Boundary conditions on internal three-body wave functions

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For a three-body system, a quantum wave function Ψ^l_m with definite l and m quantum numbers may be expressed in terms of an internal wave function χ^l_k, which is a function of three internal coordinates. This article provides necessary and sufficient constraints on χ^l_k to ensure that the external wave function Ψ^l_m is analytic. These constraints effectively amount to boundary conditions on χ^l_k and its derivatives at the boundary of the internal space. Such conditions find similarities in the (planar) two-body problem where the wave function (to lowest order) has the form $r^{|m|}$ at the origin. We expect the boundary conditions to prove useful for constructing singularity free three-body basis sets for the case of nonvanishing angular momentum.

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I. INTRODUCTION

Consider a wave function Ψ^l_m for a system of three bodies that is an eigenfunction of L_s^2 and L_{sz} with quantum numbers l and m, respectively, where $\mathbf{L}_s$ is the space-fixed orbital angular momentum. (The s subscript stands for ''space-fixed.'') We regard Ψ^l_m, the ''external wave function,'' as a function of the two Cartesian Jacobi vectors. It is well known [1–3] that such a wave function can be written in the form

$$\Psi^l_m = \sum_k \mathcal{D}^{l*}_{mk} \chi^l_k, \tag{1.1}$$

where the Wigner rotation matrix $\mathcal{D}^l_{mk}$ is a function of the three Euler angles and where χ^l_k, the ''internal wave function,'' is a function of three internal or shape coordinates. As usual, k is regarded as the quantum number of the body-fixed L_z. The wave function Ψ^l_m need not be an energy eigenfunction; for example, it could be an element of a basis set in terms of which an unknown energy eigenfunction is to be expanded. The basis sets we have in mind include standard orthonormal bases, hyperspherical harmonics [4,5], discrete variable representation (DVR) bases [6–11], and wave packet [12] or wavelet [13] bases.

This paper concerns boundary conditions that the internal wave function χ^l_k must satisfy, given that the external wave function Ψ^l_m is a smooth function of the Cartesian Jacobi vectors. The boundary in question is the boundary of shape space, which consists of the collinear configurations. (Our definition of ''boundary conditions'' excludes consideration of the string or body-frame singularities of the wave function, which are discussed more fully below.) The applications we have in mind are mainly molecular (either bound states of triatomic molecules or triatomic scattering problems), but the considerations we raise also apply to atoms or other systems of bodies with Coulomb interactions (with certain qualifications discussed below). We ignore spin in this paper. We consider only three-body systems in this paper, but an important reason for studying boundary conditions in three-body systems is that it is good practice for the analogous problem for systems of four or more bodies, which is generally more difficult and much less well understood.

There are at least two practical reasons for being interested in boundary conditions. First, if one attempts to expand some unknown function in terms of a given basis, and if there are boundary conditions satisfied by the unknown function that are not satisfied by the basis functions, then the convergence will be slow. In important cases, the coefficient of the nth term in the expansion will fall off either exponentially or algebraically with n, depending on whether the basis does or does not satisfy the required boundary conditions, respectively. For example, it is a bad idea to use the ordinary Legendre polynomials to expand a function whose θ dependence has the boundary conditions of one of the associated Legendre functions for $m>0$. The importance of properly treating such boundary conditions in three-body problems has been discussed previously by Kendrick *et al.* [14]

Sometimes basis functions are created on the internal space simply by writing down some internal wave functions χ^l_k that are considered convenient, for example, distributed Gaussians or wave packets. From the given internal wave functions, one can construct the corresponding external wave functions according to Eq. (1.1). The question then arises, will these external wave functions have the same smoothness and analyticity properties as some unknown wave function (usually an energy eigenfunction) that one wishes to find? If not, the convergence will be poor. For another example, it is common practice to create internal basis functions by writing down the exact internal Hamiltonian, and then carving out some piece of it that has eigenfunctions which can be determined analytically. Again there is a question as to whether the basis functions created in this manner have the boundary conditions required of the desired unknown eigenfunction. The answer to this question depends in part on whether the operator created by carving out a piece of the Hamiltonian is itself well behaved. The analysis of this paper will show how to answer these questions.

A second reason for being interested in boundary conditions is that numerical methods for solving partial differential equations on a grid must generally take careful account of boundary conditions, in order to guarantee reasonable accuracy and convergence. Grid and basis set methods are related, since grid methods implicitly involve a set of localized basis functions associated with the grid points. For example, DVR methods involve a basis set consisting of localized

wave functions, resembling diffraction patterns from a narrow slit. The often cited ''unexpected accuracy'' (that is, rapid convergence) of DVR methods is closely related to satisfying the right boundary conditions. For example, the trapezoidal rule converges exponentially (rapidly) when an analytic, periodic function is integrated over a period, but has only power law (slow) convergence if the function is analytic but not periodic, or if it is integrated only over a partial period. Similarly, if the wrong DVR basis set is used for a given problem, the (by now expected) unexpected accuracy will be lost. We will have more to say about boundary conditions and rates of convergence in future publications, but this paper will concentrate on the boundary conditions themselves.

We will momentarily present the principal results of our analysis of boundary conditions in three-body systems, but first it is well to recall some facts about two-body systems with rotational invariance. Thinking of energy eigenfunctions, we will speak first of the problem of central force motion. In three spatial dimensions, the energy eigenfunction can be written $\Psi_m^l(\mathbf{r})=Y_m^l(\theta,\phi)\chi_l(r)$, where $\chi_l(r)$ is the internal or radial wave function, defined on the radial half-line $0\leqslant r<\infty$, which is the internal space. According to the standard textbook analysis [15], the radial wave function behaves as r^l near $r=0$. This behavior holds when the true potential $V(r)$ is analytic at $r=0$, but also in other cases such as that of the singular Coulomb potential.

The standard analysis that produces these results proceeds by expanding the radial wave function in a Taylor series about $r=0$ and balancing terms on the two sides of the Schrödinger equation. Unfortunately, this analysis leaves the impression that the behavior $\chi_l\sim r^l$ of the radial wave function near $r=0$ applies only to energy eigenfunctions. Actually this behavior is much more general. Consider any wave function $\Psi_m^l(\mathbf{r})$, which is an eigenfunction of L^2 and L_z and which is analytic at $\mathbf{r}=0$ when expressed in terms of the Cartesian coordinates (x,y,z). This would apply to the eigenfunctions of any rotationally invariant operator that is well behaved at $r=0$, including Hamiltonians with central potentials $V(r)$ which are analytic at $r=0$. With standard assumptions about phase conventions the wave function can be written $\Psi_m^l(\mathbf{r})=Y_m^l(\theta,\phi)\chi_l(r)$, where $\chi_l(r)$ is the radial wave function. We note that this form follows from the standard theory of rotations and the fact that Ψ_m^l is an eigenfunction of L_s^2 and L_{sz}; we do not invoke separation of variables, since we are not necessarily separating any wave equation. Then it turns out that $\chi_l(r)$ is analytic at $r=0$, and that its Taylor series begins with the r^l term and thereafter contains only the powers r^{l+2n}, $n=1,2,\ldots$, that is, every other integer power of r. Energy eigenfunctions in the Coulomb problem do not fit this pattern, since $\Psi_m^l(\mathbf{r})$ has a cusp at $r=0$ and is not analytic there. This is because $V(r)$ is not analytic at $r=0$. Although Coulomb radial wave functions χ_l do go as r^l near $r=0$, the Taylor series of χ_l contains every subsequent power of r, not every other one.

It is also worthwhile mentioning the case of two bodies in two spatial dimensions, since planar two-body boundary conditions bear a strong analogy to the boundary conditions in three-body systems. For the planar problem, an eigenfunction of L_{sz} can be written $\Psi_m(\mathbf{r})=e^{im\phi}\chi_m(r)$, where $\mathbf{r}=(x,y)$, ϕ is the azimuthal angle, and $m=0,\pm1,\pm2,\ldots$ is the quantum number of L_{sz}. If Ψ_m is analytic in the two Cartesian coordinates (x,y) at $\mathbf{r}=0$, then the radial wave function $\chi_m(r)$ is analytic at $r=0$, its Taylor series begins with the $r^{|m|}$ term, and it subsequently contains only every other power of r, $r^{|m|+2n}$, $n=1,2,\ldots$.

At this point a reader who works with three-body molecular problems may wonder what the relevance is of two-body boundary conditions at $r=0$, since $r=0$ is the two-body collision and the collision of atoms in molecular problems does not happen at ordinary energies. The answer is that in three-body systems the collinear configurations play somewhat the same role as the two-body collision in the planar two-body problem, insofar as boundary conditions are concerned. This is why it is important to know about two-body boundary conditions at $r=0$, even for molecular problems. Collinear configurations are not necessarily suppressed in three-body molecular problems, and are often important.

On the other hand, collisional configurations are important in Coulomb problems, where the wave function has cusplike singularities [16,17], again because of the nonanalyticity of the potential. Since this paper studies the boundary conditions on the internal wave function that result from the analyticity of the external wave function, and since the external wave function in Coulomb problems is not analytic at collisions, the analysis of this paper does not apply to collisional configurations in Coulomb problems. But of course Coulomb problems also have collinear configurations, and our analysis does apply to these, as long as they are not also collisional. We also exclude string or body frame singularities (discussed momentarily) from consideration. We can summarize by saying that the analysis of this paper applies to all the important boundary conditions in three-body molecular problems, and to some of them (the collinear, noncollisional configurations) in Coulomb problems.

Regarding string or body frame singularities, some researchers would include them in their definition of ''boundary conditions.'' These are the singularities of the three-body wave function which occur along a curve (the string) in shape space emanating from the three-body collision. (This string contains points where the body frame is not well defined.) Certainly these singularities are important in practice, but we prefer not to regard them as a part of the issue of boundary conditions. This is because they do not occur at the boundary of shape space and because the locations where they do occur depends on the choice of body frame. (Thus, they can be moved around by a change of frame.) We have discussed string singularities separately in two recent papers [18,19]. Pack has also studied these body frame singularities [20].

We now summarize the main results of this paper, which relate the analyticity of the three-body external wave function Ψ_m^l to the behavior of the internal wave function χ_k^l at the boundary of the internal space. The boundary of collinear shapes is a plane specified by $\Theta=0$ in Smith's [21] hyperspherical coordinates, or $w_3=0$ in the coordinates to be introduced below. One point of this plane is the three-body

collision, which is excluded from our analysis. At other points of this plane, we have established necessary and sufficient conditions on χ_k^l such that the external wave function Ψ_m^l should be analytic functions of the six Cartesian components of the two Jacobi vectors. If Ψ_m^l is analytic at a collinear configuration (not the three-body collision), then the internal wave function χ_k^l satisfies the following properties. First, χ_k^l is itself analytic at the collinear shape, when expressed in terms of certain internal coordinates to be described below. Suffice it for now to say that one of these coordinates, call it w_3, measures the mass-weighted distance from the plane $w_3=0$ of collinear shapes, while the other two coordinates, w_1 and w_2, indicate where we are on this plane.

The second property involves a modified version of the internal wave function χ_μ^l (in contrast to χ_k^l). The distinction is that k is the eigenvalue of body-fixed L_z whereas μ is the eigenvalue of body-fixed $\hat{\mathbf{n}}\cdot\mathbf{L}$, where $\hat{\mathbf{n}}$ is the body-referred unit vector specifying the axis of a collinear shape. The vector $\hat{\mathbf{n}}$ is defined on the boundary plane of the internal space (excluding the triple collision), and is a function of where we are on that plane. Both k and μ range from $-l$ to $+l$, and the two internal wave functions are related by a rotation that maps the body $\hat{\mathbf{z}}$ axis into the $\hat{\mathbf{n}}$ axis. Then, as we shall show, it turns out that if χ_μ^l is expanded in powers of w_3, corresponding to movement in the internal space away from the boundary in the direction of increasing w_3, then the first nonvanishing power is $w_3^{|\mu|}$, and subsequently only every other power occurs in the Taylor series, $w_3^{|\mu|+2n}$, $n=1,2,\ldots$.

The converse is also true: if χ_k^l satisfies these two properties at a collinear shape (not the triple collision), then the external wave function Ψ_m^l is analytic. Obviously, these boundary conditions are like those of the planar two-body problem at $r=0$, with w_3 playing the role of r. We have also proved the (plausible) fact that at configurations that are not at the boundary of the internal space (noncollinear configurations), the external wave function Ψ_m^l is analytic if and only if χ_k^l is analytic. This concludes the summary of our main results.

In current practice it seems that when questions of boundary conditions of three-body internal wave functions have arisen it has been assumed that the wave functions of interest have the same leading order behavior near the boundary as that of the hyperspherical harmonics. This in fact is usually true, but we know of no study that proves this in a general context or that otherwise is devoted specifically to the boundary conditions themselves. In our work the boundary conditions have been derived rigorously and to all orders. We would especially like to point out that our results were obtained on the basis of analyticity and symmetry arguments alone, and that they are independent of the Hamiltonian and applicable to all reasonable coordinate systems and choices of body frame.

