Molecular resonances and regularization

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Modelling molecular resonances

1. *Ab initio* we have to consider a multi-body problem, consisting of the nuclei and the electrons that form the molecule, and the scattering particle.
2. We are rather interested in ground states of the molecule, and the interaction of a fast particle with the molecular potential V. For n nuclei at $s_1, \ldots, s_n \in \mathbb{R}^3$, this is of the form

$$V(q) = \sum_{\ell=1}^{n} \frac{Z_\ell}{\|q - s_\ell\|} + W(q) \qquad (q \in \mathbb{R}^3 \setminus \{s_1, \ldots, s_n\}),$$

   where $W : \mathbb{R}^3 \to \mathbb{R}$ is the electronic potential.
3. In a semiclassical setting, we consider the Schrödinger operator

$$H_\hbar := -\tfrac{\hbar^2}{2}\Delta + V \qquad \text{on } L^2(\mathbb{R}^3).$$

4. resonances are, as usual, poles of the resolvent $z \mapsto (H_\hbar - z\mathbb{1})^{-1}$.

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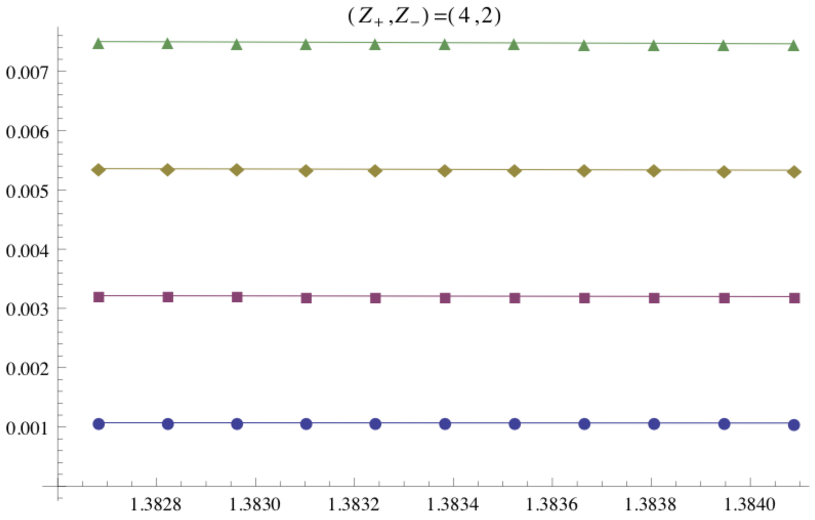
❶ Resonances for a diatomic molecule

For diatomic molecules ($V(q) = -\frac{Z_1}{|q-s_1|} - \frac{Z_2}{|q-s_2|}$)

- the resonances are enumerated (for $d = 2$) by $\mathbb{Z} \times \mathbb{N}$.
- up to a small error, their positions $E \in \mathbb{C}$ are determined by
  - the length of the unique closed orbit of energy $\Re(E) > 0$
  - and its Liapunov exponent.

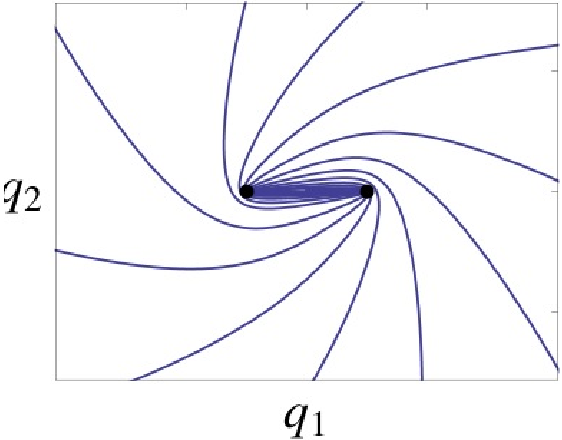
M. Seri, AK, M. Degli Esposti, Th. Jecko: *Resonances in the Two-Centers Coulomb System*, Reviews in Mathematical Physics **28**, 1650016, (2016)

