Classical and Quantum Mechanics of Non-holonomic Constraints

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Based on:
A Rothkopf and WAH, arXiv:2409.11063

Introduction

- Recall Hamilton's Principle of Extremized Action

$$\delta S = 0,$$

$$S[q^i(t), \dot{q}^i(t)] \equiv \int_{t_i}^{t_f} dt \, L\left(q^i(t), \dot{q}^i(t), t\right)$$

Euler-Lagrange Equations

- One may then derive the EL eqns for unconstrained motion:

$$\delta S = \int_{t_i}^{t_f} dt \; \frac{\partial L}{\partial q^i}\delta q^i + \frac{\partial L}{\partial \dot{q}^i}\delta \dot{q}^i$$

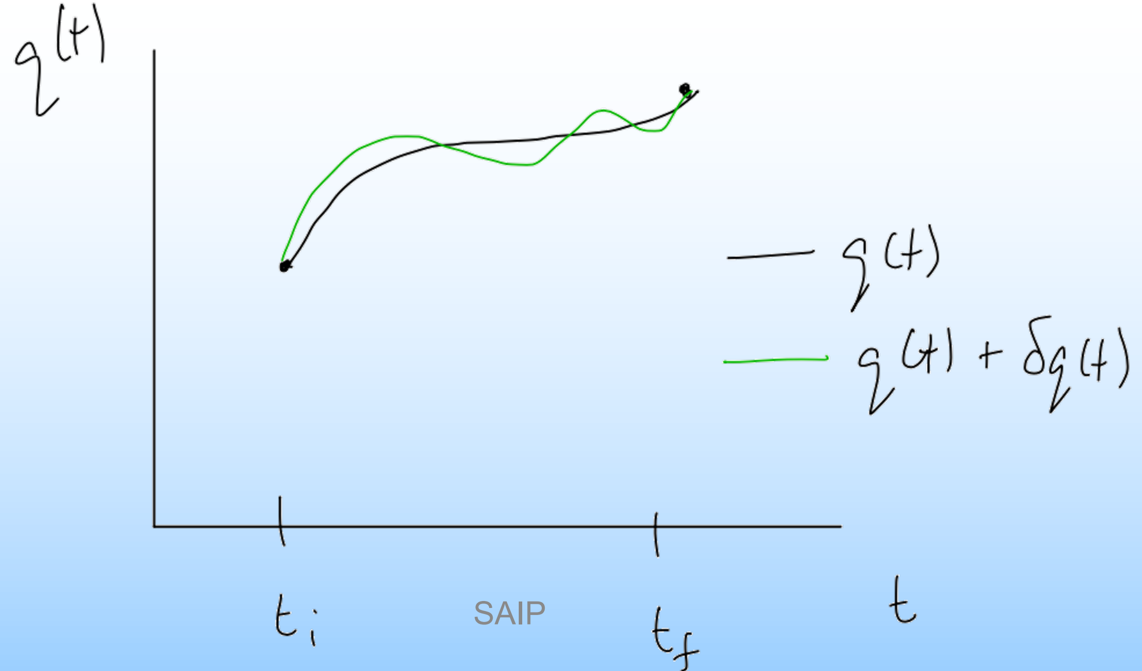
$$= \int_{t_i}^{t_f} dt \; \frac{\partial L}{\partial q^i}\delta q^i + \frac{\partial L}{\partial \dot{q}^i}\frac{d}{dt}\left(\delta q^i\right)$$

$$= \int_{t_i}^{t_f} dt \left[\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right]\delta q^i + \frac{\partial L}{\partial \dot{q}^i}\delta q^i \Big|_{t_i}^{t_f}$$

$$= 0$$

Boundary Terms

- Under the assumption that the start and end points of the motion are fixed, then $\delta q^i(t_i) = \delta q^i(t_f) = 0$, and the boundary term vanishes
- We envision the paths as



Unconstrained Motion

- Variations $\delta q(t)$ are independent and arbitrary
- Fundamental Theorem of the Calculus of Variations =>

$$\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} = 0$$

- Notice the crucial use of the "transposition rule"

$$\delta \dot{q}^i(t) = \frac{d}{dt}\left[\delta q^i(t)\right]$$

Constrained Motion

- Suppose we require that

$$g(q^i, \dot{q}^i, t) = 0$$

- Examples:
  - Mass on the end of a rod
  - Bead on a rotating hoop
  - Rolling without slipping

