Monodromy in the Kepler Problem

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Geometric aspects of momentum maps and integrabiliy
CSF Ascona, April 2018

joint work with Holger Waalkens, Groningen

HRD, Waalkens, PRL 120:020507 (2018)

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Plan

- Review of Kepler problem
- (super) integrable systems
- Quantum integrable systems, joint spectrum
- Quantum monodromy in Kepler
- Toric and semi-toric systems
- Spheroidal harmonics (Laplacian)

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Kepler problem (in 3D)

$$\mathbf{r} = (x, y, z)^t, \mathbf{p} = (\dot{x}, \dot{y}, \dot{z})^t, r = |\mathbf{r}|, \quad \dot{\mathbf{r}} = \mathbf{p}, \dot{\mathbf{p}} = -\frac{\mathbf{r}}{r^3}$$

- Liouville integrable: $H = \frac{1}{2}\mathbf{p}^2 - \frac{1}{r}, \quad \mathbf{L} = \mathbf{r} \times \mathbf{p}$
  (H, $|L|^2$, L_z) three integrals in involution

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  (H, $|L|^2$, L_z) three integrals in involution
- more integrals (super-integrable): $\mathbf{e} = \mathbf{p} \times \mathbf{L} - \frac{\mathbf{r}}{r}$
  Runge-Lenz vector
- 7 integrals? Only 5 independent (in 6D)
  => EVERY orbit is periodic
- very special, but very important; similarly:
  isotropic harmonic oscillator, free particle,
  geodesic flow on spheres

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Hydrogen atom

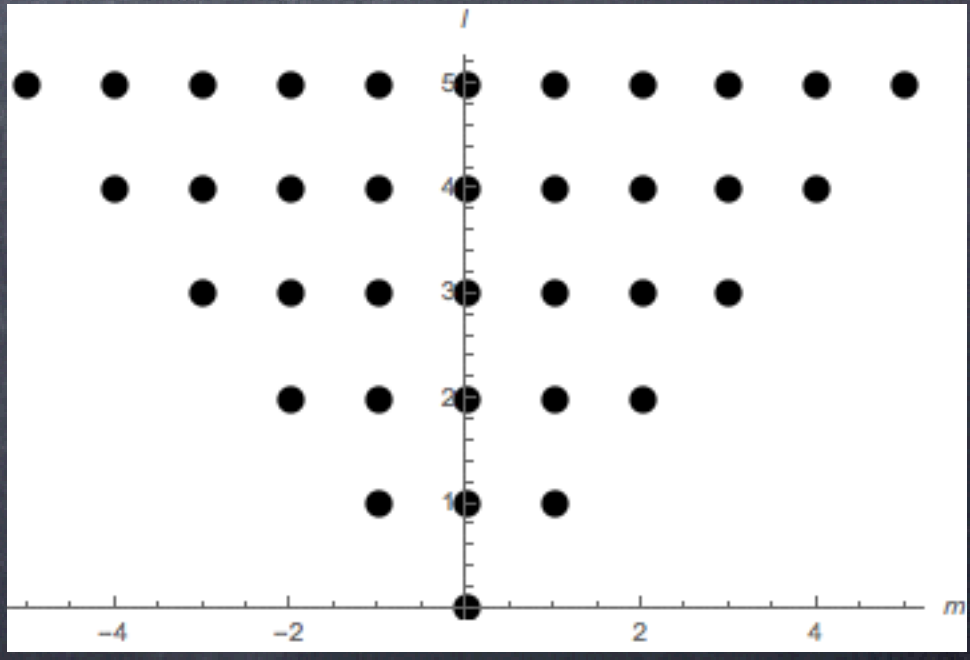
$$\mathbf{r} = (x, y, z)^t, \mathbf{p} = (\dot{x}, \dot{y}, \dot{z})^t, r = |\mathbf{r}|, \quad \dot{\mathbf{r}} = \mathbf{p}, \dot{\mathbf{p}} = -\frac{\mathbf{r}}{r^3}$$

- $H = \frac{1}{2}p^2 - \frac{1}{r}$ (Kepler in 3D)
- $\hat{H} = -\frac{1}{2}\hbar^2\nabla^2 - \frac{1}{r}$ (Schrödinger operator)
- $\hat{H}\psi = E\psi$ (Schrödinger equation, PDE)
- eigenvalues $E = -1/(2n^2)$, n=1,2,3,...
- degenerate eigenspace, multiplicity n^2

Quantum Integrable System

- quantum integrable system with classical limit
- separation of variables in spherical coordinates gives 3 commuting 2nd order differential operators $(H, |L|^2, L_z)$ on $L^2(R^3)$
- joint spectrum of $(H, |L|^2, L_z)$ is lattice $(-1/(2n^2), l(l+1), m)$, $n=1,2,\ldots$, $l=0,1,\ldots,n-1$, $m=-l,\ldots,l$
- for fixed n (e.g. n=6):

