Kinematic geometry of mass-triangles and reduction of Schrödinger's equation of three-body systems to partial differential equations solely defined on triangular parameters

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ABSTRACT Schrödinger's equation of a three-body system is a linear partial differential equation (PDE) defined on the 9-dimensional configuration space, $\mathbb{R}^9$, naturally equipped with Jacobi's kinematic metric and with translational and rotational symmetries. The natural invariance of Schrödinger's equation with respect to the translational symmetry enables us to reduce the configuration space to that of a 6-dimensional one, while that of the rotational symmetry provides the quantum mechanical version of angular momentum conservation. However, the problem of maximizing the use of rotational invariance so as to enable us to reduce Schrödinger's equation to corresponding PDEs solely defined on triangular parameters—i.e., at the level of $\mathbb{R}^6/SO(3)$ —has never been adequately treated. This article describes the results on the orbital geometry and the harmonic analysis of $(SO(3), \mathbb{R}^6)$ which enable us to obtain such a reduction of Schrödinger's equation of three-body systems to PDEs solely defined on triangular parameters.

In atomic and molecular physics, one naturally encounters the quantum mechanics of three-body systems such as helium atom He, the hydrogen molecular ion H_2^+ , the negative ion of hydrogen atom H^- , etc. The fundamental equation for studying the physics of such systems is *Schrödinger's equation*, namely

$$-\frac{\hbar^2}{2} \sum_{j=1}^3 \frac{1}{\mu_j} \Delta_j \Psi + U \cdot \Psi = E \Psi, \quad [1]$$

where U is the potential function, E is the energy level of a stationary state, and μ_j and Δ_j are, respectively, the individual mass and the Laplace-operator with respect to the coordinates of the individual particle, $j = 1, 2, 3$.

The study of the above Schrödinger's equation of three-body systems has a long history, dating back to Hylleraas' work on this subject in the 1930s, and there are an extensive literature and various approaches in the study of its solutions. The book of Bethe and Salpeter (1) and the Festschrift volume of *Review of Modern Physics* in honor of Hylleraas (2) contain many basic references on this topic.

The problem of maximizing the use of angular momentum conservation has, however, never been adequately treated. The usual procedure is to introduce approximations such as approximate reduced masses, etc. In this short article, I shall describe a geometric approach to the three-body problem which does not use any approximation or perturbation and hence applies just as well to general mass distributions as to

lopsided ones. Following Jacobi, it is natural to introduce a Riemannian metric on the configuration space of a given mechanical system such that the *kinetic energy* of a motion is given by half of the square of speed. Such a *kinematic Riemannian manifold* is actually the *geometric encoding of the kinetic energy* of the given system and it always inherits an *SO(3)-isometry* from the rotational symmetry of the physical space. Moreover, the *space of SO(3)-orbits* also has an *induced metric* which measures the distances among neighboring orbits. We thus call it the *orbital distance metric*. In the special case of three-body systems, the orbit space, M , is exactly the “space of triangles” (i.e., each point of M represents a class of congruent triangles) and the above orbital distance metric, $d\bar{s}^2$, provides a natural geometric measurement of the difference in size and shape among triangles. Let I be the *moment of inertia*. Then $\rho = \sqrt{I}$ is equal to the distance between the given triangle and the point-triangle, thus ρ provides a natural measurement of the size, while the 2-dimensional subspace $M^* \subset M$ defined by setting $\rho = 1$ is the natural geometric representation of all possible *shapes* of triangles. It is a remarkable intrinsic beauty of the kinematic geometry of triangles that M^* is *always isometric* to the euclidean hemisphere of radius $1/2$, $S_+^2(1/2)$, (i.e., independent of the mass distribution).

The Schrödinger equation is naturally *SO(3)-invariant*, and this is the origin of angular momentum conservation in quantum mechanics. The above setting of *SO(3)-orbital geometry* of the configuration space enables us to maximize the use of *angular momentum conservation* [or rather, the *SO(3)-invariance* of three-body system] to reduce the Schrödinger equation to a system of $l + 1$ (resp l) PDEs at the level of $(M, d\bar{s}^2)$, namely, solely in terms of *triangular parameters*, cf. Eqs. 20 and 20*.

A combination of the sphericity of M^* and the above reduced equations will enable us to further reduce the solution of Eq. 1 to that of an infinite system of *algebraic* linear equations (3, 4).