The outline of this paper is as follows. Section II contains the main result of the paper, Theorem 1, which concerns the boundary conditions satisfied by the internal wave function. We have stated this theorem in as nontechnical language as possible. Section II also contains a description of how the boundary conditions are to be applied and discusses several explicit conventions for internal coordinates and body frame. Sections III and IV are more technical, and are devoted to proving Theorem 1. Section III states and proves boundary conditions for the simpler case of the planar two-body problem. Section IV uses the results of Sec. III to prove the conditions for the three-body problem. Section V contains the conclusions. An Appendix collecting several facts about the representations of $SO(2)$ is included for reference.

II. THE THREE-BODY BOUNDARY CONDITIONS

A. Review of three-body formalism

Before stating the boundary conditions on three-body wave functions, we review some necessary facts about the three-body problem. We closely follow the notation and spirit of Littlejohn and Reinsch [3]. A three-body configuration in the center of mass frame is described by two (mass-weighted) Jacobi vectors $\mathbf{r}_{s\alpha}$, $\alpha=1,2$. Jacobi vectors are a standard topic in n-body problems [22,3]. The s subscript indicates that $\mathbf{r}_{s\alpha}$ is referred to the space, or laboratory, frame. For obvious reasons, we will call the space of Jacobi vectors ''configuration space.''

It is often convenient to specify a configuration by its shape and orientation. By the shape, we mean the configuration modulo physical rotations; it is parameterized by three rotationally invariant quantities (called internal, or shape, coordinates). We will denote shape coordinates in general by q_μ, $\mu=1,2,3$. A specific and particularly useful set of such coordinates is (w_1,w_2,w_3) (henceforth called the ''w-coordinates'') defined by

$$w_1=r_{s1}^2-r_{s2}^2=\rho^2\cos 2\Theta\cos 2\Phi, \tag{2.1}$$

$$w_2=2\mathbf{r}_{s1}\cdot\mathbf{r}_{s2}=\rho^2\cos 2\Theta\sin 2\Phi, \tag{2.2}$$

$$w_3=2|\mathbf{r}_{s1}\times\mathbf{r}_{s2}|=\rho^2\sin 2\Theta, \tag{2.3}$$

where we have expressed the w-coordinates both in terms of the Jacobi vectors and in terms of Smith's [21,23] symmetric hyperspherical coordinates (ρ,Θ,Φ). Here $\rho=(r_{s1}^2+r_{s2}^2)^{1/2}$ is the hyperradius. The w-coordinates have been used by many researchers over the years, including Gronwall [24], Smith [21], Dragt [25], Iwai [26], Aquilanti *et al.* [23], and others. The w-coordinates have ranges $-\infty<w_1$, $w_2<\infty$, $0\leqslant w_3<\infty$ and are in one-to-one correspondence with three-body shapes. Thus shape space is the closed half-space containing the physical region of coordinate space $w_3\geqslant 0$. Sometimes it will also be convenient to consider the region of coordinate space $w_3<0$, which we call the unphysical region. The boundary plane $w_3=0$ consists of all collinear shapes. The boundary conditions to be presented below occur along this plane. We define $w=(w_1^2+w_2^2+w_3^2)^{1/2}$ to be the ''radius'' in $w_1w_2w_3$-space and note the identity,

$$w=(w_1^2+w_2^2+w_3^2)^{1/2}=\rho^2. \tag{2.4}$$

The origin $w=0$ is the three-body collision and is an especially singular point.

The orientation of a configuration is defined relative to some convention for body frame. A body frame convention may be defined by specifying the functions $\mathbf{r}_\alpha(q)$, where $\mathbf{r}_\alpha$ represents the body components of the Jacobi vectors and where q represents an arbitrary shape. [Equivalently, q stands for (q_1,q_2,q_3)]. Our rule is to attach an s subscript to quantities referred to the space frame, and to omit this subscript for quantities referred to the body frame. The quantities $\mathbf{r}_\alpha(q)$ can also be thought of as specifying a reference orientation for a given shape q, relative to which other orientations of the same shape are referred. In the reference orientation, the space frame is identical to the body frame. The orientation of the configuration is defined as the rotation matrix $\mathsf{R}\in SO(3)$ which rotates the reference configuration into the actual configuration,

$$\mathbf{r}_{s\alpha}=\mathsf{R}\mathbf{r}_\alpha(q). \tag{2.5}$$

We discuss several common choices of body frame in Sec. II C, but for now we leave the body frame unspecified.

For collinear shapes, R is not uniquely determined by Eq. (2.5) and there is no unique body frame associated with a particular choice of reference orientation. Nevertheless, the functions $\mathbf{r}_\alpha(q)$ are normally well defined at collinear shapes, and the assignment of a reference orientation for a collinear shape will prove to be a useful concept. We will have more to say in Sec. II B about the singular nature of the body frame at collinear shapes.

We now turn to the three-body wave function Ψ and give a quick derivation of Eq. (1.1) from angular momentaum theory. The wave function Ψ depends on the two Jacobi vectors $\mathbf{r}_{s\alpha}$. Rotations act on such wave functions by

$$(\mathcal{R}(\mathsf{Q})\Psi)(\mathbf{r}_{s\alpha})=\Psi(\mathsf{Q}^T\mathbf{r}_{s\alpha}), \tag{2.6}$$

where $\mathcal{R}$ is the rotation operator parameterized by the rotation matrix $\mathsf{Q}\in SO(3)$, and T is the transpose. We consider a collection of $2l+1$ wave functions Ψ^l_m, $-l\leqslant m\leqslant l$, with definite total angular momentum l and transforming under the action of $SO(3)$ via the standard representation,

$$\Psi^l_m(\mathsf{Q}^T\mathbf{r}_{s\alpha})=(\mathcal{R}(\mathsf{Q})\Psi^l_m)(\mathbf{r}_{s\alpha})=\sum_k \mathcal{D}^l_{km}(\mathsf{Q})\Psi^l_k(\mathbf{r}_{s\alpha}), \tag{2.7}$$

where $\mathcal{D}^l_{km}(\mathsf{Q})$ is the Wigner rotation matrix of Q. We use the (active) conventions of Messiah [15] and Biedenharn and Louck [27]. We define the internal wave function by

$$\chi^l_k(q)=\Psi^l_k(\mathbf{r}_\alpha(q)). \tag{2.8}$$

The internal wave function is a multicomponent wave function which we call a ''spinor.'' The spinor index is k, $-l\leqslant k\leqslant l$. Using Eqs. (2.5), (2.7), and (2.8) we obtain the final result

$$\Psi^l_m(\mathbf{r}_{s\alpha})=\Psi^l_m(\mathsf{R}\mathbf{r}_\alpha(q))=\sum_k \mathcal{D}^{l*}_{mk}(\mathsf{R})\chi^l_k(q). \tag{2.9}$$

The importance of Eq. (2.9) is that it completes the one-to-one correspondence between the external and internal wave functions. Equation (2.8) gives the internal wave function in terms of the external wave function while Eq. (2.9) gives the external wave function in terms of the internal wave function. One must realize, however, that all $2l+1$ components of χ^l_k must be specified to construct Ψ^l_m, whereas only one Ψ^l_m is needed to construct χ^l_k. This is because the different Ψ^l_m's are not independent but related by raising and lowering operations, whereas the χ^l_k's are not.

B. Statement of boundary conditions

We now turn to the principal question addressed in this paper: What are necessary and sufficient conditions on the internal wave function $\chi^l_k(q)$ that ensure that the external wave function $\Psi^l_m(\mathbf{r}_{s\alpha})$ is analytic? Naively, one might expect the only condition to be that $\chi^l_k(q)$ is itself analytic, but this is not sufficient as we now explain.

First, we review some fundamental issues regarding analyticity. Further clarification of these points may be found in any basic reference on differential geometry, for example Refs. [28] and [29]. To say that a function of several variables is analytic at a point means that the function agrees with its Taylor series in a neighborhood of that point. To say that a function defined on a smooth manifold is analytic at a point means that the function, when represented in a suitable choice of coordinates, is an analytic function of those coordinates at that point. The choice of coordinates is critical since a function analytic with respect to one set of coordinates may not be analytic with respect to another. Thus, whenever we say that a function defined on a smooth manifold is analytic, we must be careful to say with respect to what set of coordinates. Now, if two sets of coordinates are related to one another by an invertible analytic function (with analytic inverse) then these two sets of coordinates are said (in standard mathematical terminology) to be ''compatible.'' A function analytic with respect to one set of coordinates is also analytic with respect to a compatible set of coordinates. Thus, the analyticity of a function is defined relative to an entire set of compatible coordinates.

As an example, consider the plane $\mathbb{R}^2$, and take the standard (x,y) coordinates as the privileged coordinates defining analyticity. Polar coordinates (r,θ) are compatible with (x,y) everywhere except at the origin (and on a radial line). Thus, a function such as $f(r,\theta)=r$ which is an analytic function of the polar coordinates may still not be an analytic function at the origin of $\mathbb{R}^2$. One needs additional boundary conditions at the origin to guarantee that a function analytic in polar coordinates is truly analytic on $\mathbb{R}^2$. This example contains the core idea of why boundary conditions may be needed to guarantee analyticity of a function. We explore this example further in Sec. III.

When considering the three-body wave function Ψ^l_m, we take the privileged set of coordinates defining analyticity to be the Jacobi coordinates $r_{s\alpha k}, \alpha=1,2, k=x,y,z$. The reason for choosing these coordinates is that in practice the potential energy and the wave functions are typically analytic (except at collisions) with respect to these coordinates. So long as

one only uses Jacobi coordinates, this fact is sufficient and the rest of this paper could be skipped. However, as already pointed out, a shape and orientation description of configuration space is often advantageous and this naturally involves expressing Ψ^l_m in shape and orientation coordinates as in Eq. (2.9). An important fact is that shape and orientation coordinate are never compatible at collinear shapes, because the rotation matrix R is not defined by Eq. (2.5). This is much like the relation between rectangular and polar coordinates at the origin of the plane, discussed earlier, and it explains why the analyticity of χ^l_k alone is not sufficient to guarantee the analyticity of Ψ^l_m at collinear shapes.

We will also be interested in the analyticity of functions defined on the internal space (such as the internal wave function χ^l_k). We have found it most useful to take the w-coordinates as the privileged coordinate system with respect to which the analyticity of such functions is defined. All internal coordinate systems in common use are compatible with the w-coordinates at most locations in shape space. On the internal space there is the additional issue of what we mean by analyticity at the boundary $w_3=0$. We will say that a function defined on the internal space is analytic at a particular point on the boundary if the function has an analytic continuation into the nonphysical region $w_3<0$ in the neighborhood of that point.

The analyticity of the functions $\mathbf{r}_\alpha(q)$ requires special comment. These functions have singularities on certain curves (''strings'') in $w_1w_2w_3$-space, which emanate from the three-body collision $w=0$ and go out to infinity. The location of these strings depends on the convention for body frame [18–20]. In the following we wish to work with body frame conventions that remove the strings from the region of interest in the internal space.

The reader may wonder about the analyticity of the Euler angles, or of functions of them. As it turns out, we never need to worry about such issues, because the main result of this paper, which is the establishment of necessary and sufficient conditions for the analyticity of Ψ^l_m, only involves the analytic properties of χ^l_k. The results we prove below are valid for arbitrary conventions for Euler angles.

Turning away now from general notions of analyticity, we observe that at a collinear shape, which is not the triple collision, there is a well-defined (up to sign) unit vector, denoted by $\hat{\mathbf{n}}$, pointing along the body-referred axis of collinearity. The vector $\hat{\mathbf{n}}$ depends on the position along the boundary plane and is undefined off of the plane. We therefore choose a convention for extending $\hat{\mathbf{n}}$ off of the boundary plane. That is, we choose a function $\hat{\mathbf{n}}(q)$, defined on shape space, which points along the collinear axis when evaluated at a collinear shape. When evaluated at a noncollinear shape, we only require that $\hat{\mathbf{n}}(q)$ lie in the plane spanned by $\mathbf{r}_1(q)$ and $\mathbf{r}_2(q)$.