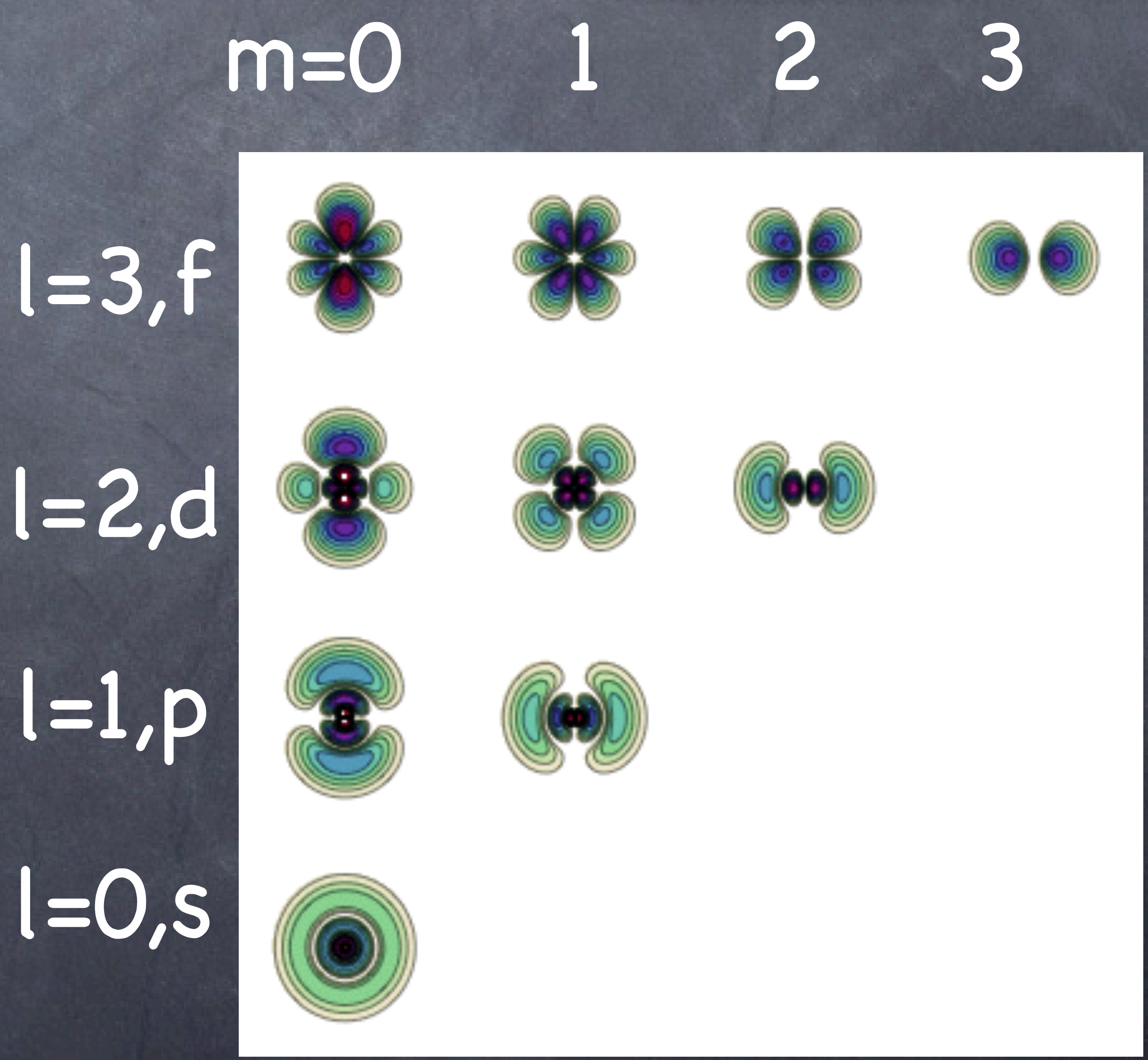
n=6:



Hydrogen Orbitals

- separation of variables in spherical coordinates
- Laguerre polynomials for radial part
- spherical harmonics $Y_l^m()$
- wave function Ψ_{nlm}
- slice of $|\Psi_{nlm}|$:

n=4:



Super-integrable Kepler

- integrals: $H = \frac{1}{2}\mathbf{p}^2 - \dfrac{1}{r}, \quad \mathbf{L} = \mathbf{r} \times \mathbf{p}$
- more integrals: $\mathbf{e} = \mathbf{p} \times \mathbf{L} - \mathbf{r}/r$
  Laplace-Runge-Lenz vector
- full symmetry algebra so(4): $\mathbf{L}, \mathbf{K} = n\mathbf{e}, \quad H = -\dfrac{1}{2n^2}$
- Casimirs $\mathbf{L} \cdot \mathbf{K} = 0, \quad \mathbf{L}^2 + \mathbf{K}^2 = n^2$
- maximally super-integrable
  every orbit is periodic
  Integrals do not all have vanishing Poisson bracket!

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so(4) algebra

- either with {,} (or in QM similarly with [,]):
- $\{ L_i, L_j \} = e_{ijk} L_k$
  $\{ L_i, K_j \} = e_{ijk} K_k$
  $\{ K_i, K_j \} = e_{ijk} L_k$
- Casimirs $(K+L)^2 = n^2$ and $(K-L)^2 = n^2$
- hence symplectic leaf is $S^2 x S^2$
- a compact symplectic manifold
  NB: reduction of maximally superintegrable systems with respect to Hamiltonian flow typically leads to compact symplectic mflds.

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Super- vs. Liouville-integrable

- Liouville-integrable: n independent commuting integrals
- Conjecture that non-commutative integrability implies Liouville integrability (Mischenko-Fomenko '78)
- proved by Sadetov '03, Bolsinov '05 (but not proven in the same functional class)
- key to our analysis is this simple observation:

A superintegrable system may be Liouville integrable in non-equivalent ways

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Liouville integrable realisations

- Definition: Given a super-integrable Hamiltonian H, a Liouville integrable realisation of H is a collection of functions $(H, F_2, \ldots, F_n)$ in involution, independent almost everywhere.
- For maximally super-integrable H there are infinitely many Liouville integrable realisations

Another Liouville integrable realisation of Kepler

- $(H, |L|^2, L_z)$ is the standard Liouville integrable realisation of the Kepler problem
- (H, G, L_z) with $G = |L|^2+2ae_z$ is another Liouville integrable realisation of the Kepler problem
- a is deformation parameter, for $a=0$: $G=|L|^2$
- corresponding statements for the quantum case; use quantum Laplace-Runge-Lenz vector