Kinematic Geometry of Triangles and Specific Choice of Coordinates of the Configuration Space

Let $\mu = \sum \mu_j$ be the total mass, $m_j = \mu_j/\mu$ be the percentages of mass, $j = 1, 2, 3$, and $\mathbf{a}_j$ be the position vectors. Following Jacobi, the *kinematic metric* on $\mathbb{R}^3 \oplus \mathbb{R}^3 \oplus \mathbb{R}^3$ is defined by setting

$$\langle \{\mathbf{a}_j\}, \{\mathbf{b}_j\} \rangle = \sum_{j=1}^3 m_j \mathbf{a}_j \mathbf{b}_j. \quad [2]$$

Moreover, fixing the origin at the center of gravity enables us to reduce the *configuration space* to the 6-dimensional linear subspace $\mathbb{R}^6$ given by $\sum m_j \mathbf{a}_j = 0$. The Laplace-operators on both $\mathbb{R}^9$ and the above $\mathbb{R}^6$ are given by

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Abbreviation; PDE, partial differential equation.

$$\Delta f = \sum_{j=1}^3 \frac{1}{m_j} \Delta_j f. \quad [3]$$

Thus, Schrödinger's equation (1) can be rewritten as

$$-\frac{\hbar^2}{2\mu} \Delta \Psi + U\Psi = E\Psi. \quad [1']$$

An important starting point for achieving the “ $SO(3)$ -reduction” of Eq. 1' is the following specific, intrinsic choice of coordinate system in $\mathbb{R}^6$, namely, setting

$$\begin{aligned} \mathbf{x} &= \sqrt{\frac{m_2 m_3}{1-m_1}} (\mathbf{a}_2 - \mathbf{a}_3), \mathbf{y} = -\sqrt{\frac{m_1}{1-m_1}} \mathbf{a}_1 \\ \iota_1(\mathbf{x}) &= \left(0, \sqrt{\frac{m_3}{m_2(1-m_1)}} \mathbf{x}, -\sqrt{\frac{m_2}{m_3(1-m_1)}} \mathbf{x} \right) \in \mathbb{R}^6 \\ \iota_2(\mathbf{y}) &= \left(-\sqrt{\frac{1-m_1}{m_1}} \mathbf{y}, \sqrt{\frac{m_1}{1-m_1}} \mathbf{y}, \sqrt{\frac{m_1}{1-m_1}} \mathbf{y} \right) \in \mathbb{R}^6. \end{aligned} \quad [4]$$

Then

$$\iota_1(\mathbf{x}) + \iota_2(\mathbf{y}) = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3) \in \mathbb{R}^6$$

$$\langle \iota_1(\mathbf{x}), \iota_1(\mathbf{x}) \rangle = |\mathbf{x}|^2, \langle \iota_2(\mathbf{y}), \iota_2(\mathbf{y}) \rangle = |\mathbf{y}|^2, \langle \iota_1(\mathbf{x}), \iota_2(\mathbf{y}) \rangle = 0.$$

[5]

Thus $\mathbb{R}^6 \equiv \{(\mathbf{x}, \mathbf{y}) = (\xi_1, \xi_2, \xi_3, \eta_1, \eta_2, \eta_3), \xi_j, \eta_j \in \mathbb{R}\}$ provides a nice cartesian coordinate system of $(SO(3), \mathbb{R}^6)$ which is advantageous for the $SO(3)$ -harmonic analysis on its function space. Set

$$f_1 = |\mathbf{x}|^2 = \sum \xi_j^2, f_2 = |\mathbf{y}|^2 = \sum \eta_j^2, f_3 = \mathbf{x} \cdot \mathbf{y} = \sum \xi_j \eta_j. \quad [6]$$

