,m,U)$; dashed lines—the eigenvalues of Eq. (10b) given by $-A_{n_\xi}(\pi/2-\gamma,m,U)$. The eigenvalues are plotted as functions of U for several representative values of the parameters γ and m. The lowest (the highest) curves in solid (dashed) manifolds correspond to $n_\eta=0$ ($n_\xi=0$) and are shown by thicker lines. The points of the intersections between solid and dashed curves shown by solid circles indicate the values of U and A for which Eqs. (10) are satisfied simultaneously, which corresponds to the HSE harmonics.

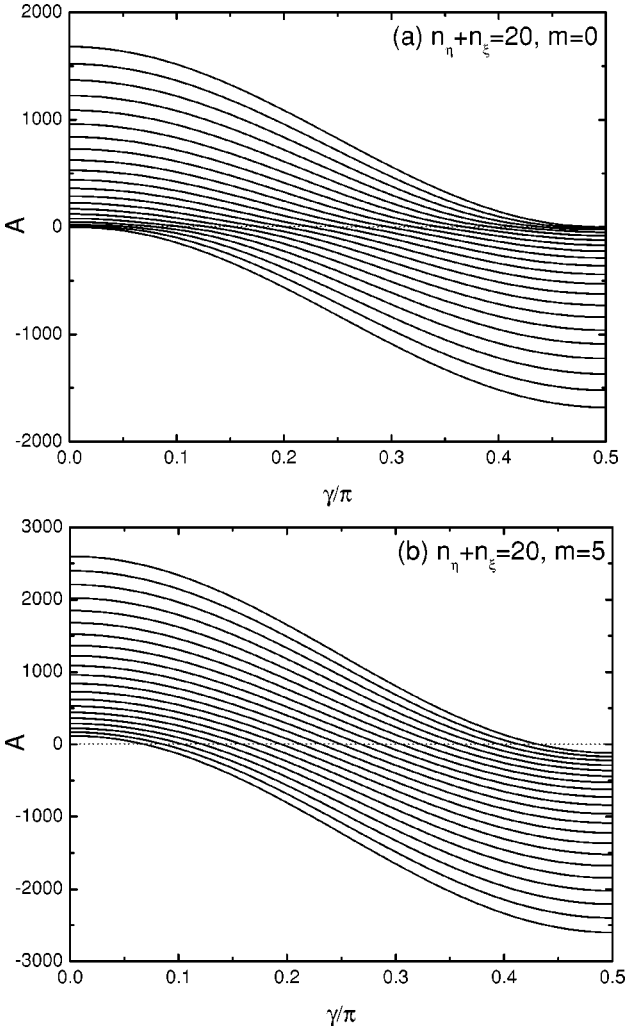

FIG. 2. The separation constants (35b) for the HSE harmonics with $n_\eta+n_\xi=20$ are plotted as functions of γ for two representative values of *m*. The lowest (the highest) curves correspond to $n_\eta=0$ $(n_\xi=0)$.

$$T_n(\tau;\gamma,m,U)\big|_{\gamma\to 0}=(1-t^2)^{m/2}\tilde{P}_n^{(m,m)}(t), \qquad (34b)$$

$$n=0,1,2\ldots,$$

where $\tilde{P}_n^{(m,m)}(t)$ are the normalized Jacobi polynomials. Equations (15) and (34b) define our standardization for the functions $T_n(\tau;\gamma,m,U)$. Note that the eigenvalues (34a) could be obtained from Eqs. (28) in the limit $\gamma\to 0$. The limit $\gamma\to\pi/2$ can also be analyzed analytically, but this leads to a rather complicated transcendental equation for the eigenvalues which we do not discuss here.

IV. HYPERSPHERICAL ELLIPTIC HARMONICS

Let us return to Eqs. (10). Following the approach used in the preceding section, we can consider these equations separately, treating γ, *m*, and *U* as parameters and *A* as an eigenvalue. As follows from the above results, thus defined eigenvalues of Eqs. (10a) and (10b) are given by $A_{n_\eta}(\gamma,m,U)$ and $-A_{n_\xi}(\pi/2-\gamma,m,U)$, respectively, where n_η and n_ξ are the numbers of zeros of the corresponding eigenfunctions. These eigenvalues as functions of *U* are shown in Figs. 1 for several representative values of γ and *m*. Note that such plots for two values of γ related by $\gamma_2=\pi/2-\gamma_1$ can be obtained from each other by inverting the sign of *A* and interchanging the types of lines used to draw the two sets of eigenvalues, hence it is sufficient to consider the interval $0\leqslant\gamma\leqslant\pi/4$. For $\gamma\to 0$, the eigenvalues of Eq. (10a) are given by Eq. (34a), so the solid curves in Figs. 1(a) and 1(b) are almost independent of *U*; for $\gamma=\pi/4$, the solid and dashed curves are symmetric with respect to the axis $A=0$, as can be seen from Figs. 1(c) and 1(d). The values of *U* and *A* for which Eqs. (10) are satisfied simultaneously are given by the coordinates of the intersections between the solid and dashed curves; conversely, each solid circle in Fig. 1 represents a HSE harmonic.