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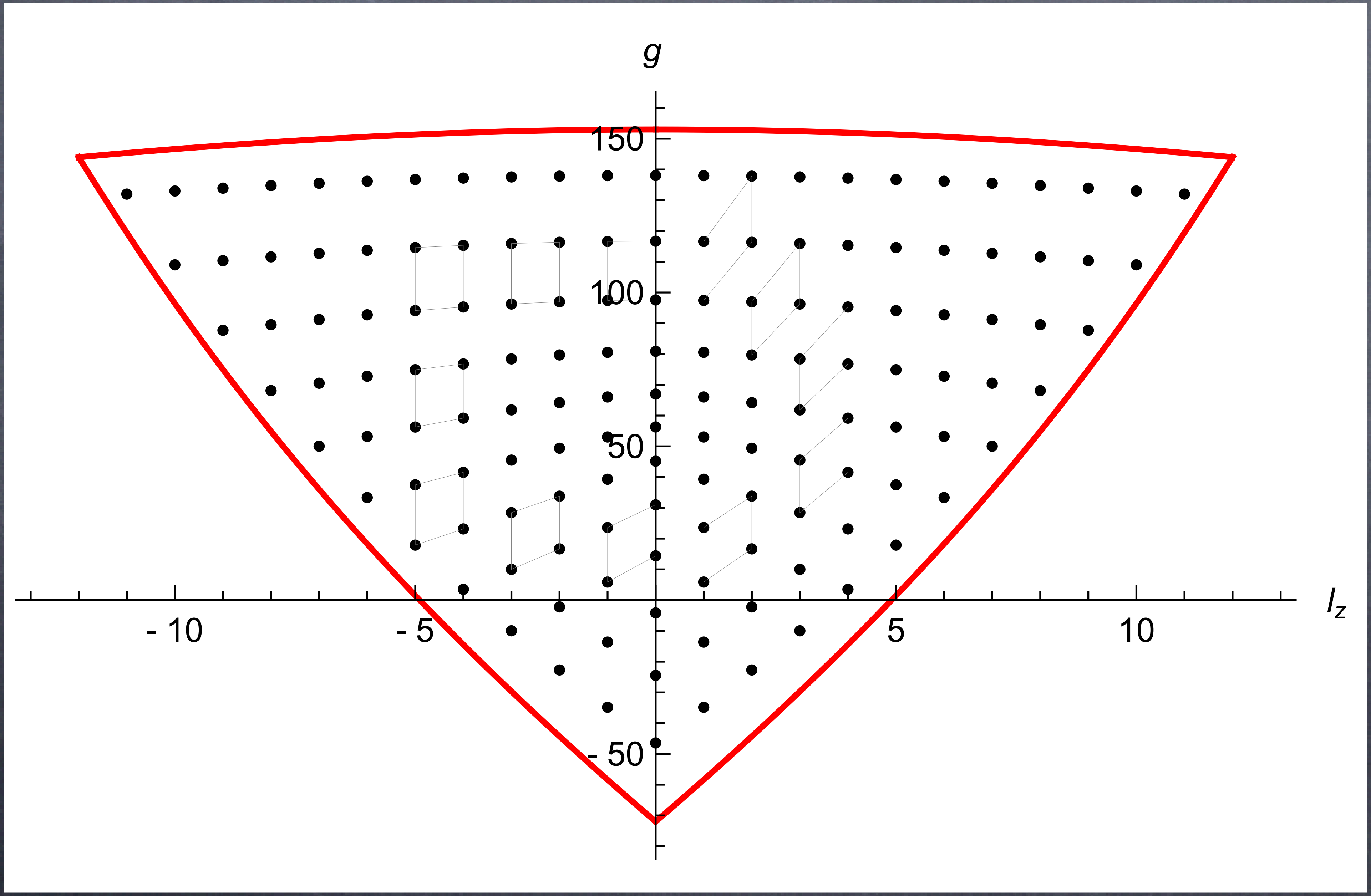
- classical: it appears arbitrary to consider Liouville integrable realisations of a super-integrable system
- quantum: each realisation should be studied since each gives a set of commuting observables, which can hence be **measured simultaneously**
- can measure $(H, |L|^2, L_z)$ simultaneously and can measure (H, G, L_z) simultaneously, but cannot measure $(H, |L|^2, G, L_z)$ simultaneously

Joint spectrum (G, L_z)

$H=-1/(2n^2)$ fixed



n=12

a=28.8

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Monodromy in Hydrogen

- Consider the quantum integrable system (H,G,L_z) in the semiclassical limit.
- Theorem (Waalkens and HRD): For fixed n with $n^2 > a$ the joint spectrum of (G,L_z) has quantum monodromy. The joint spectrum is locally a lattice, but there is only one globally well defined quantum number m, the eigenvalue of L_z.

HRD, Waalkens, PRL 120:020507 (2018)

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The Kepler system on $S^2 x S^2$

- commuting fct. in K,L-variables: $G = |L|^2 + 2aK_z/n$, L_z
- on $S^2 x S^2$: Coordinates $S_1=(x_1,y_1,z_1)$, $S_2=(x_2,y_2,z_2)$
  radius of spheres: n
  $G = |S_1+S_2|^2 + 2a(z_1-z_2)/n$, $L_z = z_1+z_2$
- commuting fct. $x_1x_2+y_1y_2+z_1z_2 + f(z_1,z_2)$ and z_1+z_2;
  here $f(z_1,z_2) = b(z_1-z_2)$
- other systems on $S^2 x S^2$ with different f:
  * coupled spins: Zhilinskii & Sadovski '99, Floch & Pelayo '16, Jaume Alonso & HRD & Hohloch '18, Jaume Alonso's poster
  * geodesic flow on S^3: Diana Nguyen's poster
  * Hydrogen EM field: Cushman & Sadovskii '99, & Efstathiou '07
  * 2FF: Hohloch & Palmer '18