It is well known that every $SO(3)$ -invariant polynomial of $\{\xi_j, \eta_j\}$ can be uniquely expressed as a polynomial of $\{f_1, f_2, f_3\}$. Thus (f_1, f_2, f_3) also constitutes a natural coordinate system of the orbit space $\bar{M}$. Set

$$(g^{ij}) = (\nabla f_i \cdot \nabla f_j) = \begin{pmatrix} 4f_1 & 0 & 2f_3 \\ 0 & 4f_2 & 2f_3 \\ 2f_3 & 2f_3 & f_1 + f_2 \end{pmatrix} \quad [7]$$

and let (g_{ij}) be the inverse matrix of (g^{ij}) . Then the orbital distance metric, $d\bar{s}^2$, on $\bar{M}$ is given by

$$d\bar{s}^2 = \sum_{i,j} g_{ij} df_i df_j. \quad [8]$$

LEMMA 1. Let $\Psi = \Psi(f_1, f_2, f_3)$ be an $SO(3)$ -invariant function and $\Delta, \bar{\Delta}$ be the Laplace operator on $(\mathbb{R}^6, ds^2), (\bar{M}, d\bar{s}^2)$ respectively. Then

$$\Delta \Psi = \bar{\Delta} \Psi + \sum_{i,j} g^{ij} \frac{\partial \Psi}{\partial f_i} \frac{\partial}{\partial f_j} \ln v, \quad [9]$$

where $v = [\det(g^{ij})]^{1/2}$ is a constant multiplier of the volume function of $SO(3)$ -orbits.

THEOREM (ref. 5). Set

$$\begin{aligned} \rho &= \sqrt{f_1 + f_2}, \quad \cos \theta = 2 \frac{[f_1 f_2 - f_3^2]^{1/2}}{f_1 + f_2}, \quad \tan \phi = \frac{f_1 - f_2}{2f_3} \\ (\rho \geq 0, \quad 0 \leq \theta \leq \pi/2, \quad -\pi \leq \phi \leq \pi). \end{aligned} \quad [10]$$

Then

$$d\bar{s}^2 = d\rho^2 + \rho^2 d\sigma^2 = d\rho^2 + \frac{1}{4} \rho^2 (d\theta^2 + \sin^2 \theta d\phi^2).$$

$$v = c\rho^3 \cos \theta \text{ (the volume function, cf. Lemma 1)}. \quad [11]$$

Moreover, the subset of $\theta = \pi/2$ represents degenerate m -triangles and it contains three specific points with $\phi = \phi_i, i = 1, 2, 3$, representing the three shapes of binary collisions, where

$$\cos(\phi_i - \phi_j) = \frac{m_i m_j - m_k}{m_i m_j + m_k}, \quad (i, j, k) \sim (1, 2, 3). \quad [12]$$

Furthermore, the distance, r_{ij} , between the i th and j th particles is given by

$$r_{ij}^2 = \frac{1}{2} \frac{(1 - m_k)}{m_i m_j} (1 - \sin \theta \cos(\phi - \phi_k)) \rho^2. \quad [13]$$

Remarks. There are three sets of basic coordinates (i.e., triangular parameters) on $\bar{M}$, namely, $\{I_j\}$ is the natural one for kinematics, $\{f_j\}$ is the natural one for algebra [such as $SO(3)$ -representation] while (ρ, θ, ϕ) is geometrically the optimal one which reveals the sphericity of $(\bar{M}, d\bar{s}^2)$. Therefore, the coordinates (ξ_j, η_j) on $\mathbb{R}^6$ and (f_j) on $\bar{M}$ that are used in the next section are the advantageous ones for obtaining the reduction of Schrödinger's equation from the level of $\mathbb{R}^6$ to the level of $\bar{M} = \mathbb{R}^6/SO(3)$. However, after such a reduction has already been achieved, it is then natural to change to the spherical coordinates (ρ, θ, ϕ) . For example, Lemma 1 can be rewritten as follows.

LEMMA 1'. Let $f = F(\rho, \theta, \phi)$ be an $SO(3)$ -invariant function of $\mathbb{R}^6$. Then

$$\Delta f = \frac{\partial^2 F}{\partial \rho^2} + \frac{5}{\rho} \frac{\partial F}{\partial \rho} + \frac{4}{\rho^2} A F,$$

$$A F = \frac{\partial^2 F}{\partial \theta^2} + (\cot \theta - \tan \theta) \frac{\partial F}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2 F}{\partial \phi^2}. \quad [9']$$

The Reduction of Schrödinger's Equation (1') to PDE Solely in Terms of Triangular Parameters