Resonances for a diatomic molecule



$d = 2$

Diatomic molecules: trapped and closed orbits



Trapped orbits in configuration place for energy $E = 1$

Resonances for n–atomic molecules

- On the one hand, a result like this had to be expected, considering results for Schrödinger operators with non-singular potentials:

  Christian Gérard, Johannes Sjoestrand: *Semiclassical resonances generated by a closed trajectory of hyperbolic type*. Comm. Math. Phys. **108**, 391–421 (1987)

- On the other hand, the closed orbit of the 2-center problem exists only *after* regularization of the classical flow.
  So regularization *is* an issue here.
- The result relied on integrability (in a stronger sense than in [1]!) of the two-center problem.
- By analogy, for $n \geq 3$ centers one would expect a density estimate of resonances $\mathcal{O}(\hbar^{-\nu})$ in a small strip near the real axis, with ν affine in the fractal dimension of the trapped set.

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Hamiltonian, attractive case ($I < 0$):

$$\widehat{H} : T^*\left(\mathbb{R}^d \setminus \{0\}\right) \to \mathbb{R} \quad , \quad \widehat{H}(p,q) = \frac{\|p\|^2}{2m} + \frac{I}{\|q\|}$$

Why another regularisation?

There are already regularisations by
Levi-Civita, Kustaanheimo-Stiefel, Moser, Souriau, Ligon-Schaaf

Advantages:

- All dimensions $d \geq 1$
- simultaneously for all energies
- no change of time parameter
- symplectic extension of phase space.

❷ Regularisation of the Kepler Problem

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What kind of regularity?

- regularity of the single collision orbits, *e.g.* analyticity in $t^{1/3}$
- regularity of a Poincaré map (block regularity)
- regularity of the flow.

Theorem

For all $d \in \mathbb{N}$ there exists a complete, real-analytic extension (P, ω, H) of the Hamiltonian system $\left(T^*(\mathbb{R}^d \setminus \{0\}),\, dq \wedge dp,\, \widehat{H}\right)$.

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Regularisation by phase space extension: Kepler case

- ε–neighborhood of the excluded fiber $T_0^*\mathbb{R}^d$

$$\widehat{U}^\varepsilon := \left\{(p,q) \in T^*\left(\mathbb{R}^d \backslash \{0\}\right) \,\middle|\, \|q\| < \varepsilon,\ \frac{\|p\|^2}{2m} > \frac{3}{4}\frac{|I|}{\|q\|}\right\}$$

- $\widehat{T} : \widehat{U}^\varepsilon \to \mathbb{R}$: the time elapsed since the closest encounter of the Kepler solution with the pericentre.
- Laplace-Runge-Lenz vector (with $\hat{L}(p,q) := q \wedge p$)

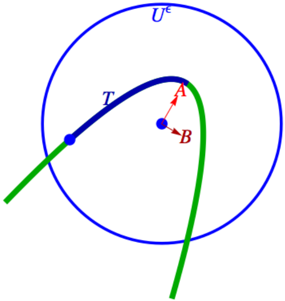
$$\tilde{A} : \widehat{U}^\varepsilon \to \mathbb{R}^d \quad , \quad \tilde{A}(p,q) := -\widehat{L}(p,q)p + mI\frac{q}{\|q\|}.$$

- its direction $\widehat{A} : \widehat{U}^\varepsilon \to S^{d-1} \quad , \quad \widehat{A} := \tilde{A}/\|\tilde{A}\|$.
- $\widehat{B} : \widehat{U}^\varepsilon \to \mathbb{R}^d \quad , \quad \widehat{B} := \widehat{L}\widehat{A}$

Regularisation for Kepler case

Together we obtain a real-analytic map
$\widehat{\Psi} := (\widehat{H}, \widehat{T}, \widehat{A}, \widehat{B}) : \widehat{U}^{\varepsilon} \longrightarrow T^*(\mathbb{R}_{\widehat{H}} \times S^{d-1}_{\widehat{A}}),$

- all entries except time $\widehat{T}$ are constants of the motion.
- $\mathrm{im}(\widehat{\Psi})$ misses the zero section $\cong \mathbb{R} \times S^{d-1}$ of the cotangent bundle, since the collision orbits are characterized by zero angular momentum and thus $\widehat{B} = \widehat{L}\widehat{A} = 0$, and the point of collision on such an orbit corresponds to $\widehat{T} \to 0$.