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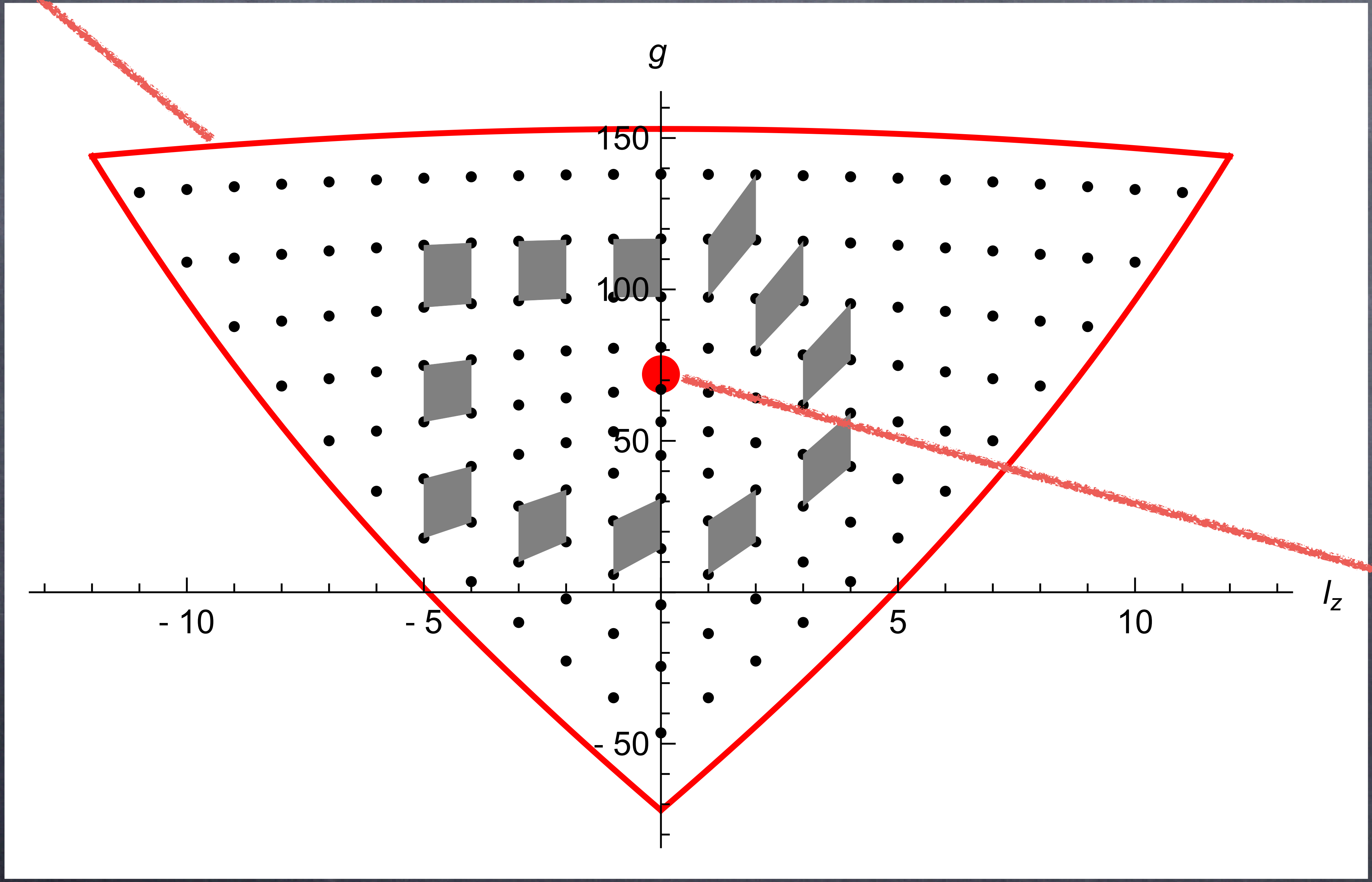
Joint spectrum (G, L_z)

critical values of classical momentum map

$H=-1/(2n^2)$ fixed



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a=28.8

focus-focus value

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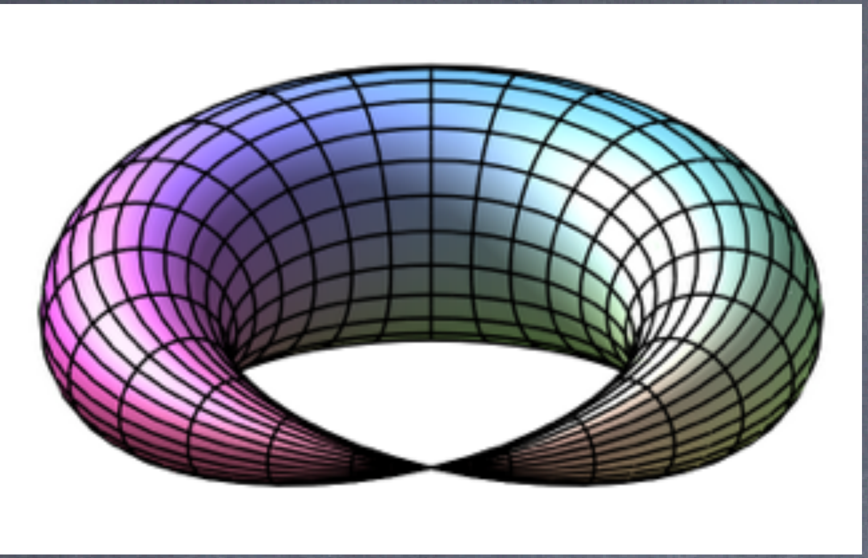
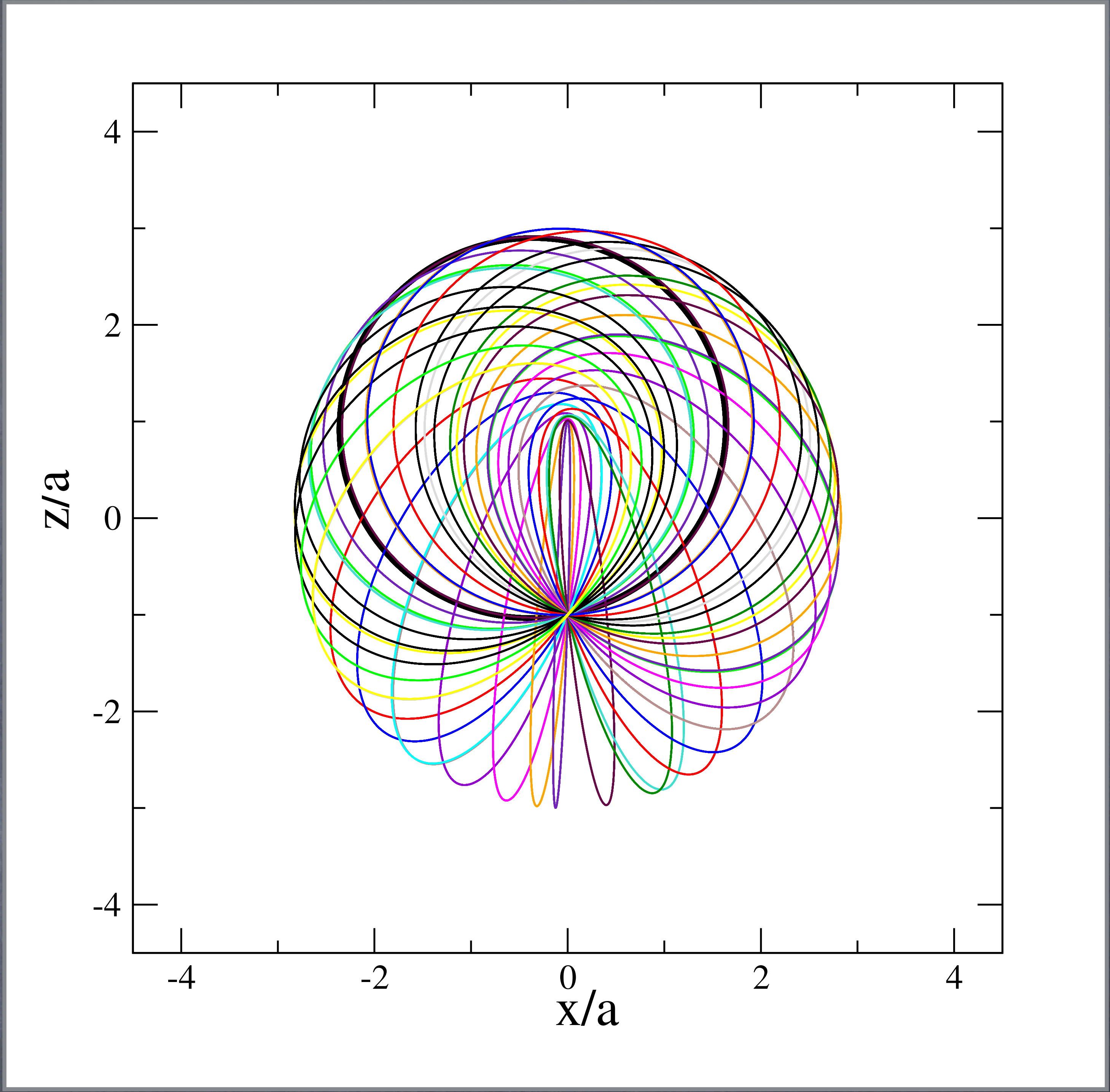
pinched torus



