Quantum Monodromy and Symplectic Invariants of the Spheroidal Harmonics System

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Introduction

Recent work by Dullin and Waalkens showed that the Hydrogen atom in prolate spheroidal coordinates has quantum monodromy [1]. Our first main result deals with this phenomena; we show that the quantum integrable system obtained by separating the Laplacian in prolate spheroidal coordinates also has quantum monodromy. We call this the spheroidal harmonics system.

Our second main result deals with the semi-global symplectic invariants. Introduced by Vu Ngoc in 2003, these invariants describe the behaviour of the actions near the Focus-Focus point [5]. The work of Pelayo and Vu Ngoc led to a global classification system of 2 dimensional semi toric systems [3, 4]. The semi-global symplectic invariants, along with 4 other symplectic invariants were shown to globally classify this class of integrable systems. We compute the semi-global symplectic invariants for the spheroidal harmonics system.

The Spheroidal Harmonics Integrable System

We study the Laplacian in 3 degrees of freedom:

$$H = \frac{1}{2}\left(p_x^2 + p_y^2 + p_z^2\right).$$

We set $\boldsymbol{Q} = (q_x, q_y, q_z)$ and $\boldsymbol{P} = (p_x, p_y, p_z)$ as the positions and linear momentum respectively. Define $\boldsymbol{L} = \boldsymbol{Q} \times \boldsymbol{P} = (l_x, l_y, l_z)$ as the vector of angular momenta. We perform a symplectic reduction that identifies the straight lines of the flow of H to points and fixes $H = 1/2$. The system is reduced by using the linear and angular momenta as new coordinates. The associated Poisson matrix is

$$B = \begin{pmatrix} \boldsymbol{0} & \hat{\boldsymbol{P}} \\ \hat{\boldsymbol{P}} & \hat{\boldsymbol{L}} \end{pmatrix} \tag{1}$$

For a vector $\boldsymbol{v} \in \mathbb{R}^3$, the corresponding hat matrix is the anti-symmetric matrix $\hat{\boldsymbol{v}}$ defined by

$$\hat{\boldsymbol{v}}\boldsymbol{u} = \boldsymbol{v} \times \boldsymbol{u} \ \forall \boldsymbol{u} \in \mathbb{R}^3.$$

This system has 2 Casimirs:

- $\mathcal{C}_1 = \boldsymbol{P}^2$ means the linear momentum space is compact. For simplicity, we set $\mathcal{C}_1 = 1$.
- $\mathcal{C}_2 = \boldsymbol{P} \cdot \boldsymbol{L}$. Since $\boldsymbol{L} = \boldsymbol{Q} \times \boldsymbol{P}$, this means $\mathcal{C}_2 = 0$. Consequently, the tangent space of the $\boldsymbol{P}$ sphere is the $\boldsymbol{L}$ space.

The reduced phase space is therefore T^*S^2.

Prolate spheroidal coordintes are defined by the transformation

$$\begin{aligned} x &= a\sqrt{\left(\xi^2 - 1\right)\left(1 - \eta^2\right)}\cos(\phi) \\ y &= a\sqrt{\left(\xi^2 - 1\right)\left(1 - \eta^2\right)}\sin(\phi) \\ z &= a\xi\eta \end{aligned} \tag{2}$$

where $\eta \in [-1, 1]$, $\xi \in [0, \infty)$ and $\phi \in [0, 2\pi)$. We may re-write H in prolate spheroidal coordinates as

$$H = \frac{1}{2a^2}\left(\frac{\left(\eta^2 - 1\right)p_\eta^2 - \left(\xi^2 - 1\right)p_\xi^2}{\left(\eta - \xi\right)\left(\eta + \xi\right)} - \frac{p_\phi^2}{\left(\eta^2 - 1\right)\left(\xi^2 - 1\right)}\right). \tag{3}$$

Separating the Hamilton-Jacobi Equation for (3) gives $L_z = l_z$ and

$$G = \frac{1}{2}\left(l_x^2 + l_y^2 + l_z^2 - a^2\left(p_x^2 + p_y^2\right)\right) \tag{4}$$

as separation constants. We call the integrable system (G, L_z) the spheroidal harmonics integrable system.