We now introduce a certain basis of spinors $\tau_\mu(q)$, $-l\leqslant\mu\leqslant l$, which are eigenspinors of the projection $\hat{\mathbf{n}}(q)\cdot\mathbf{L}$ of the body-referred angular momentum operator $\mathbf{L}$ onto the collinear axis. These spinors are chosen to satisfy

$$(\hat{\mathbf{n}}\cdot\mathbf{L})\tau_\mu=\mu\tau_\mu, \tag{2.10}$$

$$\tau^\dagger_\mu\tau_{\mu'}=\sum_k (\tau_\mu)^*_k(\tau_{\mu'})_k=\delta_{\mu\mu'}, \tag{2.11}$$

where † represents the Hermitian conjugate. Here the μ subscript does not index the components of τ_μ but rather labels the spinor; the $2l+1$ components themselves are denoted by $(\tau_\mu)_k$, $-l\leqslant k\leqslant l$ and are taken with respect to the normalized eigenbasis of L_z, using standard phase conventions. Notice that Eqs. (2.10) and (2.11) determine $\tau_\mu(q)$ only up to an overall phase, which is another convention we have the freedom to choose. We define an alternative version of the internal wave function by

$$\chi^l_\mu=\tau^\dagger_\mu\chi^l=\sum_k (\tau_\mu)^*_k\chi^l_k, \tag{2.12}$$

where χ^l is the column vector $(\chi^l_{-l},\ldots,\chi^l_l)^T$. Since the spinors τ_μ are orthonormal, Eq. (2.12) may be inverted to give

$$\chi^l_k=\sum_\mu (\tau_\mu)_k\chi^l_\mu. \tag{2.13}$$

Given some region of interest in the internal space, there are conventions involved in choosing the coordinates q_μ, the functions $\mathbf{r}_\alpha(q)$, which specify the reference orientations, the function $\hat{\mathbf{n}}(q)$, which extends the collinear axis away from the boundary, and the spinors $\tau_\mu(q)$. We will be particularly interested in a certain class of conventions which taken together we call ''valid'' conventions. At a noncollinear shape, a set of conventions is said to be valid if q_μ is compatible with the w-coordinates and the functions $\mathbf{r}_\alpha(q)$, $\hat{\mathbf{n}}(q)$, and $(\tau_\mu)_k(q)$ are analytic. In particular, this means that the shape in question does not lie on a string singularity. At a collinear shape, we still require the compatibility of the internal coordinates with the w-coordinates and the analyticity of $\mathbf{r}_\alpha(q)$, $\hat{\mathbf{n}}(q)$, and $(\tau_\mu)_k(q)$. However, we further require that the boundary plane be given by $q_3=0$. We also require that various functions be either even or odd. Specifically,

$$q_\mu(-w_3)=q_\mu(w_3),\quad \mu=1,2, \tag{2.14}$$

$$q_3(-w_3)=-q_3(w_3), \tag{2.15}$$

$$(\hat{\mathbf{n}}\cdot\mathbf{r}_\alpha)(-q_3)=(\hat{\mathbf{n}}\cdot\mathbf{r}_\alpha)(q_3), \tag{2.16}$$

$$(\mathsf{P}_\perp\mathbf{r}_\alpha)(-q_3)=-(\mathsf{P}_\perp\mathbf{r}_\alpha)(q_3), \tag{2.17}$$

$$\hat{\mathbf{n}}(-q_3)=\hat{\mathbf{n}}(q_3), \tag{2.18}$$

$$(\tau_\mu)_k(-q_3)=(\tau_\mu)_k(q_3), \tag{2.19}$$

where we have suppressed the dependence on w_1, w_2, q_1, and q_2 and where $\mathsf{P}_\perp(q)$ denotes the projection operator onto the plane orthogonal to $\hat{\mathbf{n}}(q)$.

With the preceding setup, we state the main result of this paper.

Theorem 1. Let a configuration $\mathbf{r}_{s\alpha}$ (which is not the triple collision) have shape q, and assume valid conventions for the

shape coordinates q_μ, the reference orientation $\mathbf{r}_\alpha(q)$, the vector $\hat{\mathbf{n}}(q)$, and the spinor $\tau_\mu(q)$ in the neighborhood of q.
(i) If q is noncollinear, then Ψ^l_m is analytic at $\mathbf{r}_{s\alpha}$ if and only if χ^l_μ (equivalently χ^l_k) is analytic at q.
(ii) If q is collinear, then Ψ^l_m is analytic at $\mathbf{r}_{s\alpha}$ if and only if χ^l_μ (equivalently χ^l_k) is analytic at q with the Taylor series

$$\chi^l_\mu(q_1,q_2,q_3)=\sum_{n=0}^{\infty} a_{\mu n}(q_1,q_2)q_3^{|\mu|+2n}, \qquad (2.20)$$

where $a_{\mu n}$ is an analytic function of (q_1,q_2).

The most striking aspect of this theorem is that the wave function grows as $q_3^{|\mu|}$ away from the collinear shapes. We can provide the following heuristic physical interpretation of this rule. If a classical three-body system, under the influence of a smooth potential, approaches a collinear configuration, any angular momentum about the collinear axis will create a centrifugal barrier that prevents the system from reaching the collinear configuration. Quantum mechanically, the centrifugal barrier acts to suppress the wave function in the classically forbidden region. The more quanta of angular momentum about the collinear axis, the more the wave function is suppressed resulting in the $q_3^{|\mu|}$ growth. This interpretation is dynamical in nature since it depends on the notion of a Hamiltonian. We stress, however, that the derivation of Theorem 1 will depend only on notions of analyticity and symmetry.

C. Explicit examples of boundary conditions

We analyze the boundary conditions explicitly for several common choices of valid conventions. Our purpose is to illustrate the general theory with some familiar conventions and to show how some well-known properties of certain internal wave functions, such as hyperspherical harmonics, come about. Of course, the properties we derive apply to any internal wave function for which the external wave function is analytic.

The first example uses the w-coordinates and a body frame which coincides with the principal axes. The body-referred Jacobi vectors are given parametrically by

$$\mathbf{r}_1(w_1,w_2,w_3)=\left[\frac{a+b}{2\sqrt{2}}\left(1+\frac{w_1}{ab}\right)^{1/2}\frac{w_2}{|w_2|}\right]\hat{\mathbf{z}} -\left[\frac{a-b}{2\sqrt{2}}\left(1-\frac{w_1}{ab}\right)^{1/2}\right]\hat{\mathbf{x}}, \qquad (2.21)$$

$$\mathbf{r}_2(w_1,w_2,w_3)=\left[\frac{a+b}{2\sqrt{2}}\left(1-\frac{w_1}{ab}\right)^{1/2}\right]\hat{\mathbf{z}} +\left[\frac{a-b}{2\sqrt{2}}\left(1+\frac{w_1}{ab}\right)^{1/2}\frac{w_2}{|w_2|}\right]\hat{\mathbf{x}}, \qquad (2.22)$$

$$a=\sqrt{w+w_3}, \qquad (2.23)$$

$$b=\sqrt{w-w_3}. \qquad (2.24)$$

Since the collinear axis for a collinear shape is given by $\hat{\mathbf{n}}(w_1,w_2)=\hat{\mathbf{z}}$, we define the extension to noncollinear shapes by

$$\hat{\mathbf{n}}(w_1,w_2,w_3)=\hat{\mathbf{z}}. \qquad (2.25)$$

Equations (2.21) and (2.22) exhibit a discontinuity in the function $\mathbf{r}_\alpha(w_1,w_2,w_3)$ along the w_3 axis. In fact the reference orientation approaches a continuum of different values, depending on the direction of approach. The w_3 axis forms the string singularity of the principal axis frame. This string consists of oblate symmetric tops, and the discontinuity there is a direct result of the ambiguity in the choice of the principal axes due to the degeneracy of the principal moments of inertia. Another singularity occurs in the principal axis frame, arising from the double-valued nature of the frame. Upon circling the w_3 axis once, the principal axis frame does not return to its original value, but rather has rotated by π. Thus, to make the principal-axis frame single-valued requires introducing a branch cut. In Eqs. (2.21) and (2.22), we have chosen this branch cut to be the two-dimensional surface $w_2=0$, $w_1>0$. Such string singularities and branch cuts are common to other choices of body frame as well and are discussed further in Ref. [18].

We comment briefly on the validity of the conventions introduced here. The w-coordinates are trivially valid everywhere, with the w_3 coordinate being transverse to the collinear shapes. The function $\hat{\mathbf{n}}(q)=\hat{\mathbf{z}}$ is constant and hence analytic everywhere. It obviously satisfies Eq. (2.18) as well. Away from the frame singularities discussed above, $\mathbf{r}_\alpha(q)$ is analytic, and it is straightforward to show that Eqs. (2.16) and (2.17) are satisfied. From Eq. (2.25) we may take $(\tau_\mu)_k(q)=\delta_{\mu k}$, which is clearly analytic and satisfies Eq. (2.19). Hence these conventions are valid everywhere except at the frame singularities.

Away from the frame singularities and away from the boundary of shape space, Theorem 1 tells us that analyticity of $\chi^l_k(q)$ is a necessary and sufficient condition for analyticity of $\Psi^l_m(\mathbf{r}_{s\alpha})$. In order to guarantee analyticity of $\Psi^l_m(\mathbf{r}_{s\alpha})$ on the boundary of shape space (away from the positive w_1 axis where there is a frame singularity), $\chi^l_k(q)$ must have the Taylor series

$$\chi^l_k(w_1,w_2,w_3)=\sum_{n=0}^{\infty} a_{kn}(w_1,w_2)w_3^{|k|+2n}, \qquad (2.26)$$

where of course $a_{kn}(w_1,w_2)$ is analytic.

In the next example, we keep the principal axis frame, but change coordinates from the w-coordinates to the symmetric hyperspherical coordinates (ρ, Φ, Θ) defined in Eqs. (2.1)–(2.3). The coordinate Θ is transverse to the boundary of shape space that occurs at $\Theta=0$. These hyperspherical coordinates are compatible everywhere except the w_3 axis and the two-dimensional surface $w_2=0$, $w_1>0$, where they experience a coordinate singularity. Note that the location of the coordinate singularities agrees exactly with the location of the singularities in the principal axis frame. We again choose $\hat{\mathbf{n}}(q)=\hat{\mathbf{z}}$ and $(\tau_\mu)_k=\delta_{\mu k}$. It is again true that the conventions are valid everywhere except at the frame singu-

larities. Little modification to the form of Eq. (2.26) is necessary except to change the coordinates, which gives

$$\chi_k^l(\rho,\Phi,\Theta)=\sum_{n=0}^{\infty} a_{kn}(\rho,\Phi)\Theta^{|k|+2n}. \tag{2.27}$$

Of course, the coefficients $a_{kn}(\rho,\Phi)$ in the above equation are different from those in Eq. (2.26). The form of the wave function in Eq. (2.27) can be witnessed in the results of Wolniewicz [30] for hypershperical harmonics in the symmetric representation.

In the next example, we again use the w-coordinates but choose a different body frame, called the *zxz* frame in Ref. [3] or the $\mathrm{BF}_{\tau 1}$ frame in Ref. [20]. This frame places $\mathbf{r}_1$ along the positive z axis and $\mathbf{r}_2$ in the xz plane. Explicitly, the reference configuration $\mathbf{r}_\alpha(w_1,w_2,w_3)$ for the *zxz* frame is

$$\mathbf{r}_1(w_1,w_2,w_3)=(1/\sqrt{2})(w+w_1)^{1/2}\hat{\mathbf{z}}, \tag{2.28}$$

$$\mathbf{r}_2(w_1,w_2,w_3)=(1/\sqrt{2})\frac{1}{(w+w_1)^{1/2}}(w_3\hat{\mathbf{x}}+w_2\hat{\mathbf{z}}). \tag{2.29}$$

We again take $\hat{\mathbf{n}}(q)=\hat{\mathbf{z}}$ and $(\tau_\mu)_k(q)=\delta_{\mu k}$, and it is easy to see that Eqs. (2.14)–(2.19) are again satisfied. Equations (2.28) and (2.29) exhibit a string singularity on the negative w_1 axis, which consists of shapes satisfying $\mathbf{r}_1=0$. Intuitively, we explain the location of the string by the following observation: if $\mathbf{r}_1=0$, then the orientation of $\mathbf{r}_2$ within the xz plane is not fixed. The conventions are valid everywhere off of the string; there is no branch cut for the *zxz* frame as there was for the principal axis frame. The Taylor series given in Eq. (2.26) is again applicable for the present conventions. Of course the coefficients $a_{kn}(w_1,w_2)$ are different here and the domain of validity is also different.

In the next example, we continue to use the *zxz* frame, $\hat{\mathbf{n}}(q)=\hat{\mathbf{z}}$, and $(\tau_\mu)_k(q)=\delta_{\mu k}$, but use a different set of hyperspherical coordinates (ρ,ζ,θ) defined by

$$w_1=\rho^2\sin 2\zeta, \tag{2.30}$$

$$w_2=\rho^2\cos 2\zeta\cos\theta, \tag{2.31}$$

$$w_3=\rho^2\cos 2\zeta\sin\theta. \tag{2.32}$$

These are the asymmetric hyperspherical coordinates of Smith [21,23]. They are compatible everywhere in the physical region except on the w_1 axis, where there is a coordinate singularity. Notice that this coordinate singularity includes the singularities in the *zxz* frame, which occur on the negative w_1 axis. The coordinate θ is transverse to the collinear shapes, which occur at both $\theta=0$ and $\theta=\pi$. We concentrate on the boundary $\theta=0$ first. Since the conventions are valid over the entire half-plane $\theta=0$, the Taylor series

$$\chi_k^l(\rho,\zeta,\theta)=\sum_{n=0}^{\infty} a_{kn}(\rho,\zeta)\theta^{|k|+2n} \tag{2.33}$$

is sufficient to guarantee analyticity of the external wave function. With regards to the half-plane $\theta=\pi$, by our definition the conventions are not valid there because we require the boundary be given by $q_3=0$. Nevertheless, by using new coordinates $(\rho,\zeta,\theta'=\pi-\theta)$, the conventions are valid on this half-plane. If the external wave function is to be analytic on this half-plane, χ_k^l must satisfy a Taylor series in θ' identical in form to Eq. (2.33) for θ. One set of functions that do satisfy the appropriate conditions at both $\theta=0$ and $\theta=\pi$ are the associated Legendre polynomials $P_k^l(\theta)$. An internal wave function $\chi_k^l(\rho,\zeta,\theta)=b_k(\rho,\zeta)P_k^l(\theta)$, with $b_k(\rho,\zeta)$ analytic, therefore lifts to an analytic external wave function (in the region of validity). Internal wave functions of this form arise naturally when constructing hyperspherical harmonics. (See, for example, Aquilanti *et al.* [5,4].)