pre-image of
focus-focus value



Kepler ellipses forming
the pinched torus

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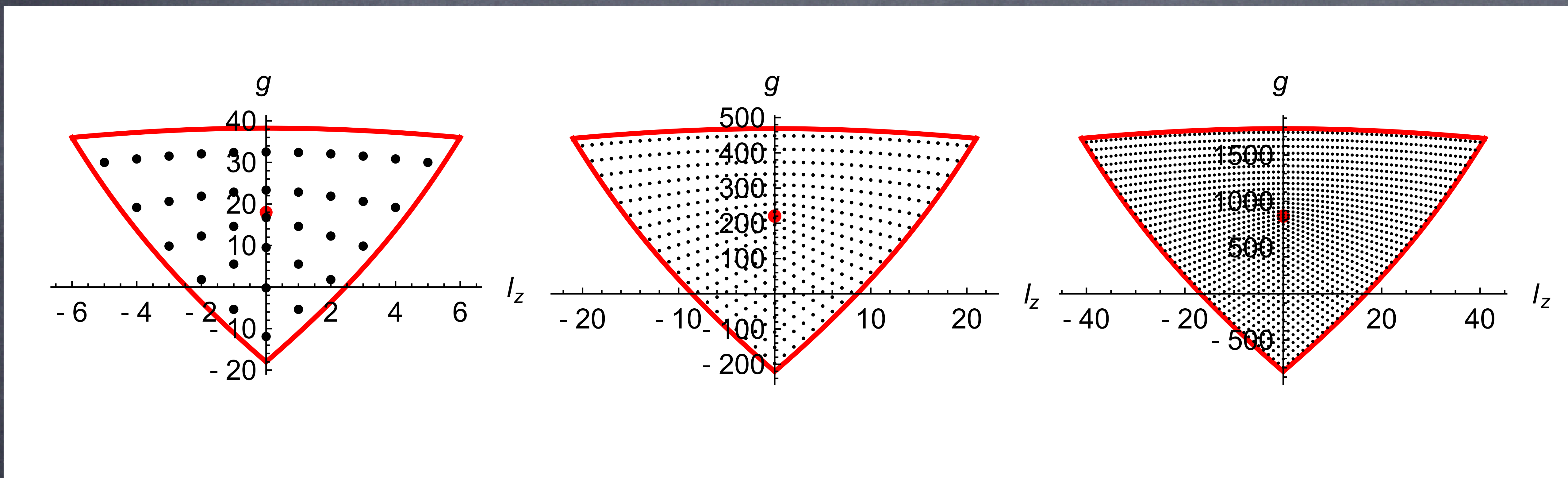
Semiclassical limit



n = 6 n = 21 n = 41

$a=n^2/4$: keeping the relative position of focus-focus point fixed

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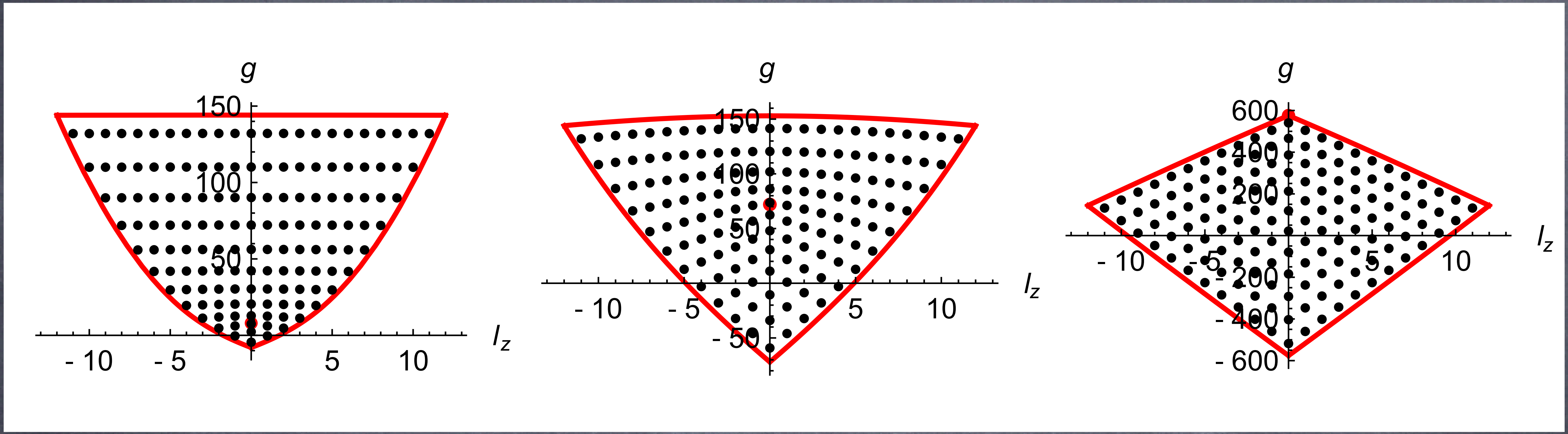
Dependence on a