As has been noticed above, Eqs. (10a) and (10b) amount to the same differential equation considered in the intervals $[-2\gamma,2\gamma]$ and $[2\gamma,2\pi-2\gamma]$, respectively. This means that HSE harmonics are given by the solutions of Eq. (10a), which are regular at $\eta=\pm 2\gamma$ *and* at $\eta=2\pi-2\gamma$, which corresponds to polynomial solutions of Eqs. (13). This situation is similar to the case of spherical elliptic harmonics in three-dimensional space [9,10,13]: the regularity boundary conditions can be satisfied simultaneously at *three* singular points due to the presence of *two* spectral parameters, the energy eigenvalue *U* and the separation constant *A*. Thus we can summarize our construction of the HSE harmonics as follows:

$$U_{n_\eta n_\xi}=2(n_\eta+n_\xi+m)(n_\eta+n_\xi+m+2), \qquad (35a)$$

$$A_{n_\eta n_\xi}=A_{n_\eta}^{(n_\eta+n_\xi)}(\gamma,m)=-A_{n_\xi}^{(n_\eta+n_\xi)}(\pi/2-\gamma,m), \qquad (35b)$$

$$\Phi_{n_\eta n_\xi}(\eta,\xi)=\mathcal{N}\times T_{n_\eta}^{(n_\eta+n_\xi)}(\eta;\gamma,m)\,T_{n_\xi}^{(n_\eta+n_\xi)}(\xi;\pi/2-\gamma,m), \qquad (35c)$$

$$n_\eta=0,1,\ldots, \quad n_\xi=0,1,\ldots,$$

where n_η and n_ξ are the HSE quantum numbers and $\mathcal{N}$ is a normalization factor. As follows from Eq. (35a), the energy eigenvalues $U_{n_\eta n_\xi}$ do not depend on γ, and HSE harmonics with the same values of $n_\eta+n_\xi+m$ are degenerate. The separation constants $A_{n_\eta n_\xi}$ for $n_\eta+n_\xi=0$, 1, and 2 are given in Table I; in the general case their dependence on the HSE quantum numbers n_η and n_ξ and the parameters γ and *m* cannot be found analytically. Figure 2 illustrates the dependence of $A_{n_\eta n_\xi}$ on γ for $n_\eta+n_\xi=20$ and two representative values of *m*. Functions (35c) are orthogonal with the weight $(\cos\eta-\cos\xi)$ and we normalize them by [15,22]

$$\frac{\pi^2}{4s}\int_{-2\gamma}^{2\gamma} d\eta \int_{2\gamma}^{2\pi-2\gamma} d\xi (\cos\eta - \cos\xi) \times \Phi_{n_\eta n_\xi}(\eta,\xi)\Phi_{n'_\eta n'_\xi}(\eta,\xi) = \delta_{n_\eta n'_\eta}\delta_{n_\xi n'_\xi}. \quad (36)$$

For any m, these functions form a complete basis in the space of functions of two shape angles Ω_s satisfying appropriate boundary conditions at collinear configurations. The transformations between thus constructed HSE harmonics and the more familiar sets of HSP harmonics obtained by separating variables in Eq. (8) in Delves and Smith-Whitten coordinates, as well as their application for expanding the internal wave functions of a three-body system with $L \neq 0$, will be discussed elsewhere.

V. CONCLUSIONS

In this paper we have introduced a special set of HSE harmonics in six-dimensional space and developed an efficient algorithm to practically construct them. These functions may find applications in hyperspherical treatments of various atomic [2,3], molecular [4], and nuclear [5] three-body systems. However, because of a relation between the additional integral of motion Υ_m responsible for the separation of variables in HSE coordinates and the $O(4)$ symmetry of the Coulomb interaction, these functions are especially convenient for studying three-body Coulomb systems, as will be demonstrated in a forthcoming paper.

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