III. THE PLANAR TWO-BODY PROBLEM

Before proving the theorem on three-body boundary conditions, we discuss the two-body problem in the plane. Not only is this simpler case useful practice for the three-body problem, but in fact our proof of the three-body results relies on the the two-body results presented here.

First, we must adapt the basic concepts and notation introduced for the three-body problem for use with the two-body problem. The configuration space of a two-body system, in the center of mass frame, is just the two-dimensional plane, the relative position of one body with respect to the other being denoted here as $\mathbf{r}_s\in\mathbb{R}^2$. The shape of the two-body system depends only on the separation distance r between the bodies, and we denote the shape coordinate by $q(r)$. We assign to each shape q a reference orientation $\mathbf{r}(q)$. The reference orientation $\mathbf{r}(q)$ is simply a point on the circle of radius $r(q)$ centered at the origin of $\mathbb{R}^2$. This fact makes the reference orientations much easier to visualize here than for the three-body problem; the reference orientations all lie on a curve beginning at the origin and intersecting each concentric circle once as it moves out to infinity. An arbitrary configuration $\mathbf{r}_s$ is given by

$$\mathbf{r}_s=\mathsf{R}\mathbf{r}(q), \tag{3.1}$$

where $\mathsf{R}\in SO(2)$ denotes the orientation of the system. We will denote the rotation angle of R by θ.

As an example, one could choose the internal coordinate to be $q(r)=r$ and the reference orientation to be

$$\mathbf{r}(r)=r\hat{\mathbf{x}}. \tag{3.2}$$

This choice produces shape and orientation coordinates (r,θ), which are the usual polar coordinates on $\mathbb{R}^2$.

We now discuss the two-body wave function Ψ. The action of $\mathsf{Q}\in SO(2)$ on Ψ is

$$(\mathcal{R}(\mathsf{Q})\Psi)(\mathbf{r}_s)=\Psi(\mathsf{Q}^T\mathbf{r}_s). \tag{3.3}$$

We denote by Ψ_m a wave function which transforms according to the irrep m of $SO(2)$,

$$\Psi_m(\mathsf{Q}^T\mathbf{r}_s)=(\mathcal{R}(\mathsf{Q})\Psi_m)(\mathbf{r}_s)=e^{-im\alpha}\Psi_m(\mathbf{r}_s), \tag{3.4}$$

where α is the rotation angle of Q. The internal wave function $\chi_m(q)$ is defined by

$$\chi_m(q)=\Psi_m(\mathbf{r}(q)). \tag{3.5}$$

Given $\chi_m(q)$ we may recover the external wave function $\Psi_m(\mathbf{r}_s)$ with the aid of Eqs. (3.1), (3.4), and (3.5),

$$\Psi_m(\mathbf{r}_s)=\Psi_m(\mathsf{R}\mathbf{r}(q))=e^{im\theta}\chi_n(q). \tag{3.6}$$

Equations (3.3)–(3.6) are obviously analogous to Eqs. (2.6)–(2.9) for the three-body problem.

We take the Cartesian coordinates (r_{sx},r_{sy}) [that is, the usual space-fixed (x,y)] as the privileged coordinates for defining analyticity of functions on configuration space. We take the radial coordinate r as the privileged coordinate for defining analyticity of functions on shape space. Since r is a positive quantity, we must give special consideration to the boundary $r=0$. A function on shape space is said to be analytic at $r=0$ if it can be analytically continued (as a function of r) into the region $r<0$.

For the three-body problem, there were four different conventions that had to be specified. For the two-body problem, we need only specify two conventions: the shape coordinate q and the reference orientation $\mathbf{r}(q)$; there is no analog of $\hat{\mathbf{n}}(q)$ or $\tau_\mu(q)$ for the two-body problem. Away from the two-body collision, these two conventions are said to be ''valid'' if the shape coordinate q is compatible with r and if $\mathbf{r}(q)$ is analytic. At the two-body collision, q must still be compatible with r and $\mathbf{r}(q)$ must still be analytic. However, we also require that $q=0$ coincide with the two-body collision and that the following conditions be met

$$q(-r)=-q(r), \tag{3.7}$$

$$\mathbf{r}(-q)=-\mathbf{r}(q). \tag{3.8}$$

We now state the following two-body theorem, which is analogous to Theorem 1 for the three-body problem.

Theorem 2. Let a configuration $\mathbf{r}_s$ have shape q, and assume valid conventions for the shape coordinate q and the reference orientation $\mathbf{r}(q)$ in the neighborhood of q.
(i) If $q\neq 0$, then Ψ_m is analytic at $\mathbf{r}_s$ if and only if χ_m is analytic at q.
(ii) If $q=0$, then Ψ_m is analytic at $\mathbf{r}_s=0$ if and only if χ_m is analytic at 0 with the Taylor series

$$\chi_m(q)=\sum_{n=0}^{\infty} a_{mn}q^{|m|+2n}, \tag{3.9}$$

where the a_{mn} are constant complex coefficients.

Proof. For the entirety of this proof, when we say that a function of either the Cartesian coordinates or shape coordinate is analytic, we mean only that it is locally analytic at the specific points, $\mathbf{r}_s$ or q respectively, mentioned in the statement of the theorem.

Equation (3.4) shows that if Ψ_m is analytic at an arbitrary $\mathbf{r}_s$, then Ψ_m is analytic at any other orientation $\mathsf{Q}^T\mathbf{r}_s$ with $\mathsf{Q}\in SO(2)$ arbitrary. We therefore assume without loss that the specific configuration $\mathbf{r}_s$ in the statement of the Theorem is the reference orientation $\mathbf{r}$.

(i) Assume $q\neq 0$. Assume $\Psi_m(\mathbf{r}_{s\alpha})$ is analytic. From Eq. (3.5), the fact that $\mathbf{r}(q)$ is analytic, and the fact that the composition of analytic functions is analytic, $\chi_m(q)$ is analytic.

Next assume $\chi_m(q)$ is analytic. By the assumption of compatibility, $q(r)$ is analytic. Furthermore, $r(\mathbf{r}_s)=(r_{sx}^2+r_{sy}^2)^{1/2}$ is an analytic function of the Cartesian coordinates. Hence, $q(\mathbf{r}_s)=q(r(\mathbf{r}_s))$ is analytic. Turning to the rotation matrix R in Eq. (3.1), its rotation angle θ is given by $\theta(\mathbf{r}_s,\mathbf{r})=\arcsin\,(\hat{\mathbf{z}}\cdot(\mathbf{r}\times\mathbf{r}_s/r^2))$, which is an analytic function of $\mathbf{r}_s$ and $\mathbf{r}$. (We only consider θ in the range $-\pi/2<\theta<\pi/2$ since we are only checking for analyticity at the reference orientation $\theta=0$.) Furthermore, $\mathbf{r}(\mathbf{r}_s)=\mathbf{r}(q(\mathbf{r}_s))$ is analytic since $\mathbf{r}(q)$ is analytic by the validity assumption and $q(\mathbf{r}_s)$ was shown to be analytic above. Hence,

$$\theta(\mathbf{r}_s)=\theta(\mathbf{r}_s,\mathbf{r}(\mathbf{r}_s)) \tag{3.10}$$

is analytic. Since $\exp(im\theta)$ is an analytic function of θ, we conclude that

$$\Psi_m(\mathbf{r}_s)=e^{im\theta(\mathbf{r}_s)}\chi_m(q(\mathbf{r}_s)) \tag{3.11}$$

is an analytic function of the Cartesian coordinates.

(ii) Assume $q=0$. Assume $\Psi_m(\mathbf{r}_{s\alpha})$ is analytic. By the same argument as in case (i), $\chi_m(q)$ is analytic at $q=0$. To prove Eq. (3.9), we differentiate Eq. (3.4) d times with respect to $\mathbf{r}_s$,

$$\sum_{k_1\ldots k_d} Q_{j_1k_1}\ldots Q_{j_dk_d}\left(\frac{\partial}{\partial r_{sk_1}}\cdots\frac{\partial}{\partial r_{sk_d}}\Psi_m\right)(\mathsf{Q}^T\mathbf{r}_s)$$
$$=e^{-im\alpha}\left(\frac{\partial}{\partial r_{sj_1}}\cdots\frac{\partial}{\partial r_{sj_d}}\Psi_m\right)(\mathbf{r}_s), \tag{3.12}$$

where Q_{jk}, $j,k=x,y$, are the components of Q. Evaluating Eq. (3.12) at $\mathbf{r}_s=0$ produces

$$\sum_{k_1\ldots k_d} Q_{j_1k_1}\ldots Q_{j_dk_d}\left(\frac{\partial}{\partial r_{sk_1}}\cdots\frac{\partial}{\partial r_{sk_d}}\Psi_m\right)(0)$$
$$=e^{-im\alpha}\left(\frac{\partial}{\partial r_{sj_1}}\cdots\frac{\partial}{\partial r_{sj_d}}\Psi_m\right)(0). \tag{3.13}$$

Equation (3.13) shows that the rank d tensor $(\partial/\partial r_{sj_1}\ldots\partial/\partial r_{sj_d}\Psi_m)(0)$ transforms under the completely symmetrized action of $SO(2)$ as an irrep of $SO(2)$ labeled by m. (See Appendix.) The decomposition of the fully symmetrized action of $SO(2)$ on rank d tensors decomposes into irreps as shown in Eq. (A1). If m does not label one of the irreps included in Eq. (A1), that is, if $m\neq d,\ d-2,\ldots,-(d-2),-d$, then $(\partial/\partial r_{sj_1}\ldots\partial/\partial r_{sj_d}\Psi_m)(0)=0$. Consequently, the chain rule and Eq. (3.5) show that

$$\left(\frac{d^d}{dq^d}\chi_m\right)(0)=\sum_{k_1\ldots k_d}\frac{dr_{sk_1}}{dq}(0)\cdots\frac{dr_{sk_d}}{dq}(0)\times\left(\frac{\partial}{\partial r_{sk_1}}\cdots\frac{\partial}{\partial r_{sk_d}}\Psi_m\right)(0)=0 \tag{3.14}$$

when $m\neq d,d-2,\ldots,-(d-2),-d$. This shows that the appropriate Taylor coefficients vanish in order to produce the Taylor series in Eq. (3.9).

Now assume that χ_m is analytic at $q=0$ with Taylor series shown in Eq. (3.9). We first complete the proof of Theorem 2 assuming the internal coordinate $q(r)=r$ and the reference configuration $\mathbf{r}(r)=r\hat{\mathbf{x}}$. We explicitly construct a function $\tilde{\Psi}_m(\mathbf{r}_s)$ by

$$\tilde{\Psi}_m(\mathbf{r}_s)=\sum_{n=0}^{\infty}\sum_{k_1\ldots k_{|m|+2n}}\times a_{mn}(t_m^{|m|+2n})_{k_1\ldots k_{|m|+2n}}r_{sk_1}\ldots r_{sk_{|m|+2n}}, \tag{3.15}$$

where the a_{mn} are the same Taylor coefficients as in Eq. (3.9) and the $t_m^{|m|+2n}$ are the rank $|m|+2n$ tensors defined by Eq. (A2). Clearly the transformation property Eq. (A3) of the $t_m^{|m|+2n}$ shows that $\tilde{\Psi}_m$ satisfies Eq. (3.4). Hence, we may apply the same analysis to $\tilde{\Psi}_m$ as we have for Ψ_m. In particular, $\tilde{\Psi}_m$ is uniquely determined via Eq. (3.6) by the internal wave function $\tilde{\chi}_m$ defined by Eq. (3.5)

$$\tilde{\chi}_m(r)=\tilde{\Psi}_m(r\hat{\mathbf{x}})=\sum_{n=0}^{\infty}a_{mn}r^{|m|+2n}, \tag{3.16}$$

where we have used Eqs. (3.15) and (A4). Since χ_m and $\tilde{\chi}_m$ have the same Taylor series, $\chi_m=\tilde{\chi}_m$. Furthermore, the unique correspondence between internal and external wave functions guarantees that $\Psi_m=\tilde{\Psi}_m$. From Eq. (3.15), we see that $\Psi_m=\tilde{\Psi}_m$ is analytic at 0 by construction. This completes the proof of Theorem 2 for the specific conventions chosen above.