n=12



a=4 a=36 a=288

$n^2>a$: monodromy, semi-toric systems

$n^2<a$: no monodromy, a toric system

parabolic quantum numbers n_1, n_2, m

$n = n_1+n_2+|m|+1$

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multi-separability

- separability in different coordinate systems; implies super-integrability
- gives natural realisations of Liouville integrable systems, similarly in quantum mechanics
- Kepler problem (Hydrogen) is multi-separable
  1) spherical coordinates ($a=0$)
  2) parabolic coordinates ($a=\infty$)
  3) spheroidal coordinates
  4) sphero-conical coordinates
- The family (H,G,L_z) contains the first three

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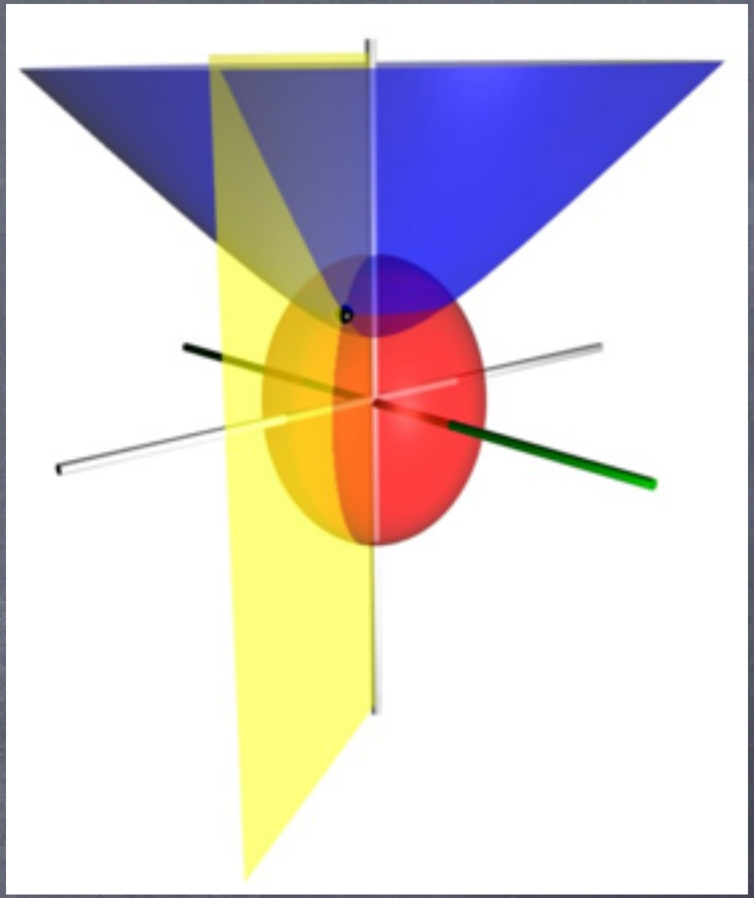
prolate spheroidal coordinates

- confocal ellipses, focus points at ±a
- classical: separation constant G, as before $G = |L|^2 + 2ae_z$
- quantum: separation gives spheroidal wave equation (confluent Heun)
- finite expansion of spheroidal harmonics in terms of spherical harmonics (Coulson & Robinson '58)