Quantum Monodromy in the Spheroidal Harmonics System

Separating the Schrödinger equation in prolate spheroidal coordinates yields 2 ordinary differential equations. The eigenvalues of these ODES define a quantum integrable system when written in the $(\boldsymbol{P}, \boldsymbol{L})$ coordinates. The first of these equations gives L_z; the second is the spheroidal wave equation:

$$\psi_\nu\left(g - \frac{l^2}{1 - \nu^2} + \frac{2\mu}{\hbar^2}Ea^2\left(1 - \nu^2\right)\right) + \left(1 - \nu^2\right)\psi_\nu'' - 2\nu\psi_\nu' = 0 \tag{5}$$

Thus, G is the eigenvalue of the spheroidal wave equation. Using the `SpheroidalEigenvalue` function in Mathematica, we produce the lattice of the joint spectrum (G, L_z) in Figure (1), which possesses quantum monodromy about the origin. If 2 basis vectors are v_1 (vertical) and v_2 (horizontal), then over one cycle, we have a basis transformation

$$\begin{pmatrix} v_1' \\ v_2' \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ k & 1 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \tag{6}$$

where in this case $k = 2$; implying the existence of a doubly pinched torus in the phase space.

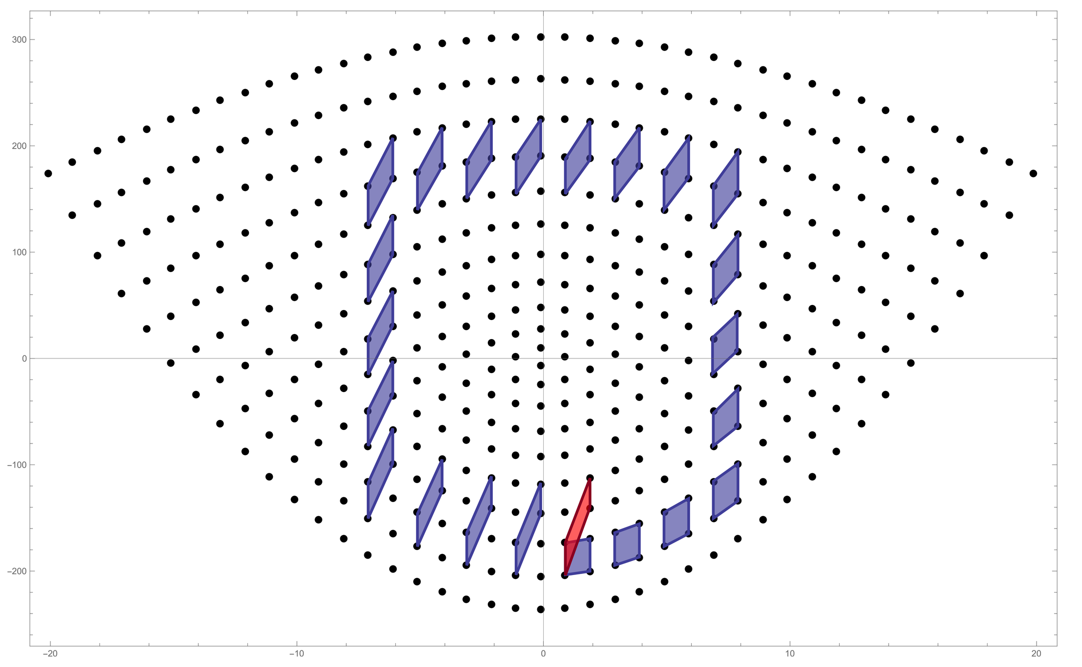

Figure 1: Joint spectrum of the spheroidal harmonics system (G, L_z). When transported around the Focus-Focus point, the unit cell is transformed according to (6).

Critical Points

Critical points of the combined system are found by solving

$$B\nabla G + \beta B\nabla L_z = 0$$

where $\beta \in \mathbb{R} \setminus \{0\}$. For a given $L_z = l$, the critical points of the combined (G, L_z) system are:

1. $\boldsymbol{P} = (0, 0, \pm 1)$ and $\boldsymbol{L} = (0, 0, 0)$ with β free. The critical value is $(G, L_z) = (0, 0)$.
2. $\boldsymbol{P} = (p_x, p_y, 0)$ and $\boldsymbol{L} = (0, 0, l)$ with $\beta = l$. The critical value is $(G, L_z) = \left(\frac{1}{2}\left(l^2 - a^2\right), l\right)$.