We mention two noteworthy special cases of Theorem 2, which the above analysis has now proven. First, if $f(r)$ is an even analytic function, then $f(\mathbf{r}_s)=f(r(\mathbf{r}_s))$ is an analytic function of the Cartesian coordinates. (This fact is quite trivial to prove from scratch by simply considering the Taylor series of the two functions.) Second, if $f(r)$ is an odd analytic function, then $f(\mathbf{r}_s)=f(r,\theta)=\exp(i\theta)f(r)$ is an analytic function of the Cartesian coordinates, where (r,θ) are the standard polar coordinates.

We now assume arbitrary valid conventions $\mathbf{r}(q)$ and $q(r)$ for the reference orientation and shape coordinate respectively. To complete the proof of Theorem 2 for these conventions, we first define and discuss three useful functions $\mathsf{F}(\mathbf{r}_s)$, $\mathbf{G}(\mathbf{r}_s)$, and $\mathbf{H}(\mathbf{r}_s)$ related to these conventions. By the validity assumptions, $\mathbf{r}(r)$ is an odd analytic function in the neighborhood of $r=0$, and hence $\hat{\mathbf{r}}(r)=\mathbf{r}(r)/r$ is an even analytic function in the neighborhood of $r=0$. Define the matrix-valued function $\mathsf{F}(r)$ by

$$\mathsf{F}(r)=\hat{\mathbf{x}}\hat{\mathbf{r}}^T(r)+\hat{\mathbf{y}}(\hat{\mathbf{z}}\times\hat{\mathbf{r}}(r))^T. \tag{3.17}$$

Notice that $\mathsf{F}(r)$ is the unique matrix in $SO(2)$ satisfying

$$\mathsf{F}(r)\hat{\mathbf{r}}(\mathbf{r})=\hat{\mathbf{x}}. \tag{3.18}$$

Since $\hat{\mathbf{r}}(r)$ is an even analytic function, we see from Eq. (3.17) that $\mathsf{F}(r)$ is an even analytic function. Hence, from the first of the two special cases of Theorem 2 mentioned above, $\mathsf{F}(\mathbf{r}_s)=\mathsf{F}(r(\mathbf{r}_s))$ is also analytic. Notice of course that $\mathsf{F}(\mathbf{r}_s)$ is invariant under all rotations $\mathsf{Q}\in SO(2)$,

$$\mathsf{F}(\mathsf{Q}\mathbf{r}_s)=\mathsf{F}(\mathbf{r}_s). \tag{3.19}$$

By the validity assumptions, $q(r)$ is an odd analytic function of r. Hence, from the second of the two special cases of Theorem 2 mentioned above, the function

$$G(\mathbf{r}_s)=e^{i\theta}q(r) \tag{3.20}$$

is an analytic function of the Cartesian coordinates. [Here (θ,r) are the standard polar coordinates in $\mathbb{R}^2$.] We define a vector-valued version of $G(\mathbf{r}_s)$, denoted $\mathbf{G}(\mathbf{r}_s)$, by

$$\mathbf{G}(\mathbf{r}_s)=\mathrm{Re}(G(\mathbf{r}_s))\hat{\mathbf{x}}+\mathrm{Im}(G(\mathbf{r}_s))\hat{\mathbf{y}}=q(r)\hat{\mathbf{r}}_s. \tag{3.21}$$

Obviously, $\mathbf{G}(\mathbf{r}_s)$ is also an analytic function of the Cartesian coordinates. Recall that the compatibility of the coordinate q guarantees that $q(r)$ has an inverse, which we denote by q^{-1}, that is, $q^{-1}(q(r))=r$. The function $\mathbf{G}(\mathbf{r}_s)$ therefore has an inverse given by

$$\mathbf{G}^{-1}(\mathbf{r}_s)=q^{-1}(r)\hat{\mathbf{r}}_s, \tag{3.22}$$

as may be verified by inserting this formula into Eq. (3.21). Equations (3.21) and (3.22) easily admit the following results

$$\mathbf{G}(\mathsf{Q}\mathbf{r}_s)=\mathsf{Q}\mathbf{G}(\mathbf{r}_s), \tag{3.23}$$

$$\mathbf{G}^{-1}(\mathsf{Q}\mathbf{r}_s)=\mathsf{Q}\mathbf{G}^{-1}(\mathbf{r}_s), \tag{3.24}$$

where $\mathsf{Q}\in SO(2)$ is arbitrary.

We define a new function $\mathbf{H}(\mathbf{r}_s)$ by

$$\mathbf{H}(\mathbf{r}_s)=\mathsf{F}(\mathbf{r}_s)\mathbf{G}(\mathbf{r}_s). \tag{3.25}$$

This function has several important properties. First, since both $\mathbf{G}(\mathbf{r}_s)$ and $\mathsf{F}(\mathbf{r}_s)$ are analytic, $\mathbf{H}(\mathbf{r}_s)$ is analytic. Second,

$$\mathbf{H}(\mathbf{r}(q))=\mathsf{F}(\mathbf{r}(q))\mathbf{G}(\mathbf{r}(q))=q\hat{\mathbf{x}}, \tag{3.26}$$

which follows from Eqs. (3.18) and (3.21). A third fact is that $\mathbf{H}$ is invertible. This fact requires more work to prove, which we do by explicitly constructing $\mathbf{H}^{-1}$. Let $\mathbf{r}_s'=\mathbf{H}(\mathbf{r}_s)$. Then,

$$\mathbf{r}_s=\mathbf{G}^{-1}(\mathsf{F}^{-1}(\mathbf{r}_s)\mathbf{r}_s')=\mathsf{F}^{-1}(\mathbf{r}_s)\mathbf{G}^{-1}(\mathbf{r}_s'), \tag{3.27}$$

where we use the definition of $\mathbf{H}$ and the fact that $\mathbf{G}$ is invertible in the first equality and the second equality follows from Eq. (3.24). Now, the magnitudes of $\mathbf{r}_s'$ and $\mathbf{r}_s$ are related by

$$|\mathbf{r}_s'| = |\mathsf{F}(\mathbf{r}_s)\mathbf{G}(\mathbf{r}_s)| = |\mathbf{G}(\mathbf{r}_s)| = q(|\mathbf{r}_s|), \tag{3.28}$$

where we have used Eq. (3.21) in the final equality. Turning this relation around and using Eq. (3.22) we have,

$$|\mathbf{r}_s| = q^{-1}(|\mathbf{r}_s'|) = |\mathbf{G}^{-1}(\mathbf{r}_s')|. \tag{3.29}$$

As witnessed by Eq. (3.19), $\mathsf{F}(\mathbf{r}_s)$ depends only on the magnitude of its argument, and hence Eqs. (3.27) and (3.29) combine to produce

$$\mathbf{r}_s = \mathsf{F}^{-1}(\mathbf{G}^{-1}(\mathbf{r}_s'))\mathbf{G}^{-1}(\mathbf{r}_s'), \tag{3.30}$$

which gives $\mathbf{r}_s$ in terms of $\mathbf{r}_s'$. Hence,

$$\mathbf{H}^{-1}(\mathbf{r}_s') = \mathsf{F}^{-1}(\mathbf{G}^{-1}(\mathbf{r}_s'))\mathbf{G}^{-1}(\mathbf{r}_s'). \tag{3.31}$$

Another fact regarding $\mathbf{H}$ is that if $\mathsf{Q} \in SO(2)$ is arbitrary, then

$$\begin{aligned}\mathbf{H}(\mathsf{Q}\mathbf{r}_s) &= \mathsf{F}(\mathsf{Q}\mathbf{r}_s)\mathbf{G}(\mathsf{Q}\mathbf{r}_s) = \mathsf{F}(\mathbf{r}_s)\mathsf{Q}\mathbf{G}(\mathbf{r}_s) \\ &= \mathsf{Q}\mathsf{F}(\mathbf{r}_s)\mathbf{G}(\mathbf{r}_s) = \mathsf{Q}\mathbf{H}(\mathbf{r}_s),\end{aligned} \tag{3.32}$$

where the second equality follows from Eqs. (3.19) and (3.23) and the third equality follows from the commutativity of the group $SO(2)$. From Eq. (3.32) follows an analogous identity for $\mathbf{H}^{-1}$

$$\mathbf{H}^{-1}(\mathsf{Q}\mathbf{r}_s) = \mathsf{Q}\mathbf{H}^{-1}(\mathbf{r}_s). \tag{3.33}$$

We now have the proper background to complete the proof. Since $\mathbf{H}$ is invertible, we introduce the function $\tilde{\Psi}_m$ by

$$\tilde{\Psi}_m(\mathbf{r}_s) = \Psi_m(\mathbf{H}^{-1}(\mathbf{r}_s)), \tag{3.34}$$

$$\Psi_m(\mathbf{r}_s) = \tilde{\Psi}_m(\mathbf{H}(\mathbf{r}_s)). \tag{3.35}$$

We see from Eq. (3.33) that $\tilde{\Psi}_m$ satisfies Eq. (3.4) since Ψ_m satisfies Eq. (3.4). We define the internal wave function $\tilde{\chi}_m(q)$ using the old convention $\mathbf{r}(q) = q\hat{\mathbf{x}}$,

$$\tilde{\chi}_m(q) = \tilde{\Psi}_m(q\hat{\mathbf{x}}). \tag{3.36}$$

Using the new convention $\mathbf{r}(q)$, we have $\chi_m(q)$ given by

$$\chi_m(q) = \Psi_m(\mathbf{r}(q)) = \tilde{\Psi}_m(\mathbf{H}(\mathbf{r}(q))) = \tilde{\Psi}_m(q\hat{\mathbf{x}}), \tag{3.37}$$

where the second equality follows from Eq. (3.35) and the third from Eq. (3.26). Thus, the functional form of $\chi_m(q)$ and $\tilde{\chi}_m(q)$ are identical. Since we have assumed that χ_m is analytic at $q=0$ with the Taylor series in Eq. (3.9), $\tilde{\chi}_m$ is also analytic with the identical Taylor series. Now since we have proved Theorem 2 for the old conventions used to define $\tilde{\chi}_m(q)$, we have that $\tilde{\Psi}_m(\mathbf{r}_s)$ is an analytic function of the Cartesian coordinates. Furthermore, since $\mathbf{H}(\mathbf{r}_s)$ is analytic, Eq. (3.35) implies that $\Psi_m(\mathbf{r}_s)$ is analytic. ■

IV. PROOF OF THREE-BODY BOUNDARY CONDITIONS

In this section, we prove Theorem 1.

Proof. For the entirety of this proof, when we say that a function of either the Jacobi coordinates or shape coordinates is analytic, we mean only that it is locally analytic at the specific points, $\mathbf{r}_{s\alpha}$ or q respectively, mentioned in the theorem.

A common fact we will use several times is that the Wigner matrices $\mathcal{D}^l_{mk}(\mathsf{Q})$ are analytic functions of the rotation matrices $\mathsf{Q} \in SO(3)$. Equation (2.7) thus shows that if Ψ^l_m is analytic at an arbitrary $\mathbf{r}_{s\alpha}$, then Ψ^l_m is analytic at any other orientation $\mathsf{Q}^T\mathbf{r}_{s\alpha}$ with $\mathsf{Q} \in SO(3)$ arbitrary. We therefore assume without loss that the specific configuration $\mathbf{r}_{s\alpha}$ in the statement of the Theorem is the reference orientation $\mathbf{r}_\alpha$.

(i) Assume q is noncollinear. The proof here is a straightforward generalization of the proof of part (i) of Theorem 2. First assume $\Psi^l_m(\mathbf{r}_{s\alpha})$ is analytic. From Eqs. (2.8) and (2.12), the fact that both $\mathbf{r}_\alpha(q)$ and $(\tau_\mu)_k(q)$ are analytic, and the fact that the composition of analytic functions is analytic, $\chi^l_\mu(q)$ and $\chi^l_k(q)$ are both analytic.

Next assume $\chi^l_\mu(q)$ is analytic. From Eq. (2.13) and the fact that $(\tau_\mu)_k(q)$ is analytic, $\chi^l_k(q)$ is also analytic. The validity assumption guarantees that $q(w_\mu)$ is analytic. From Eqs. (2.1)–(2.3) it is evident that the functions $w_\mu(\mathbf{r}_{s\alpha})$ are themselves analytic. Therefore, $q(\mathbf{r}_{s\alpha}) = q(w_\mu(\mathbf{r}_{s\alpha}))$ is analytic.