Regularisation: Kepler case

- We now complete phase space by adding a cylinder

$$P := T^*\left(\mathbb{R}^d \setminus \{0\}\right) \ \dot{\cup} \ \mathbb{R} \times S^{d-1}$$

and introducing a second chart Ψ with domain

$$U^\varepsilon := \widehat{U}^\varepsilon \ \dot{\cup} \ \mathbb{R} \times S^{d-1} \ \subseteq \ P,$$

$$\Psi \equiv \left(H, T, A, B\right) : U^\varepsilon \to T^*(\mathbb{R} \times S^{d-1}),$$

$$\Psi\restriction_{\widehat{U}^\varepsilon} := \widehat{\Psi} \quad \text{and} \quad \Psi\restriction_{\mathbb{R}\times S^{d-1}}(h, a) := (h, 0, a, 0).$$

- The Poisson structure corresponding to ω is the one of the Dirac bracket for $T^*S^{d-1} \subseteq T^*\mathbb{R}^d$.
- Except for dimension $d = 1$, the symplectic manifold (P, ω) is *not* a cotangent bundle.

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Regularisation and semiclassics

Although the Kepler potential is singular, in many cases one obtains results like in smooth situations, where one can directly apply pseudodifferential operator techniques.
One would like to have a meta-theorem telling this.

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❸ n–center problem in $d = 3$ dimensions

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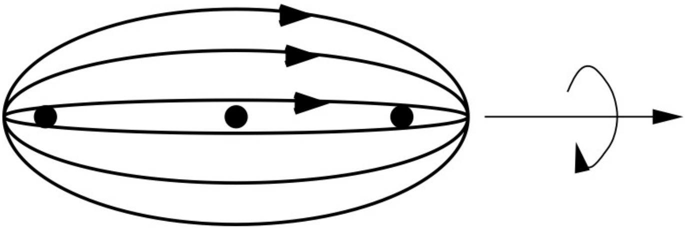
Problem: System need not be hyperbolic for energies $E > 0$.
Example: Three centers on a line lead to neutral stability:



Assumptions:

- Non-collinear configurations $s_1, \ldots, s_n$
- Charges $Z_l \neq 0$ (so applicable for molecules)

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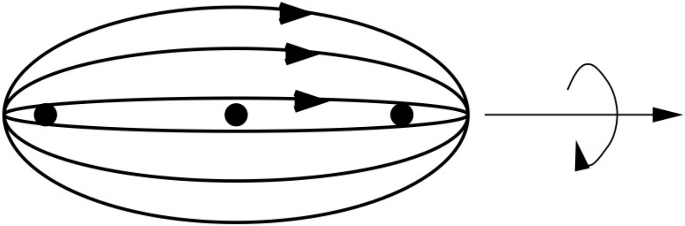

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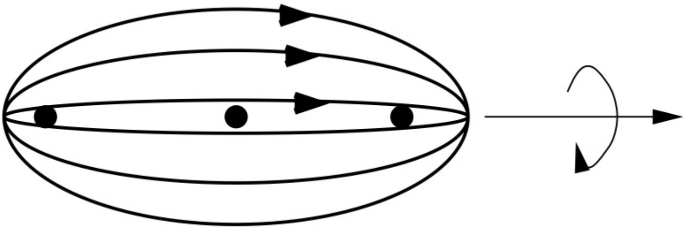

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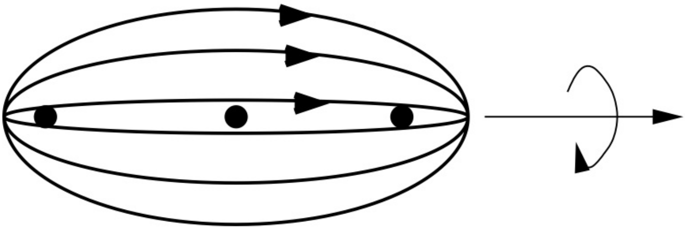

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Symbolic Dynamics (3D):

Set b_E of bounded orbits of energy $E > 0$, for large enough E:

- $n = 1 : b_E = \emptyset$,
- $n = 2 : b_E \cong S^1$,
- $n \geq 3$: b_E is locally homeomorphic to product of a Cantor set and an interval.