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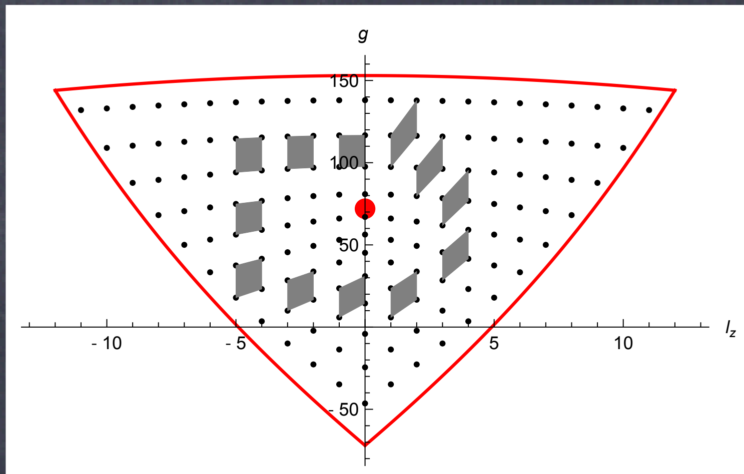
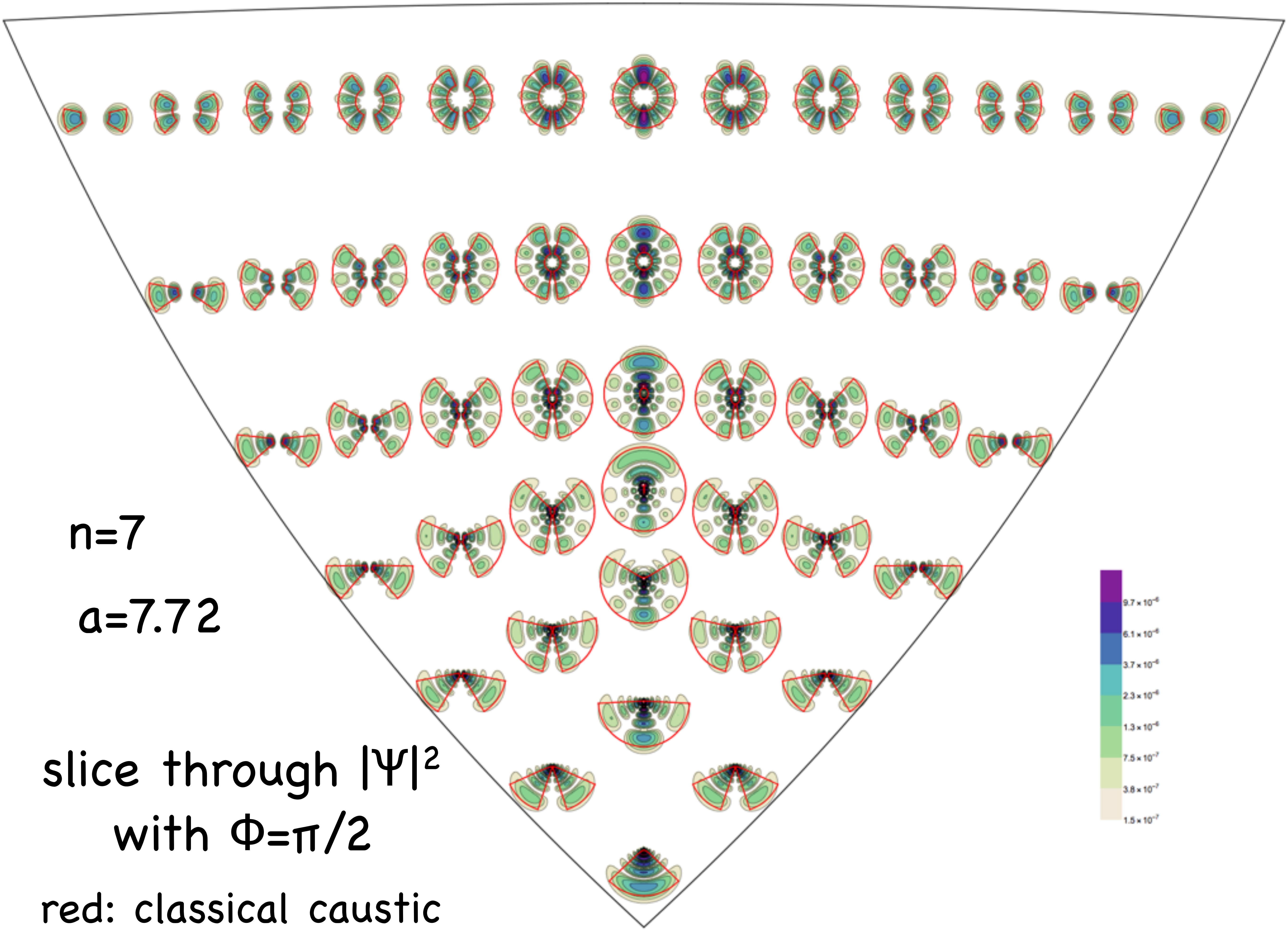
Spectrum and Orbitals

- Classical and Quantum system on $S^2 \times S^2$
- Obtained from quotient by flow of H
- Joint spectrum determined by eigenvalues of tri-diagonal matrix A, fixed eigenvalue m of L_z
- non-zero matrix entries for $l = |m|, |m|+1, \ldots, n-1$ for fixed n, m

$$A_{l,l} = l(l+1), \quad A_{l+1,l} = \frac{a}{n}\sqrt{(n^2 - l^2)(l^2 - m^2)/(l^2 - \tfrac{1}{4})}$$





$n=7$

$a=7.72$

slice through $|\Psi|^2$
with $\Phi=\pi/2$

red: classical caustic

Regularisation

- Moser regularisation: maps system to geodesic flow on S^3. Clearly SO(4) symmetric. Quotient by flow of H leads to system on $S^2 x S^2$.
- Kustaanheimo-Stiefel regularisation: maps system to isotropic harmonic oscillator in R4. Quotient by flow of H and flow of bi-linear integral leads to system on $S^2 x S^2$.
- Liouville integrable realisations obtained from separation of variables are the same as before.

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Laplacian

- remove the potential -> just free particle, QM = Laplace operator
- separates in many coordinate system
- separated equations define special functions spherical harmonics, spheroidal harmonics,...
- quotient by free particle dynamics leads to integrable systems on T^*S^2
- with Diana Nguyen and Sean Dawson: Monodromy in spheroidal harmonics, Sean's poster

free particle quotient

- $r = (x,y,z)^\dagger$, $p=(p_x,p_y,p_z)^\dagger$, $L=r \times p$ ang. momentum
- $H = (p_x^2+p_y^2+p_z^2)/2$, flow of H: straight lines in R^3
- Fix H: sphere in momentum space
- Components of linear momentum p and angular momentum $L=r \times p$ satisfy SE(3) algebra
- reduced phase space is T^*S^2
- spheroidal integrable system:
  $G = |L|^2 - a^2(p_x^2+p_y^2)$, L_z