We now focus on the orientation matrix R in Eq. (2.5), which may be expressed in terms of the vectors $\mathbf{r}_{s\alpha}$ and $\mathbf{r}_\alpha$ as

$$\mathsf{R}(\mathbf{r}_{s\alpha},\mathbf{r}_\alpha) = \frac{1}{|\mathbf{r}_1\times\mathbf{r}_2|^2}[\mathbf{r}_{s1}\mathbf{v}_1^T + \mathbf{r}_{s2}\mathbf{v}_2^T + (\mathbf{r}_{s1}\times\mathbf{r}_{s2})(\mathbf{r}_1\times\mathbf{r}_2)^T], \tag{4.1}$$

$$\mathbf{v}_1 = -\mathbf{r}_2\times(\mathbf{r}_2\times\mathbf{r}_1), \tag{4.2}$$

$$\mathbf{v}_2 = -\mathbf{r}_1\times(\mathbf{r}_1\times\mathbf{r}_2). \tag{4.3}$$

To confirm the above expression for R, we need only verify Eq. (2.5) and show that $\mathsf{R}(\mathbf{r}_1\times\mathbf{r}_2) = \mathbf{r}_{s1}\times\mathbf{r}_{s2}$, both of which follow easily from the simple identities

$$\mathbf{v}_\alpha\cdot\mathbf{r}_\alpha = |\mathbf{r}_1\times\mathbf{r}_2|^2, \tag{4.4}$$

$$\mathbf{v}_\alpha\cdot(\mathbf{r}_1\times\mathbf{r}_2) = 0, \tag{4.5}$$

$$\mathbf{v}_1\cdot\mathbf{r}_2 = \mathbf{v}_2\cdot\mathbf{r}_1 = 0. \tag{4.6}$$

Since $\mathbf{r}_1\times\mathbf{r}_2$ does not vanish, it is clear that $\mathsf{R}(\mathbf{r}_{s\alpha},\mathbf{r}_\alpha)$ is an analytic function of the vectors $\mathbf{r}_{s\alpha}$ and $\mathbf{r}_\alpha$. Since both $\mathbf{r}_\alpha(q)$ and $q(\mathbf{r}_{s\alpha})$ are analytic, the function $\mathbf{r}_\alpha(\mathbf{r}_{s\alpha}) = \mathbf{r}_\alpha(q(\mathbf{r}_{s\alpha}))$ is analytic. Hence, $\mathsf{R}(\mathbf{r}_{s\alpha}) = \mathsf{R}(\mathbf{r}_{s\alpha},\mathbf{r}_\alpha(\mathbf{r}_{s\alpha}))$ is also analytic. Recalling that the Wigner matrices are analytic functions of R and that $q(\mathbf{r}_{s\alpha})$ is analytic, we see that

$$\Psi^l_m(\mathbf{r}_{s\alpha})=\sum_k \mathcal{D}^{l*}_{mk}(\mathsf{R}(\mathbf{r}_{s\alpha}))\chi^l_k(q(\mathbf{r}_{s\alpha})) \tag{4.7}$$

is an analytic function of the Jacobi coordinates.

(ii) Assume q is collinear. We define a new set of coordinates on configuration space consisting of two shape coordinates, two orientation coordinates, and two coordinates constructed from the one remaining shape coordinate and the one remaining orientation coordinate. We call these coordinates the ''mixed coordinates.'' The majority of the remainder of the proof will be dedicated to defining the mixed coordinates and proving the most important fact about them, that they are compatible with the Jacobi coordinates at the collinear configuration.

First, we discuss the parameterization of the rotation matrix R in Eq. (2.5). Consider an arbitrary unit vector $\hat{\mathbf{e}}$ lying in the northern hemisphere (excluding the equator), with $\hat{\mathbf{n}}(q)$ as the north pole. We define $\mathsf{U}(q,\hat{\mathbf{e}})\in SO(3)$ to be the unique rotation such that

$$\mathsf{U}(q,\hat{\mathbf{e}})\hat{\mathbf{n}}(q)=\hat{\mathbf{e}} \tag{4.8}$$

and such that its rotation axis lies on the equator. Specifically, the rotation axis of U lies in the direction of

$$\mathbf{a}(q,\hat{\mathbf{e}})=\hat{\mathbf{n}}(q)\times\hat{\mathbf{e}}, \tag{4.9}$$

and the rotation angle of U has the value $\arcsin|\mathbf{a}|$. Thus, $\mathsf{U}(q,\hat{\mathbf{e}})$ is explicitly given by

$$\mathsf{U}(q,\hat{\mathbf{e}})=\exp[f(|\mathbf{a}(q,\hat{\mathbf{e}})|)(\mathbf{a}(q,\hat{\mathbf{e}})\times)], \tag{4.10}$$

$$f(x)=\frac{\arcsin x}{x}, \tag{4.11}$$

where we have introduced the notation $\mathbf{a}\times$ for the 3×3 matrix which maps an arbitrary vector $\mathbf{v}$ into $\mathbf{a}\times\mathbf{v}$. The purpose of Eqs. (4.10) and (4.11) is to demonstrate the analyticity of $\mathsf{U}(q,\hat{\mathbf{e}})$. Observe that $\arcsin(x)$ is an odd analytic function on the interval $(-1,1)$, and hence, $f(x)$ is an even analytic function on $(-1,1)$. This in turn implies that $f(\mathbf{a})=f(|\mathbf{a}|)$ is an analytic function of $\mathbf{a}$. From Eq. (4.9) and the fact that $\hat{\mathbf{n}}(q)$ is analytic at $q_3=0$, $\mathbf{a}(q,\hat{\mathbf{e}})$ is analytic at $q_3=0$ and at all $\hat{\mathbf{e}}$ in the northern hemisphere defined by the north pole $\hat{\mathbf{n}}(q_3=0)$. The analyticity of the exponential function permits the following final statement. The function $\mathsf{U}(q,\hat{\mathbf{e}})$ expressed in Eq. (4.10) is an analytic function at $q_3=0$ and at all $\hat{\mathbf{e}}$ in the northern hemisphere with $\hat{\mathbf{n}}(q_3=0)$ as the north pole.

For an arbitrary rotation angle θ we define $\mathsf{V}(q,\theta)$ to be the rotation by θ about $\hat{\mathbf{n}}(q)$. Explicitly, this rotation is given by

$$\mathsf{V}(q,\theta)=\hat{\mathbf{n}}(q)\hat{\mathbf{n}}^T(q)+[\sin\theta(\hat{\mathbf{n}}(q)\times)+\cos\theta]\mathsf{P}_\perp(q). \tag{4.12}$$

We now express the rotation matrix R in Eq. (2.5) by

$$\mathsf{R}(\hat{\mathbf{e}},\theta)=\mathsf{U}(q,\hat{\mathbf{e}})\mathsf{V}(q,\theta), \tag{4.13}$$

where we have parameterized R by the quantities $\hat{\mathbf{e}}$ and θ.

We assume without loss of generality that $\hat{\mathbf{n}}(q_3=0)=\hat{\mathbf{z}}$. (This assumption simply amounts to a judicious choice of space frame.) We may thus define $\mathsf{W}(q)\in SO(3)$ in the neighborhood of $q_3=0$ to be the unique matrix such that

$$\mathsf{W}(q)\hat{\mathbf{z}}=\hat{\mathbf{n}}(q) \tag{4.14}$$

and such that its axis of rotation lies in the xy plane. In fact, we see from Eq. (4.8) that

$$\mathsf{W}(q)=\mathsf{U}^T(q,\hat{\mathbf{z}}). \tag{4.15}$$

The analyticity property of U implies that $\mathsf{W}(q)$ is analytic at $q_3=0$. We use $\mathsf{W}(q)$ to define an orthonormal frame $\hat{\mathbf{n}}_i(q)$, $i=1,2,3$, by

$$\hat{\mathbf{n}}_1(q)=\mathsf{W}(q)\hat{\mathbf{x}}, \tag{4.16}$$

$$\hat{\mathbf{n}}_2(q)=\mathsf{W}(q)\hat{\mathbf{y}}, \tag{4.17}$$

$$\hat{\mathbf{n}}_3(q)=\mathsf{W}(q)\hat{\mathbf{z}}=\hat{\mathbf{n}}(q). \tag{4.18}$$

The functions $\hat{\mathbf{n}}_i(q)$ are of course analytic.

The unit vector $\hat{\mathbf{e}}$ is determined by only two of its components, of which we choose $\hat{e}_1=\hat{\mathbf{e}}\cdot\hat{\mathbf{n}}_1$ and $\hat{e}_2=\hat{\mathbf{e}}\cdot\hat{\mathbf{n}}_2$. The third component $\hat{e}_3(\hat{e}_1,\hat{e}_2)=(\hat{e}_1^2+\hat{e}_2^2)^{1/2}$ is an analytic function of the other two in the northern hemisphere. The function

$$\hat{\mathbf{e}}(q_1,\hat{e}_1,\hat{e}_2)=\hat{e}_1\hat{\mathbf{n}}_1(q)+\hat{e}_2\hat{\mathbf{n}}_2(q)+\hat{e}_3(\hat{e}_1,\hat{e}_2)\hat{\mathbf{n}}_3(q) \tag{4.19}$$

is of course analytic.

We next define a pair of vectors $\mathbf{s}_\alpha(q,\theta)$, $\alpha=1,2$, by

$$\begin{aligned}\mathbf{s}_\alpha(q,\theta)&=\mathsf{V}(q,\theta)\mathbf{r}_\alpha(q)\\&=(\hat{\mathbf{n}}\cdot\mathbf{r}_\alpha)(q)\hat{\mathbf{n}}(q)+[\sin\theta(\hat{\mathbf{n}}(q)\times)+\cos\theta](\mathsf{P}_\perp\mathbf{r}_\alpha)(q),\end{aligned} \tag{4.20}$$

where we have used Eq. (4.12). We introduce two new variables u_1 and u_2 by

$$u_1=q_3\cos\theta, \tag{4.21}$$

$$u_2=q_3\sin\theta. \tag{4.22}$$

We define $u=q_3$, which is convenient notation since when u is positive, it is the radial coordinate in u_1u_2-space, that is, $u=(u_1^2+u_2^2)^{1/2}$. The vectors $\mathbf{s}_\alpha$ are conveniently parameterized by the new coordinates

$$\mathbf{s}_\alpha(u_1,u_2)=(\hat{\mathbf{n}}\cdot\mathbf{r}_\alpha)(u)\hat{\mathbf{n}}(u)+[u_2(\hat{\mathbf{n}}(u)\times)+u_1]\times\left[\frac{(\mathsf{P}_\perp\mathbf{r}_\alpha)(u)}{u}\right], \tag{4.23}$$

where we have dropped the explicit dependence on q_1 and q_2. Since $f(u)$ is an even analytic function of u, $f(u_1,u_2)=f((u_1^2+u_2^2)^{1/2})$ is analytic in u_1 and u_2. This fact, together with Eqs. (2.16)–(2.18), shows that $\hat{\mathbf{n}}$, $\hat{\mathbf{n}}\cdot\mathbf{r}_\alpha$, $(\mathsf{P}_\perp\mathbf{r}_\alpha)/u$, and

hence $\mathbf{s}_\alpha$ are all analytic functions of u_1 and u_2. Reintroducing the explicit dependence on q_1 and q_2, we see that $\mathbf{s}_\alpha(q_1,q_2,u_1,u_2)$ is analytic.

Using similar arguments as above, from Eqs. (4.9) and (4.10) we see that both $\mathbf{a}(q_1,q_2,u_1,u_2,\hat{\mathbf{e}}=\hat{\mathbf{z}})$ and $\mathsf{U}(q_1,q_2,u_1,u_2,\hat{\mathbf{e}}=\hat{\mathbf{z}})$ are analytic. Hence, Eq. (4.15) shows that $\mathsf{W}(q_1,q_2,u_1,u_2)$ is analytic, from which follows, using Eqs. (4.16)–(4.18), that the $\hat{\mathbf{n}}_i(q_1,q_2,u_1,u_2)$, $i=1,2,3$, are analytic. Hence, Eq. (4.19) shows that $\hat{\mathbf{e}}(q_1,q_2,u_1,u_2,\hat{e}_1,\hat{e}_2)$ is analytic. From this result we also have, using Eqs. (4.9) and (4.10), that

$$\mathbf{a}(q_1,q_2,u_1,u_2,\hat{e}_1,\hat{e}_2) = \mathbf{a}(q_1,q_2,u_1,u_2,\hat{\mathbf{e}}(q_1,q_2,u_1,u_2,\hat{e}_1,\hat{e}_2))$$

and

$$\mathsf{U}(q_1,q_2,u_1,u_2,\hat{e}_1,\hat{e}_2) = \mathsf{U}(q_1,q_2,u_1,u_2,\hat{\mathbf{e}}(q_1,q_2,u_1,u_2,\hat{e}_1,\hat{e}_2))$$

are both analytic.

We define the mixed coordinates to be the variables $(q_1,q_2,u_1,u_2,\hat{e}_1,\hat{e}_2)$. We can express $\mathbf{r}_{s\alpha}$ in terms of the mixed coordinates as follows

$$\begin{aligned}\mathbf{r}_{s\alpha}(q_1,q_2,u_1u_2,\hat{e}_1,\hat{e}_2) &= \mathsf{R}\mathbf{r}_\alpha = \mathsf{UV}\mathbf{r}_\alpha \\ &= \mathsf{U}(q_1,q_2,u_1,u_2,\hat{e}_1,\hat{e}_2)\mathbf{s}_\alpha(q_1,q_2,u_1,u_2),\end{aligned} \tag{4.24}$$

where we have used Eqs. (2.5), (4.13), and (4.20). Since we have already shown that both $\mathsf{U}(q_1,q_2,u_1,u_2,\hat{e}_1,\hat{e}_2)$ and $\mathbf{s}_\alpha(q_1,q_2,u_1,u_2)$ are analytic, we see that the Jacobi coordinates are analytic functions of the mixed coordinates.