The reduction of Schrödinger's equation (1') from the level of $\mathbb{R}^6$ to the level of $\bar{M}$ can be regarded as an improvement and a refinement of the usual version of “angular momentum conservation” in quantum mechanics. In terms of the above coordinates, the angular momentum operator is the following vector-value operator, namely

$$\mathbf{J} = (J_1, J_2, J_3) = -\sqrt{-1} \{ \mathbf{x} \times \nabla_\xi + \mathbf{y} \times \nabla_\eta \},$$

$$\nabla_\xi = \left(\frac{\partial}{\partial \xi_1}, \frac{\partial}{\partial \xi_2}, \frac{\partial}{\partial \xi_3} \right), \quad \nabla_\eta = \left(\frac{\partial}{\partial \eta_1}, \frac{\partial}{\partial \eta_2}, \frac{\partial}{\partial \eta_3} \right). \quad [14]$$

Moreover,

$$J^2 = J_1^2 + J_2^2 + J_3^2, \quad J_+ = J_1 + \sqrt{-1} J_2, \quad J_- = J_1 - \sqrt{-1} J_2 \quad [15]$$

are some of its associated operators often useful in the study

of angular momentum in quantum mechanics. Set

$$\begin{aligned}\Delta_\xi &= \sum \frac{\partial^2}{\partial \xi_j^2}, \quad \Delta_\eta = \sum \frac{\partial^2}{\partial \eta_j^2}, \quad \Delta_{\xi\eta} = \sum \frac{\partial^2}{\partial \xi_j \partial \eta_j} \\ u &= \xi_1 + \sqrt{-1}\xi_2, \quad v = \eta_1 + \sqrt{-1}\eta_2, \\ w &= (\xi_2\eta_3 - \xi_3\eta_2) + \sqrt{-1}(\xi_3\eta_1 - \xi_1\eta_3) \\ h_{\alpha,\beta} &= \frac{1}{\alpha!\beta!} u^\alpha v^\beta, \quad h_{\alpha,\beta}^* = \frac{1}{(\alpha-1)!(\beta-1)!} u^{\alpha-1} v^{\beta-1} w \\ h_{\alpha,\beta}^{(k)} &= J^k h_{\alpha,\beta}, \quad 0 \leq k \leq 2(\alpha + \beta); \quad h_{\alpha,\beta}^{*(k)} \\ &= J^k h_{\alpha,\beta}^*, \quad 0 \leq k \leq 2(\alpha + \beta - 1).\end{aligned}\quad [16]$$

Then, it is easy to check that

$$[J_i, \Delta_\xi] = [J_i, \Delta_\eta] = [J_i, \Delta_{\xi\eta}] = 0, \quad i = 1, 2, 3 \quad [17]$$

and both $h_{\alpha,\beta}$ and $h_{\alpha,\beta}^*$ are common zeros of Δ_ξ , Δ_η , and $\Delta_{\xi\eta}$. Hence, it follows from Eqs. 16 and 17 that all $h_{\alpha,\beta}^{(k)}$ and $h_{\alpha,\beta}^{*(k)}$ are common zeros of Δ_ξ , Δ_η , and $\Delta_{\xi\eta}$.

THEOREM 1 (ref. 6). *Let $\mathbb{C}[\xi, \eta]$ be the ring of complex coefficient polynomials in $\{\xi_j\}$ and $\{\eta_j\}$ and $\mathcal{R}$ be the sub-ring of $SO(3)$ -invariant ones (i.e., polynomials in $\{f_j\}$). Then $\mathbb{C}[\xi, \eta]$ is a “vector space” over $\mathcal{R}$ with $\{h_{\alpha,\beta}^{(k)}; h_{\alpha,\beta}^{*(k)}\}$ as a specific basis, meaning that every element of $\mathbb{C}[\xi, \eta]$ can be uniquely expressed as a linear combination of $\{h_{\alpha,\beta}^{(k)}; h_{\alpha,\beta}^{*(k)}\}$ with coefficients in $\mathcal{R}$.*

Remarks. The above specific family of basis-functions is characterized by the following properties up to constant factors:

- (i) biharmonicity—i.e., common zeros of Δ_ξ , Δ_η , and $\Delta_{\xi\eta}$,
- (ii) bihomogeneity in $\{\xi_j\}$ and $\{\eta_j\}$,
- (iii) common eigenfunctions of J^2 and J_3 , namely

$$\begin{aligned}J^2 h_{\alpha,\beta}^{(k)} &= (\alpha + \beta)(\alpha + \beta + 1) h_{\alpha,\beta}^{(k)}, \\ J^2 h_{\alpha,\beta}^{*(k)} &= (\alpha + \beta)(\alpha + \beta - 1) h_{\alpha,\beta}^{*(k)}, \\ J_3 h_{\alpha,\beta}^{(k)} &= (\alpha + \beta - k) h_{\alpha,\beta}^{(k)}, \\ J_3 h_{\alpha,\beta}^{*(k)} &= (\alpha + \beta - k - 1) h_{\alpha,\beta}^{*(k)}.\end{aligned}\quad [18]$$

THEOREM 2 (ref. 6). *For each given pair of azimuthal and magnetic quantum numbers (ℓ, m) , $|m| \leq \ell > 0$, there exist two*

separate quantum types whose wave functions are respectively given by

$$\Psi = \sum_{j=0}^{\ell} \psi_j h_{\ell-j,j}^{(k)} \text{ and } \Psi^* = \sum_{j=1}^{\ell} \psi_j h_{\ell-j+1,j}^{*(k)}, \quad [19]$$

where $k = \ell - m$ and $\{\psi_j\}$ (resp $\{\psi_j^*\}$) are $(\ell + 1)$ -tuple (resp ℓ -tuple) of $SO(3)$ -invariant functions satisfying the following systems of PDE, respectively,

$$\begin{aligned}-\frac{\hbar^2}{2\mu} \left\{ \Delta \psi_j + 4(\ell - j) \frac{\partial \psi_j}{\partial f_1} + 4j \frac{\partial \psi_j}{\partial f_2} + 2j \frac{\partial \psi_{j-1}}{\partial f_3} \right. \\ \left. + 2(\ell - j) \frac{\partial \psi_{j+1}}{\partial f_3} \right\} + U \psi_j = E \psi_j, \quad (0 \leq j \leq \ell) \quad [20] \\ -\frac{\hbar^2}{2\mu} \left\{ \Delta \psi_j^* + 4(\ell - j + 1) \frac{\partial \psi_j^*}{\partial f_1} + 4j \frac{\partial \psi_j^*}{\partial f_2} + 2(j - 1) \frac{\partial \psi_{j-1}^*}{\partial f_3} \right. \\ \left. + 2(\ell - j) \frac{\partial \psi_{j+1}^*}{\partial f_3} \right\} + U \psi_j^* = E \psi_j^*, \quad (1 \leq j \leq \ell), \quad [20^*]\end{aligned}$$

where $\Delta \psi_j$ and $\Delta \psi_j^*$ are given by formula 9).

Remarks. C. N. Yang pointed out the following correlation between the above separation into two quantum types and the parity separation. Since the invariant functions are always even functions while $h_{\alpha,\beta}^{(k)}$ and $h_{\alpha,\beta}^{*(k)}$ are even or odd according to $(\alpha + \beta)$ being even or odd, the two types of wave functions Ψ and Ψ^* of Eq. 19 are always of different parity.

The proofs of the above results as well as the next stage of reduction to a system of algebraic linear equations will occur in succeeding papers, namely refs. 3–6.

1. Bethe, H. A. & Salpeter, E. E. (1957) *Quantum Mechanics of One- and Two-Electron Atoms* (Springer, Berlin).
2. (1963) *Rev. Mod. Phys.* **35** (Festschrift in Honor of Hylleraas).
3. Hsiang, W. T. & Hsiang, W. Y. (1997) *On the Reduction of Schrödinger's Equation of Three-Body Problem to a System of ODE in Radial Parameter* (Center for Pure and Applied Mathematics, Univ. of California, Berkeley), PAM-697, preprint.
4. Hsiang, W. T. & Hsiang, W. Y. (1997) *On the Reduction of Schrödinger's Equation of Three-Body Systems to System of Linear Algebraic Equations* (Center for Pure and Applied Mathematics, Univ. of California, Berkeley), PAM-699, preprint.
5. Hsiang, W. Y. & Straume, E. (1995) *Kinematic Geometry of Triangles with Given Mass Distribution* (Center for Pure and Applied Mathematics, Univ. of California, Berkeley), PAM-636, preprint.
6. Hsiang, W. Y. (1996) *Kinematic Geometry of Mass Triangles and the Three-Body Problem in Quantum Mechanics* (Center for Pure and Applied Mathematics, Univ. of California, Berkeley), PAM-682, preprint.