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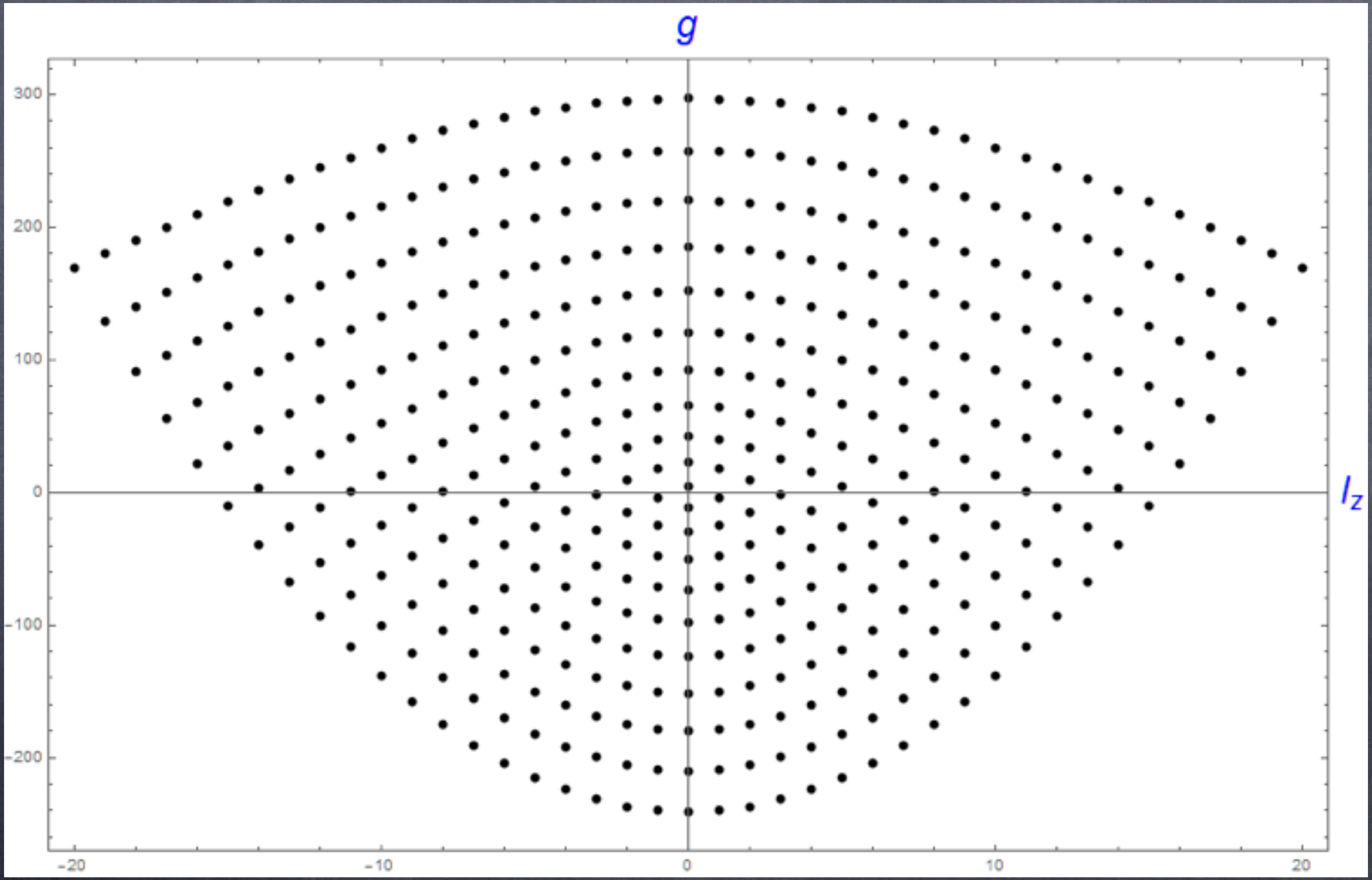
Monodromy in Spheroidal Harmonics

with Diana Nguyen and Sean Dawson

ListPlot[Flatten[Table[{l, SpheroidalEigenvalue[n, l, 16]}, {n, 0, 20}, {l, -n, n}], 1]]



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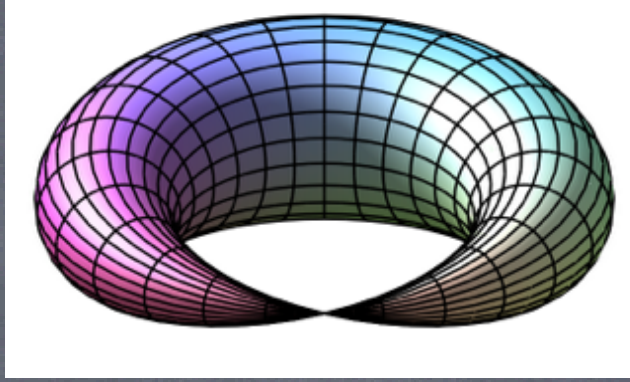
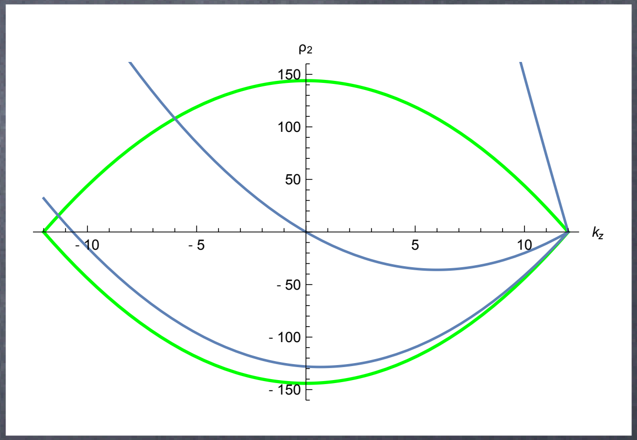


Proof of Mondromy

- Regular reduction by flow of H to $S^2 x S^2$
- Singular reduction by flow of L_z to 2-D orbifold using invariant polynomials
- Show existence of a pinched torus by reconstruction from orbifold to $S^2 x S^2$
- similar to Cushman & Sadovskii '00, & Efstathiou '04, but our "Hamiltonian" G is different
- implies classical monodromy (Matveev '96, Zung '97)
- implies quantum monodromy (Vu Ngoc '99)

singular reduction

- reduction by flow generated by L_z, rotation
- invariant polynomials:
  $I_1 = K_z$, $I_2 = L_x^2+L_y^2-K_x^2-K_y^2$, $I_3 = K_xL_y-K_yL_x$,
- $\{I_1, I_2+iI_3\} = 2i(I_2+iI_3)$, $\{I_2, I_3\} = \partial C/\partial I_1$
  Casimir $C = P(I_1)-I_2^2-I_3^2$,
- $G = I_2 + n^2+m^2 - I_1^2 + 2aI_1/n$
- C=0 defines reduced phase space, singular for m = L_z = 0 (Lemon), reconstruction gives pinched torus



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Conclusion

- Super-integrable systems have different Liouville-integrable realisations, some may have monodromy
- Same for corresponding Quantum Integrable Systems
- The most important super-integrable systems:
  * Kepler problem (PRL 120:020507 (2018))
  * 3D isotropic Harmonic Oscillator
  * Free particle (Laplace Operator) (Sean's poster)
  * geodesic flow on sphere (Diana's poster)
- All have (quantum) monodromy in spheroidal coordinates
- Program: Identify semi-toric special functions