- The Poles of the $\boldsymbol{P}$ sphere are Focus-Focus points with eigenvalues $\lambda = \pm a p_z \pm i\beta$ where $\beta \in \mathbb{R} \setminus \{0\}$ is a free parameter.
- The family of critical points along the equator are elliptic-transversal critical points.
- We show the critical points on the $\boldsymbol{P}$ sphere and the bifurcation diagram of the energy momentum map in Figure (2)

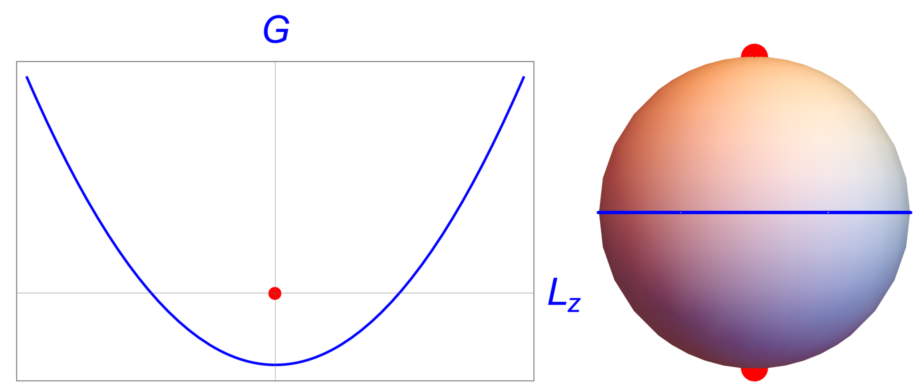

Figure 2: (a) Bifurcation diagram of the energy momentum map. (b) $\boldsymbol{P}$ sphere with the Focus-Focus (red) and elliptic-transversal (blue) critical points.

Singular Reduction

To prove the existence of quantum monodromy, we show that the pre-image of the Focus-Focus critical value is a doubly pinched torus in the $(\boldsymbol{P}, \boldsymbol{L})$ phase space.

- To do this, we use singular reduction with respect to the flow of L_z.
- The invariants of this symmetry are

$$b_1 := p_z \qquad b_2 := l_x^2 + l_y^2 \qquad b_3 := l_x p_y - l_y p_x$$

- The Poisson structure of these 3 invariants is encapsulated by the matrix

$$B_{\text{inv}} = \begin{pmatrix} 0 & 2b_3 & 1 - b_1^2 \\ -2b_3 & 0 & 2b_1 l^2 + 2b_1 b_2 \\ b_1^2 - 1 & -2b_1 l^2 - 2b_1 b_2 & 0 \end{pmatrix}.$$

- This structure has one further Casimir, $\mathcal{C}_3$, due to the b_i's being functionally dependent:

$$\mathcal{C}_3 = \left(1 - b_1^2\right)\left(b_2 + l^2\right) - l^2 - b_3^2. \tag{7}$$

By solving $\nabla\mathcal{C}_3 = 0$, we find the critical points of $\mathcal{C}_3$ are $(\pm 1, 0, 0)$ with $l = 0$ and the critical value is $\mathcal{C}_3 = 0$.

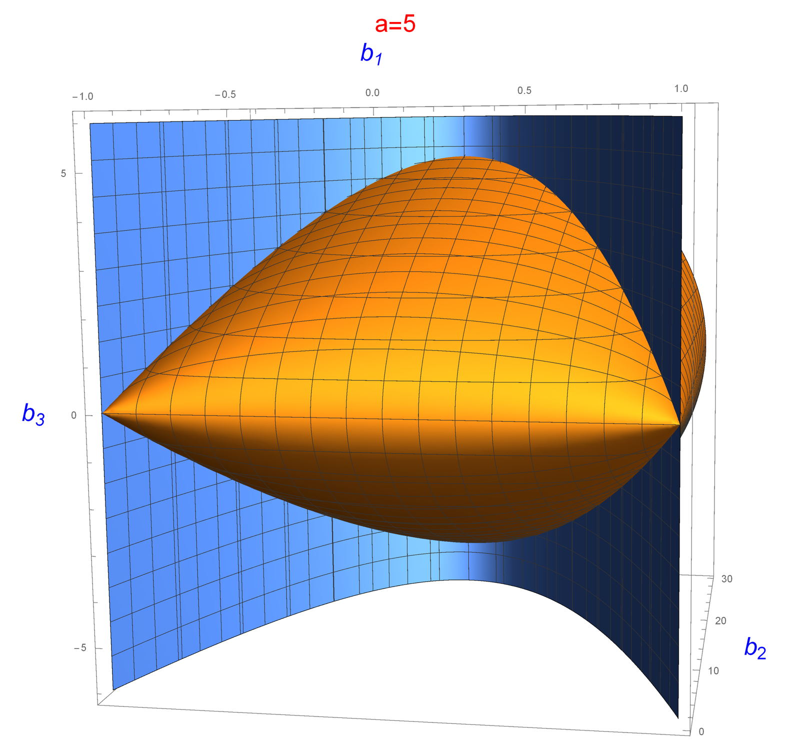

Figure 3: Blue: $G = 0$ and Orange: $\mathcal{C}_3 = 0$ for $l = 0$. Note the singular points at $(\pm 1, 0, 0)$.