All bounded orbits are hyperbolic.

b_E has Liouville measure zero.

Morse index of (closed) orbits equal to number of near-collisions.

Complete symbolic dynamics, including scattering orbits.

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Topological Entropy of Energy E Flow Φ_E:

- For $n = 1$ and $n = 2$: $h_{\text{top}}(\Phi_E) = 0$.
- For $n \geq 3$:

$$h_{\text{top}}(\Phi_E^1) = C_1\sqrt{2E} \cdot \left(1 + \frac{\ln(E)}{E} C_2 + \mathcal{O}(1/E)\right).$$

Constants $C_1 \equiv C_1(s_l)$ and $C_2 \equiv C_2(s_l, Z_l)$ are determined by solution of finite eigenvalue problem.

Bolotin, Negrini '01: $h_{\text{top}}(\Phi_E^1) > 0$ for $n \geq 3$ and *all* $E > 0$.

Topological Entropy of Energy E Flow Φ_E:

- For $n = 1$ and $n = 2$: $h_{\text{top}}(\Phi_E) = 0$.
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Fractal Dimensions of Bounded Orbits:

Bounded orbits b_E of energy $E > E_{\mathrm{th}}$.

Hausdorff dimension $\dim_{\mathcal{H}} \;\leq\;$ Minkowski dimension $\dim_{\mathcal{M}}$:

$$1 + 2d(E) \cdot \Big(1 - \mathcal{O}((E \ln E)^{-1})\Big) \leq \dim_{\mathcal{H}}(b_E) \leq$$
$$\leq \;\; \dim_{\mathcal{M}}(b_E) \leq 1 + 2d(E) \cdot \Big(1 + \mathcal{O}((E \ln E)^{-1})\Big)$$

with

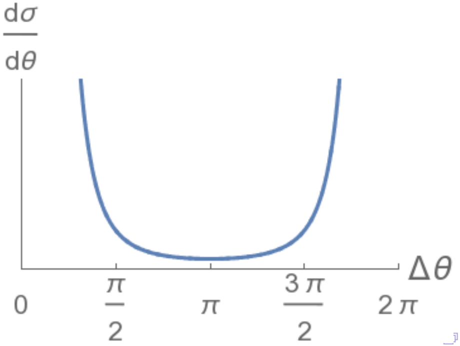
$$d(E) \equiv d(E; s_l, Z_l) = \frac{\ln(n-1)}{\ln(E)} \cdot \left(1 + \mathcal{O}\left(\frac{1}{\ln(E)}\right)\right)$$

solution of finite eigenvalue problem.

in general discontinuous in forward directon $\hat{\theta}^+ = \hat{\theta}^-$, but may be smooth for complicated dynamics:

Example (Rutherford): $V(q) = -Z/|q|$ on $\mathbb{R}^d$

$$\frac{d\sigma}{d\hat{\theta}^+}(E, \hat{\theta}^-, \hat{\theta}^+) = \left(\frac{|Z|}{4E \sin^2(\frac{1}{2}\sphericalangle(\hat{\theta}^+, \hat{\theta}^-))} \right)^{d-1} .$$



Differential Cross Section for the n–Center Problem

- **Dim. d=2:** $Z_l > 0$.
  For all n : $\frac{d\sigma}{d\hat{\theta}^+}$ smooth, up to diagonal.
  C^1-near to Rutherford cross section (that is, $n = 1$), with relative deviation of order $\mathcal{O}(1/E)$.
- **Dim. d=3:** $Z_l \neq 0$.
  Smooth and C^1-near to Rutherford cross section, *except* in cones centered at lines through s_k, s_l and forward direction. These cones have small angles $\mathcal{O}(1/\sqrt{E})$.