To show compatibility of the mixed coordinates with the Jacobi coordinates we need now only show that the mixed coordinates are analytic functions of the Jacobi coordinates. First, since the internal coordinates q_μ are valid coordinates, they are analytic functions of the w-coordinates. By inspecting Eqs. (2.1) and (2.2), we see that $w_1(\mathbf{r}_{s\alpha})$ and $w_2(\mathbf{r}_{s\alpha})$ are analytic, even at a collinear shape. However, because of the absolute value in Eq. (2.3) the same can not be said of $w_3(\mathbf{r}_{s\alpha})$. However, the function $w_3^2(\mathbf{r}_{s\alpha})$ is analytic. Thus, we have the following lemma: Any analytic function of (w_1,w_2,w_3^2) may be viewed, via composition, as an analytic function of $\mathbf{r}_{s\alpha}$. Using this lemma and noting that $q_1(w_\mu)$ and $q_2(w_\mu)$ are analytic functions which by Eq. (2.14) are also even in w_3, we see that the two mixed coordinates $q_1(\mathbf{r}_{s\alpha})$ and $q_2(\mathbf{r}_{s\alpha})$ are both analytic functions of the Jacobi coordinates.

Note that the coordinate $q_3(\mathbf{r}_{s\alpha})$ is not analytic. However, since $q_3^2(w_\mu)$ is analytic and by Eq. (2.15) also even in $w_3, q_3^2(\mathbf{r}_{s\alpha})$ is analytic. This fact allows us to generalize our previous lemma regarding the w-coordinates to arbitrary q. As we will have frequent need of this more general lemma, we record it below.

Lemma 1. If $f(q)$ is an analytic function which is even in q_3, then $f(\mathbf{r}_{s\alpha})=f(q(\mathbf{r}_{s\alpha}))$ is analytic.

This lemma, together with Eqs. (2.16)–(2.18), proves the analyticity of the following functions:

$$(\mathbf{r}_\alpha\cdot\hat{\mathbf{n}})(\mathbf{r}_{s\alpha}),|\mathsf{P}_\perp\mathbf{r}_\alpha|^2(\mathbf{r}_{s\alpha}),r_\alpha^2(\mathbf{r}_{s\alpha}),\hat{\mathbf{n}}(\mathbf{r}_{s\alpha}).$$

Furthermore, Eqs. (4.9) and (4.10) show that U is even in q_3 and hence $\mathsf{U}(\mathsf{r}_{s\alpha},\hat{\mathbf{e}})=\mathsf{U}(q(\mathbf{r}_{s\alpha}),\hat{\mathbf{e}})$ is analytic at the collinear configuration and at all $\hat{\mathbf{e}}$ in the northern hemisphere with $\hat{\mathbf{n}}(q_3=0)$ at the north pole. Equation (4.15) proves the analyticity of $\mathsf{W}(\mathbf{r}_{s\alpha})=\mathsf{W}(q(\mathbf{r}_{s\alpha}))$ and hence Eqs. (4.16)–(4.18) prove the analyticity of the basis vectors $\hat{\mathbf{n}}_i(\mathbf{r}_{s\alpha}) =\hat{\mathbf{n}}_i(q(\mathbf{r}_{s\alpha}))$, $i=1,2,3$.

The vector $\hat{\mathbf{e}}$ is determined by the equation

$$\hat{\mathbf{e}}=\mathsf{R}\hat{\mathbf{n}}, \tag{4.25}$$

which follows from Eqs. (4.12), (4.13), and (4.8). We observed earlier that away from a collinear shape, the matrix R is given by Eq. (4.1), which results in the following formula for $\hat{\mathbf{e}}$

$$\hat{\mathbf{e}}=\nu_1(q)\mathbf{r}_{s1}+\nu_2(q)\mathbf{r}_{s2}, \tag{4.26}$$

$$\nu_\alpha=\frac{\mathbf{v}_\alpha\cdot\hat{\mathbf{n}}}{\mathbf{v}_\alpha\cdot\mathbf{r}_\alpha}, \tag{4.27}$$

where we have used Eq. (4.4) and the fact that

$$(\mathbf{r}_1\times\mathbf{r}_2)\cdot\hat{\mathbf{n}}=0 \tag{4.28}$$

since $\hat{\mathbf{n}}$ is assumed to lie in the plane spanned by $\mathbf{r}_1$ and $\mathbf{r}_2$. We will now show that Eq. (4.26) is valid not only at noncollinear configurations, but at collinear configurations as well. More specifically, we will prove that $\hat{\mathbf{e}}(\mathbf{r}_{s\alpha})$ is analytic at collinear configurations.

Considering Eq. (4.26) in the neighborhood of a collinear configuration, we first assume that neither $\mathbf{r}_1$ nor $\mathbf{r}_2$ vanishes. Obviously, to show that $\hat{\mathbf{e}}(\mathbf{r}_{s\alpha})$ is analytic, we need only show that $\nu_\alpha(\mathbf{r}_{s\alpha})=\nu_\alpha(q(\mathbf{r}_{s\alpha}))$ is analytic. From Lemma 1 this amounts to showing that $\nu_\alpha(q)$ is analytic and even in q_3. That $\nu_\alpha(q)$ is even in q_3 is easily proved by inserting Eqs. (4.2) and (4.3) into Eq. (4.27) and using Eqs. (2.16) and (2.17). To show that $\nu_\alpha(q)$ is analytic requires the following observation: The ratio of two functions which are both analytic at a given point is also analytic at that point provided that the ratio is not infinite. (This fact is easily proved by considering the Taylor series of the two functions.) As q_3 tends toward 0, by our previous assumption, $\mathbf{r}_{s\alpha}$ does not vanish, nor does $\hat{\mathbf{n}}$. The quantity $\mathbf{v}_\alpha$, however, does vanish, but since it appears to first order in both the numerator and denominator of Eq. (4.27), the ratio is finite at $q_3=0$. Thus, $\nu_\alpha(q)$ is analytic, and hence $\nu_\alpha(\mathbf{r}_{s\alpha})$ and consequently $\hat{\mathbf{e}}(\mathbf{r}_{s\alpha})$ are analytic as well.

If one of the Jacobi vectors, say $\mathbf{r}_{s1}$, vanishes at the collinear configuration, the preceding analysis must be modified due to the appearance of $\mathbf{r}_1$ in the denominator of Eq. (4.27). In this case, we define a new set of vectors

$$\mathbf{t}_{s1}=\mathbf{r}_{s1}+\mathbf{r}_{s2}, \tag{4.29}$$

$$\mathbf{t}_{s2}=\mathbf{r}_{s1}-\mathbf{r}_{s2}, \tag{4.30}$$

and their counterparts $\mathbf{t}_\alpha$ in the body frame which satisfy

$$\mathbf{t}_{s\alpha}=\mathsf{R}\mathbf{t}_\alpha, \tag{4.31}$$

analogous to Eq. (2.5). Notice that neither $\mathbf{t}_1$ nor $\mathbf{t}_2$ vanishes at the collinear shape since this could only occur if $\mathbf{r}_2$ were also to vanish, which only occurs for the triple collision. Now, Eqs. (4.1)–(4.3), (4.26), and (4.27) are all valid if one replaces $\mathbf{r}_{s\alpha}$ and $\mathbf{r}_\alpha$ by $\mathbf{t}_{s\alpha}$ and $\mathbf{t}_\alpha$, respectively. We may repeat the same line of reasoning as above to show that the new $\nu_\alpha(q)$, with $\mathbf{r}_\alpha$ replaced by $\mathbf{t}_\alpha$, is analytic and even in q_3. Thus from Lemma 1, the new $\mathbf{v}_\alpha(\mathbf{r}_{s\alpha})$ and hence $\hat{\mathbf{e}}(\mathbf{r}_{s\alpha})$ are both analytic. Since $\hat{\mathbf{n}}_1(\mathbf{r}_{s\alpha})$ and $\hat{\mathbf{n}}_2(\mathbf{r}_{s\alpha})$ are analytic, we finally find that the two mixed coordinates $\hat{e}_i(\mathbf{r}_{s\alpha})=\hat{\mathbf{e}}(\mathbf{r}_{s\alpha})\cdot\hat{\mathbf{n}}_i(\mathbf{r}_{s\alpha})$, $i=1,2$, are analytic functions of the Jacobi coordinates.

We turn now to the final two mixed coordinates u_1 and u_2. They are defined by Eqs. (4.21) and (4.22), but may also be expressed as

$$\begin{aligned} u_1&=q_3\cos\theta=\hat{\mathbf{n}}_1\cdot(q_3\mathsf{V}\mathsf{P}_\perp)\hat{\mathbf{n}}_1\\ &=\hat{\mathbf{n}}_1\cdot\mathsf{U}^T(q_3\mathsf{R}\mathsf{P}_\perp)\hat{\mathbf{n}}_1=\hat{\mathbf{n}}_1\cdot\mathsf{U}^T\mathsf{M}\hat{\mathbf{n}}_1, \end{aligned} \tag{4.32}$$

$$u_2=q_3\sin\theta=\hat{\mathbf{n}}_2\cdot\mathsf{U}^T\mathsf{M}\hat{\mathbf{n}}_1, \tag{4.33}$$

where

$$\mathsf{M}=q_3\mathsf{R}\mathsf{P}_\perp. \tag{4.34}$$

The second equality in Eq. (4.32) follows from Eq. (4.12) and the orthogonality of $\hat{\mathbf{n}}_1$ and $\hat{\mathbf{n}}$. The third equality follows from Eq. (4.13).

Recall that $\mathsf{U}(\mathbf{r}_{s\alpha},\hat{\mathbf{e}})$ and $\hat{\mathbf{e}}(\mathbf{r}_{s\alpha})$ are analytic. Hence, $\mathsf{U}(\mathbf{r}_{s\alpha})=\mathsf{U}(\mathbf{r}_{s\alpha},\hat{\mathbf{e}}(\mathbf{r}_{s\alpha}))$ is also analytic. We also recall that the $\hat{\mathbf{n}}_i(\mathbf{r}_{s\alpha})$, $i=1,2,3$, are analytic. Thus, inspecting Eqs. (4.32) and (4.33), we need only show that $\mathsf{M}(\mathbf{r}_{s\alpha})$ is analytic. The matrix M may be written with the aid of Eq. (4.1) as

$$\mathsf{M}(q,\mathbf{r}_{s\alpha})=\mathbf{r}_{s1}\mathbf{p}_1(q)+\mathbf{r}_{s2}\mathbf{p}_2(q)+(\mathbf{r}_{s1}\times\mathbf{r}_{s2})\mathbf{p}_3^T(q), \tag{4.35}$$

$$\mathbf{p}_\alpha=\frac{q_3\mathsf{P}_\perp\mathbf{v}_\alpha}{\mathbf{v}_\alpha\cdot\mathbf{r}_\alpha},\quad \alpha=1,2, \tag{4.36}$$

$$\mathbf{p}_3=\frac{q_3\mathsf{P}_\perp(\mathbf{r}_1\times\mathbf{r}_2)}{|\mathbf{r}_1\times\mathbf{r}_2|^2}. \tag{4.37}$$

We first assume that $\mathbf{r}_1$ and $\mathbf{r}_2$ do not vanish at the collinear shape. To prove that $\mathsf{M}(\mathbf{r}_{s\alpha})=\mathsf{M}(q(\mathbf{r}_{s\alpha}),\mathbf{r}_{s\alpha})$ is analytic, we need only show that $\mathbf{p}_\alpha(\mathbf{r}_{s\alpha})$, $\alpha=1,2$, and $\mathbf{p}_3(\mathbf{r}_{s\alpha})$ are analytic. From Lemma 1 we must therefore show that $\mathbf{p}_\alpha(q)$, $\alpha=1,2$, and $\mathbf{p}_3(q)$ are analytic and even in q_3. Using the definitions Eqs. (4.2), (4.3), (4.36), and (4.37) and the validity conditions Eqs. (2.16) and (2.17), it is straightforward to prove that $\mathbf{p}_\alpha(\mathbf{r}_{s\alpha})$, $\alpha=1,2$, and $\mathbf{p}_3(\mathbf{r}_{s\alpha})$ are even in q_3. As with our proof of the analyticity of $\nu_\alpha(q)$, to prove that $\mathbf{p}_\alpha(q)$, $\alpha=1,2$, is analytic all we need to do is show that the ratio in Eq. (4.36) is not infinite when q_3 tends toward 0. (Both the numerator and denominator are analytic functions of q.) This fact follows readily from our assumption that $\mathbf{r}_\alpha$ does not vanish and from the fact that $\mathbf{v}_\alpha$, which does vanish at $q_3=0$, appears linearly in both the numerator and denominator. Proving that $\mathbf{p}_3(q)$ is analytic requires a bit more care. Since both the numerator and the denominator in Eq. (4.37) are analytic functions, we again need only verify that $\mathbf{p}_3(q)$ does not blow up at $q_3=0$, whence

$$\lim_{q_3\to 0}\mathbf{p}_3(q_3)=\lim_{q_3\to 0}\left[\frac{2q_3}{w_3(q_3)}\right]\lim_{q_3\to 0}\left[\mathsf{P}_\perp\left(\frac{\mathbf{r}_1\times\mathbf{r}_2}{|\mathbf{r}_1\times\mathbf{r}_2|}\right)\right](q_3), \tag{4.38}$$

where we have used the definition Eq. (2.3) of w_3. We now note

$$\lim_{q_3\to 0}\frac{q_3}{w_3(q_3)}=\frac{1}{(\partial w_3/\partial q_3)(0)}=\frac{\partial q_3}{\partial w_3}(0), \tag{4.39}$$

which cannot be infinite since q_3 is an analytic function of w_3. [We have used l'Hospital's rule in the second step of Eq. (4.39).] The second limit in Eq. (4.38) cannot be infinite either, since $\mathsf{P}_\perp$ is well-defined at $q_3=0$ and

$$\mathbf{r}_1\times\mathbf{r}_2/|\mathbf{r}_1\times\mathbf{r}_2|$$

is a unit vector. Thus, $\mathbf{p}_3(q)$ is analytic at $q_3=0$. Hence, we have shown the analyticity of $\mathbf{p}_\alpha(\mathbf{r}_{s\alpha})$, $\alpha=1,2$, and $\mathbf{p}_3(\mathbf{r}_{s\alpha})$ from which follows analyticity of $\mathsf{M}(\mathbf{r}_{s\alpha})$ and $u_i(\mathbf{r}_{s\alpha})$, $i=1,2$. If the assumption that $\mathbf{r}_1$ and $\mathbf{r}_2$ do not vanish at the collinear shape proves to be false, then we can prove the analyticity of $\mathsf{M}(\mathbf{r}_{s\alpha})$ by applying the same trick used earlier of defining the vectors $\mathbf{t}_{s\alpha}$. We omit the straightforward details of completing this argument. This finishes the proof of the compatibility of the mixed coordinates with the Jacobi coordinates.