Reconstruction

Plotting the surfaces $G = 0$ and $\mathcal{C}_3 = 0$ in Figure (3), we observe that the intersection is the union of two parabolic sections which are symmetric around the planes $b_1 = 0$ and $b_3 = 0$.

- The pre-image of each point on the intersection corresponds to a circle on the $\boldsymbol{P}$ sphere with the same p_z value and radius $r(p_z) = \sqrt{1 - p_z^2}$.
- For a given $\boldsymbol{P}$, we find l_x and l_y such that $\boldsymbol{P} \cdot \boldsymbol{L} = 0$ and $l_x p_y - l_y p_x = b_3$. These are linear equations in l_x and l_y which we can solve.
- Doing so, we find the (doubly pinched) Liouville torus parameterised by p_z and ϕ as

$$\begin{aligned} \boldsymbol{P} &= \left(r(p_z)\cos(\phi), r(p_z)\sin(\phi), p_z\right) \\ \boldsymbol{L} &= \left(\pm r(p_z)\sin\phi, \mp r(p_z)\cos\phi, 0\right) \end{aligned} \tag{8}$$

where $\phi = \arctan\left(\frac{p_y}{p_x}\right)$.

This means that each point on the $\boldsymbol{P}$ sphere (other than the poles) has 2 values of $\boldsymbol{L}$ associated with it.

Local Symplectic Coordinates and Action Variables

We introduce local symplectic coordinates on the $\boldsymbol{P}$ sphere

$$q_1 = p_z \quad q_2 = \arctan\left(\frac{p_y}{p_x}\right) \quad p_1 = \frac{l_x p_y - l_y p_x}{1 - p_z^2} \quad p_2 = l_z.$$

- In these new coordinates, we re-write G from (4) as

$$p_1^2 = \frac{1}{\left(1 - q_1^2\right)^2}\left(a^2\left(1 - q_1^2\right)^2 + 2g\left(1 - q_1^2\right) - l^2\right). \tag{9}$$

- We find that the Caustics on the $\boldsymbol{P}$ sphere are located at

$$r_{1\pm} = \pm\sqrt{1 + \frac{g - \sqrt{g^2 + a^2 l^2}}{a^2}} \quad r_{2\pm} = \pm\sqrt{1 + \frac{g + \sqrt{g^2 + a^2 l^2}}{a^2}}$$

- Due to the singularity at $q_1 = 1$, we consider q_1 and p_1 as complex variables.
- In the complex q_1 plane, we define the β cycle to encircle the interval $[r_{1-}, r_{1+}]$ and the α cycle to encircle the interval $[r_{1+}, r_{2+}]$.
- These are fundamental paths on the Riemann torus defined by the numerator of (9).
- Plotting (9) in Figure (5), we see that over the β cycle, p_1 is real (blue). Over the α cycle p_1 is imaginary (orange).
- Integrating p_1 over these cycles gives the real and imaginary actions respectively:

$$I = \frac{1}{2\pi}\oint_\beta p_1 dq_1 \quad J = \frac{1}{2\pi i}\oint_\alpha p_1 dq_1. \tag{10}$$

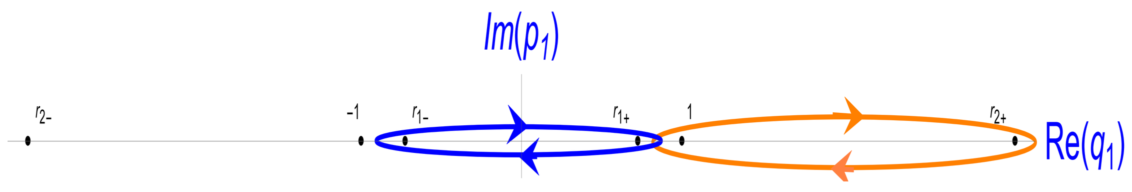

Figure 4: Complex q_1 plane with the β (blue) and α (orange) cycles.