Differential Cross Section for the *n*–Center Problem

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❹ Classical potential scattering and Dehn twists

Hamiltonian system (P, ω, H), with

- phase space $P := T^*\mathbb{R}^d$, $d \geq 2$

  symplectic form $\omega := \sum_{i=1}^{d} dq_i \wedge dp_i$

  and Hamiltonian $H : P \to \mathbb{R}$, $H(p,q) := \frac{1}{2}\|p\|^2 + V(q)$,

  with potential $V \in C^2(\mathbb{R}^d, \mathbb{R})$, decaying at infinity.
- or: $V \in C^2(\mathbb{R}^d \backslash \{0\}, \mathbb{R})$, like $V(q) = -1/\|q\|$, and smooth extension of incomplete Hamiltonian system (see below),
- or: billiard on $\mathbb{R}^d \setminus B$, with convex obstacle $B \subseteq \mathbb{R}^d$

An energy $E > 0$ is called *non-trapping*, if all energy E orbits come from and go to spatial infinity.

Index for classical potential scattering

- The set of oriented lines on $\mathbb{R}^d$ is the (co-)tangent bundle T^*S^{d-1}
- Asymptotically all solutions have the form of straight lines.
- Thus for non-trapping E: Dynamics induces symplectomorphism (*scattering map*)
$$S_E : T^*S^{d-1} \to T^*S^{d-1}.$$
- This defines a topological index $\deg(E) \in \mathbb{Z}$.
- In examples of centrally symmetric V all values ≤ 1 occur:

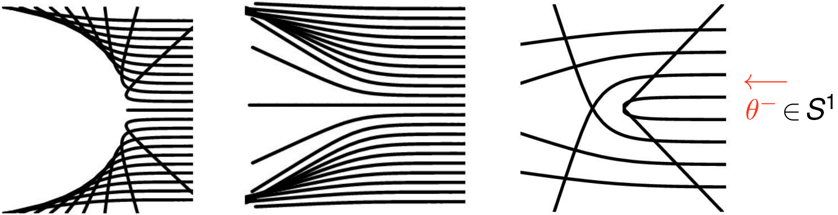

Figure: 2D scattering with degrees 1 (left), 0 (center) and -1 (right)

AK, Markus Krapf: *The non-trapping degree of scattering.* Nonlinearity **21**, 2023–2041 (2008)

Nikolay Martynchuk, Holger Waalkens: *Knauf's degree and monodromy in planar potential scattering.* (2016)

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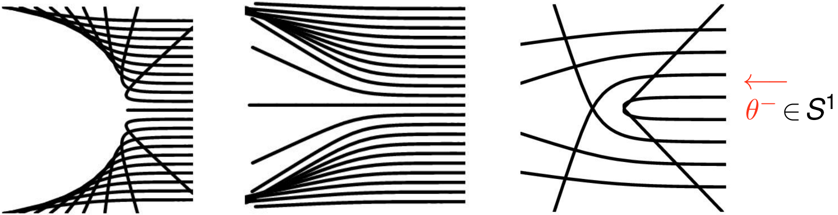

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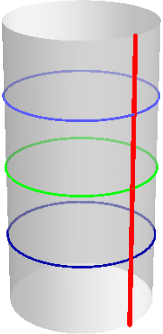
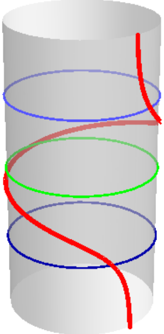
Interpretation as symplectic Dehn twist of T^*S^{d-1}



$\deg(E) = 1$



incoming, time $t \to -\infty$ $\xrightarrow{\textit{scattering}}$ outgoing, time $t \to +\infty$

- Red: Lagrangian manifold of the energy E trajectories with incoming direction $\theta^- \in S^{d-1}$
- Green: Lagrangian manifold of the energy E trajectories with incoming angular momentum 0.

Remark: This is a symplectic phenomenon, as Paul Seidel showed that the squared Dehn twist on T^*S^2 is *differentiably* isotopic to the identity.