We turn now to the eigenspinors τ_μ satisfying Eqs. (2.10) and (2.11). We denote by $(L_{si})_{mm'}$, $i=x,y,z$, $m,m'=-l,\ldots,l$, the components of the space-referred angular momentum operator L_{si} with respect to the L_{sz} eigenbasis. The matrices L_{si} transform under a rotation $\mathsf{Q}\in SO(3)$ as a vector operator,

$$\sum_j Q_{ji}L_{sj}=\mathcal{D}^l(\mathsf{Q})L_{si}\mathcal{D}^{l\dagger}(\mathsf{Q}). \tag{4.40}$$

We denote by $(L_i)_{kk'}$, $i=x,y,z$, k, $k'=-l,\ldots,l$, the components of the body-referred angular momentum operator L_i with respect to the L_z eigenbasis. The components of the two operators L_{si} and L_i, with respect to their respective bases, are related by $(L_i)_{kk'}=(L_{si})_{k'k}=(L_{si})^*_{kk'}$. (See Ref. [3], Sect. 4.H for a derivation.) Thus, the matrices L_i satisfy

$$\sum_j Q_{ji}L_j=\mathcal{D}^{l*}(\mathsf{Q})L_i\mathcal{D}^{lT}(\mathsf{Q}). \tag{4.41}$$

In view of Eqs. (4.14) and (4.41), we have

$$\hat{\mathbf{n}}\cdot\mathbf{L}=\hat{\mathbf{z}}\cdot\mathsf{W}^{T}\tilde{\mathbf{L}}=\mathcal{D}^{l*}(\mathsf{W})L_z\mathcal{D}^{lT}(\mathsf{W}). \tag{4.42}$$

From Eq. (4.42) we see that τ_μ can be expressed as

$$(\tau_\mu)_k=e^{i\sigma}\mathcal{D}^{l}_{\mu k}(\mathsf{W}^T), \tag{4.43}$$

where $\sigma(q)$ is a phase factor that must be analytic and even in q_3 in order to guarantee the same properties for $(\tau_\mu)_k(q)$. This result, together with Eqs. (2.12) and (2.13), yields

$$\chi^l_\mu=\sum_k e^{-i\sigma}\mathcal{D}^{l*}_{\mu k}(\mathsf{W}^T)\chi^l_k, \tag{4.44}$$

$$\chi^l_k=\sum_\mu e^{i\sigma}\mathcal{D}^{l*}_{k\mu}(\mathsf{W})\chi^l_\mu. \tag{4.45}$$

We may use Eq. (4.45) to rewrite Eq. (2.9) as

$$\Psi^l_m=e^{i\sigma}\sum_\mu \mathcal{D}^{l*}_{m\mu}(\mathsf{RW})\chi^l_\mu=e^{i\sigma}\sum_\mu \mathcal{D}^{l*}_{m\mu}(\mathsf{UVW})\chi^l_\mu, \tag{4.46}$$

where we have used Eq. (4.13).

We now assume that $\Psi^l_m(\mathbf{r}_{s\alpha})$ is analytic, which implies, as in part (i), that both $\chi^l_k(q)$ and $\chi^l_\mu(q)$ are analytic, and hence $\chi^l_\mu(q)$ has a Taylor series

$$\chi^l_\mu(q_1,q_2,q_3)=\sum_{n=0}^{\infty} b_{n\mu}(q_1,q_2)q_3^n, \tag{4.47}$$

where $b_{n\mu}(q_1,q_2)$ is analytic. We must now only show that the appropriate coefficients vanish in the Taylor series Eq. (4.47) to produce the Taylor series Eq. (2.20). Since $\sigma(q)$ is analytic and even in q_3, Lemma 1 shows that $\sigma(\mathbf{r}_{s\alpha})=\sigma(q(\mathbf{r}_{s\alpha}))$ is analytic. Therefore the function $\tilde{\Psi}^l_m$ defined by

$$\tilde{\Psi}^l_m(q_1,q_2,u_1,u_2)=e^{-i\sigma(q_1,q_2,u_1,u_2)}\times\Psi^l_m(q_1,q_2,u_1,u_2,\hat{\mathbf{e}}=\hat{\mathbf{z}}), \tag{4.48}$$

is analytic. Since $\hat{\mathbf{e}}=\hat{\mathbf{z}}$, we see from Eq. (4.15) that the matrix product UVW appearing in Eq. (4.46) is equal to $\mathsf{W}^T\mathsf{VW}$. From Eqs. (4.12) and (4.14) it is evident that $\mathsf{W}^T\mathsf{VW}\hat{\mathbf{z}}=\hat{\mathbf{z}}$, and hence $\mathsf{W}^T\mathsf{VW}$ is a rotation by θ about the z axis, where θ is the rotation angle of V. Therefore,

$$\mathcal{D}^{l*}_{m\mu}(\mathsf{W}^T\mathsf{VW})=\delta_{m\mu}\exp(im\theta). \tag{4.49}$$

Thus, Eqs. (4.46) and (4.48) combine to yield

$$\tilde{\Psi}^l_m(u_1,u_2)=e^{im\theta}\chi^l_m(q_3), \tag{4.50}$$

where we have dropped the explicit dependence on q_1 and q_2. From this equation and the fact that (θ,q_3) are the usual polar coordinates with respect to the Cartesian coordinates (u_1,u_2), we may apply Theorem 2. In particular, since $\tilde{\Psi}^l_m(u_1,u_2)$ is analytic, $\chi^l_m(q_3)$ has the Taylor series given in Eq. (3.9). This implies that the appropriate coefficients in Eq. (4.47) vanish.

Next assume that $\chi^l_\mu(q)$, and hence $\chi^l_k(q)$, is analytic and that $\chi^l_\mu(q)$ has the Taylor series given by Eq. (2.20). Then from Theorem 2, the function $\tilde{\Psi}^l_m(u_1,u_2)$ given in Eq. (4.50) is analytic in u_1 and u_2 and based on the analyticity of the coefficients $a_{\mu n}(q_1,q_2)$, $\tilde{\Psi}^l_m(u_1,u_2,q_1,q_2)$ is analytic in q_1 and q_2 as well. We now rewrite Eq. (4.46) as

$$\Psi^l_m=e^{i\sigma}\sum_\mu \mathcal{D}^{l*}_{m\mu}(\mathsf{UW})e^{i\mu\theta}\chi^l_\mu=e^{i\sigma}\sum_\mu \mathcal{D}^{l*}_{m\mu}(\mathsf{UW})\tilde{\Psi}^l_\mu, \tag{4.51}$$

where we have used Eq. (4.49) in the first equality and Eq. (4.50) in the second. We have already shown that σ, U, W, and $\tilde{\Psi}^l_\mu$ are analytic functions of the mixed coordinates. Thus, Ψ^l_m is an analytic function of the mixed coordinates and hence of the Jacobi coordinates as well. ■

V. CONCLUSIONS

Assuming valid conventions, Theorem 1 solves the problem of determining whether an internal wave function for the three-body problem is associated with an analytic external wave function. The criteria presented are both necessary and sufficient. The proof invoked only general concepts of analyticity and group theory and there was never any need to assume that the external wave function was an eigenfunction of a Hamiltonian or any other operator. The class of valid conventions for our results is very general and encompasses most of the conventions in common use.

We now propose several useful extensions of the present work which we plan to consider in future publications. First, Theorem 1 says nothing about the properties of the external wave function in the neighborhood of body frame singularities. Our justification for ignoring these singularities at present is that they may always be moved away from the region of interest by a change of body frame; they may even be moved into the unphysical region of shape space. However, in practice it is not always convenient to change body frames or to use a body frame that places the singularities in the unphysical region. Therefore, one should like to have a set of criteria on the internal wave function which guarantees the analyticity of the external wave function in the neighborhood of a body frame singularity.

A second desirable extension of the present work would be to develop a set of criteria applicable at the three-body collision. Such an analysis would almost certainly involve the analysis of body frame singularities mentioned above. This is because the string (or strings) of body frame singularities emanates from the three-body collision and no body frame avoids singularities at the three-body collision.

As mentioned in the introduction, the external wave function for three-body problems is not necessarily analytic at all points, the collisional configurations of Coulomb problems being an obvious example. Yet another useful extension of the present work would be to develop criteria on the internal

wave function that capture such singular behavior of the external wave function.

Finally, it is natural to try and extend our analysis to four or more bodies. The case of four bodies is certainly more challenging than that of three bodies. For the three-body problem, we can always pick valid reference orientations $\mathbf{r}_\alpha(q)$, which are well-defined analytic functions in the neighborhood of an arbitrary collinear shape (except the three-body collision). For the four-body problem, however, any reference orientation $\mathbf{r}_\alpha(q)$, $\alpha=1,2,3$, we choose will not be analytic at any collinear shape. This is because all body frames for the four body problem have singular surfaces emanating from all collinear shapes [19]. Extending the analysis of this paper to the four body problem will necessarily require a deeper consideration of frame singularities.

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APPENDIX: FACTS CONCERNING $SO(2)$

We collect some basic facts concerning $SO(2)$ that are necessary for the proof of Theorem 2. All irreducible representations (irreps) of $SO(2)$ are one-dimensional and may be labeled by an integer m, with $-\infty<m<\infty$. The components of a vector in an invariant one-dimensional carrier space labeled by m are multiplied by $\exp(-im\theta)$ when rotated by θ.

The fundamental representation of $SO(2)$, that is the representation by 2×2 real orthogonal matrices, decomposes into the direct sum of the $m=\pm 1$ irreps, which we denote $+1\oplus -1$. The two irreducible carrier spaces are spanned by the vectors $\mathbf{e}_\pm=(1,\pm i)^T$. The d-fold tensor product of the fundamental representation contains (with various multiplicities) the irreps $d, d-2, d-4, \ldots, -(d-4), -(d-2), -d$. However, exactly one irrep for each allowed value of m is totally symmetric. That is, the fully symmetrized tensor product of the fundamental representation of $SO(2)$ decomposes as

$$\mathcal{S}\bigotimes_d(+1\oplus -1)=d\oplus(d-2)\oplus(d-4)\oplus\cdots\oplus -(d-4)\oplus -(d-2)\oplus -d, \tag{A1}$$

where $\otimes$ denotes the tensor product and $\mathcal{S}$ denotes the total symmetrization operator. The irrep labeled by m is spanned by a totally symmetric rank d tensor t_m^d given by

$$t_m^d=\mathcal{S}(\underbrace{\mathbf{e}_+\otimes\cdots\otimes\mathbf{e}_+}_{u\ \text{times}}\otimes\underbrace{\mathbf{e}_-\otimes\cdots\otimes\mathbf{e}_-}_{v\ \text{times}}), \tag{A2}$$

where $m=u-v$ and $d=u+v$. Explicitly, t_m^d transforms as

$$\sum_{k_1\ldots k_2} Q_{j_1k_1}\ldots Q_{j_dk_d}(t_m^d)_{k_1\ldots k_d}=e^{-im\alpha}(t_m^d)_{j_1\ldots j_d}, \tag{A3}$$

where $(t_m^d)_{j_1\ldots j_d}$ are the components of t_m^d. A final fact we need, which follows readily from Eq. (A2), is that

$$(t_m^d)_{x\ldots x}=1. \tag{A4}$$

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