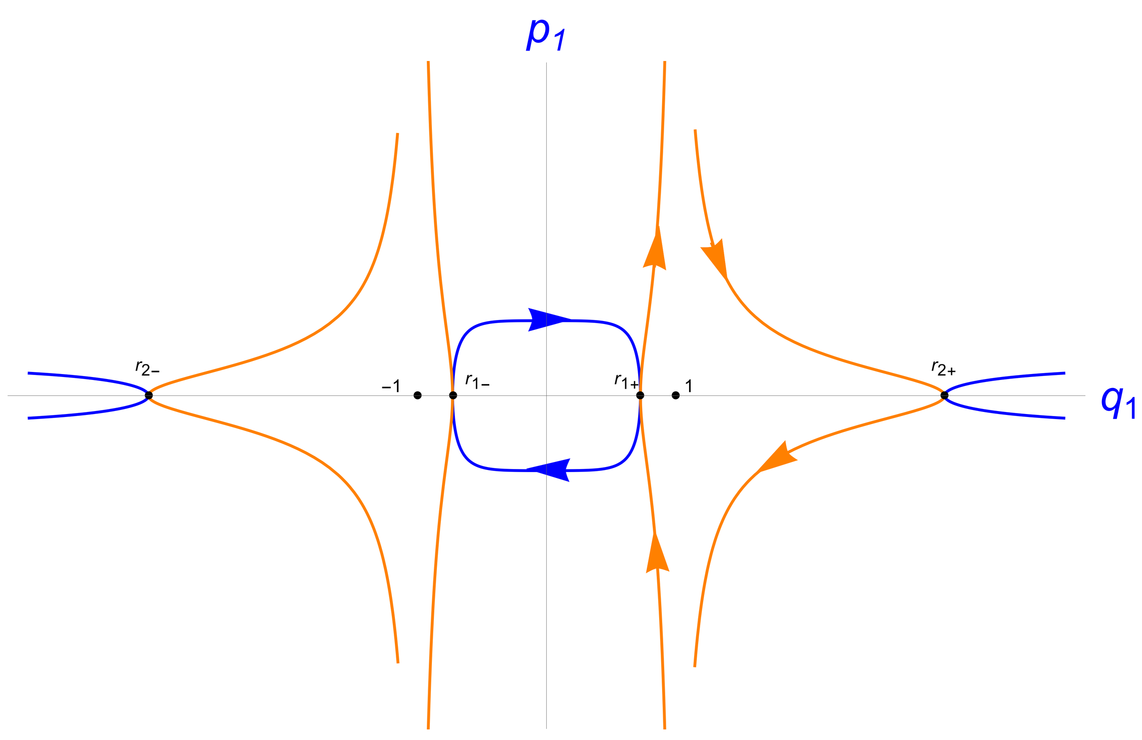

Figure 5: Phase portrait of (9) with real values of p_1 in blue and imaginary values in orange.

Discrete Symmetry Reduction

- We use discrete symmetry reduction to identify the two Focus-Focus points. We find the following 3 canonical symmetries that preserve the Casimirs

$$\begin{aligned} \mathcal{S}_1\left(p_z, l_x, l_y\right) &\to \left(-p_z, -l_x, -l_y\right) \\ \mathcal{S}_2\left(p_x, p_y, l_x, l_y\right) &\to \left(-p_x, -p_y, -l_x, -l_y\right) \\ \mathcal{S}_3\left(p_x, p_y, p_z\right) &\to \left(-p_x, -p_y, -p_z\right). \end{aligned} \tag{11}$$

- We only quotient by $\mathcal{S}_3$, otherwise the resulting space will not be smooth. The reduced phase space is $T^*\left(\mathbb{RP}^2\right)$. This reduces the β cycle by half, but leaves the α cycle unaffected.

The Semi Global Symplectic Invariants

Following [2], expanding J in the Focus-Focus Limit and inverting the series with respect to g gives the Birkhoff Normal Form:

$$g(J, l) = J + \frac{1}{4}\left(J^2 + l^2\right) - \frac{J}{16}\left(J^2 + l^2\right) + \frac{1}{128}\left(5J^4 + 6J^2 l^2 + l^4\right) + \ldots. \tag{12}$$

Expanding $I(g, l)$ in the Focus-Focus limit and substituting in the Birkhoff Normal form for g gives

$$2\pi I(J, l) = 2\pi I_0 - \Re\left(\hat{j}\ln\left(\hat{j}\right) - \hat{j}\right) + \sigma(J, l)$$

where I_0 is a constant, $\hat{j} = J + il$ and $\sigma(J, l)$ is the semi-global symplectic invariant. We therefore have the Semi-Global Symplectic Invariants of the Spheroidal Harmonics System:

$$\sigma(J, l) = J\log(8) + \frac{1}{8}\left(3J^2 + l^2\right) - \frac{1}{32}\left(5J^3 + 3Jl^2\right) + \frac{165J^4 + 138J^2 l^2 + 13l^4}{1536} + \ldots.$$

Conclusion and Further Work

- We have shown that the spheroidal harmonics system has quantum monodromy and computed its Taylor series invariants.
- **Future work**: We can use the invariants to obtain higher order approximations to the spheroidal eigenvalues using the Bohr Sommerfeld quantisation of the actions.

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