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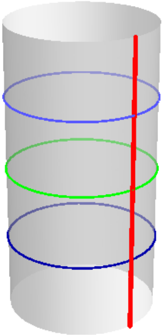

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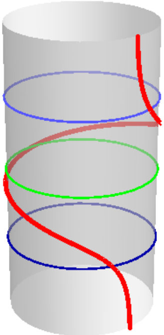

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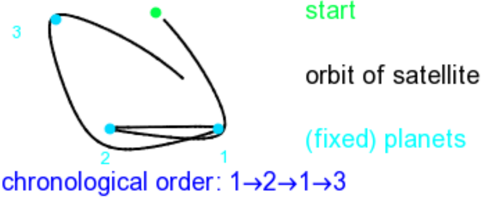
Usage of the degree

deg(E) can be used to embed symbolic dynamics for scattering in a potential $V = V_1 + \ldots + V_k$, where the V_i are assumed to carry non-zero degree, and to have *non-shadowing* supports (no line meeting more than two supports). More precisely, for any bi-infinite sequence a in

$$\left\{a \in \{1,\ldots,k\}^{\mathbb{Z}} \mid a_l \neq a_{l+1}\right\},$$

there exists an orbit of energy E, visiting the supports of the V_i in the succession prescribed by a.



Similar effects for magnetic fields:

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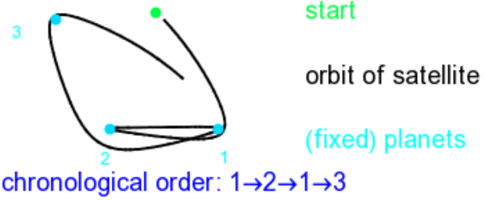

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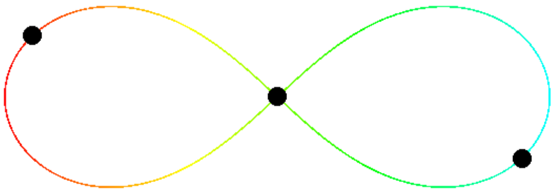
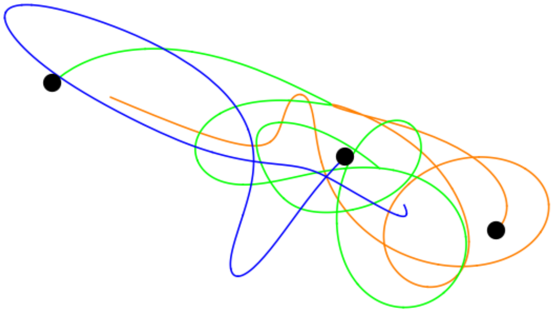
What is (not) known about the n-body problem



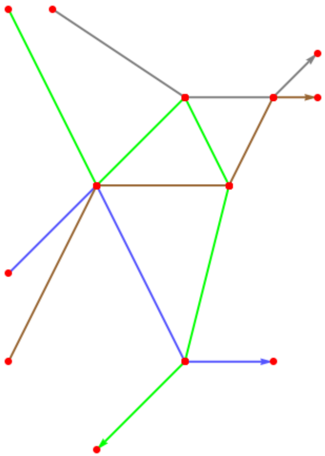
Alain Chenciner, Richard Montgomery: A remarkable periodic solution of the three-body problem in the case of equal masses. Annals of Mathematics **152**, 881–901 (2000)

But:

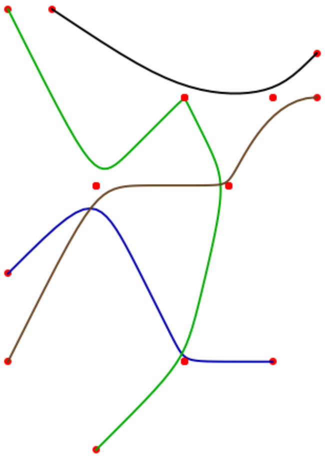


❺ n–body problem:

find solution where the celestial bodies meet at kinematically prescribed points



Ideal



reality (for Coulomb repulsion)

Jacques Féjoz, AK, Richard Montgomery: *Lagrangian relations and linear billiards.* arXiv:1606.01420 (2016)

Thank you for listening!
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