Types of Constrained Motion

- Constraints are classified:
  - Holonomic: depends only on the coordinates
  - Non-holonomic: depends on coordinates *and* velocities
- Examples:
  - Mass on the end of a rod
  - Bead on a rotating hoop
  - Rolling without slipping

Holonomic

Non-holonomic

Holonomic Constraints

- Holonomic constraints are "easy"
  - System's motion is well understood
- One may solve by
  - 1) Use $f(q^i,t) = 0$ to solve for one qi in terms of the others
    - Treat remaining q's as independent and arbitrary, proceed as in the unconstrained case

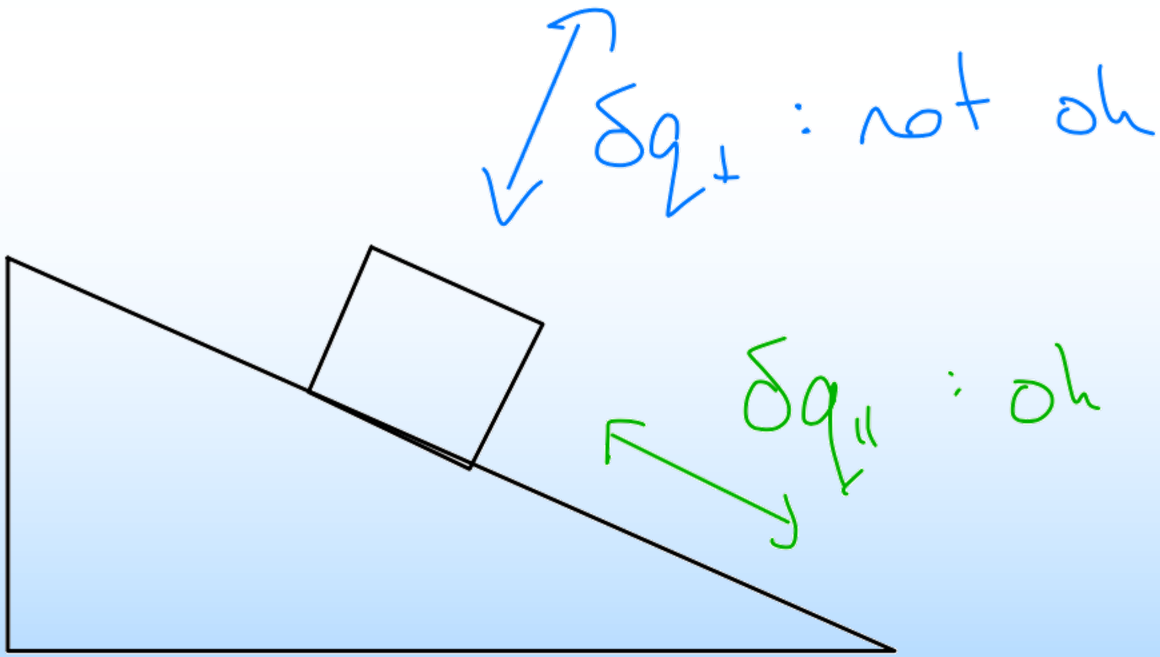
Lagrange-d’Alembert Principle

- 2) Keep all q’s, but modify Hamilton’s Principle to the Lagrange-d’Alembert Principle
  - Action is extremized, but variations must satisfy the constraint

$$\delta S = \int_{t_i}^{t_f} dt \left[\frac{\partial L}{\partial q^i}\,\delta q^i + \frac{\partial L}{\partial \dot{q}^i}\,\delta \dot{q}^i \right]_{f(q^i+\delta q^i,\, t)=0} = 0$$

Constrained Variations

- Think of a block on a wedge; variations can't push the block into or off of the wedge



Transposition Rule and IBP

- One can show that the transposition rule still holds for holonomic constraints

$$\delta\left[\frac{d}{dt}q^i(t)\right] = \frac{d}{dt}\left[\delta q^i(t)\right]$$

- And thus

$$\delta S = \int_{t_i}^{t_f} dt \left[\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right]\delta q^i \Bigg|_{f(q^i+\delta q^i,\,t)=0} = 0$$

  - Since the dqi are *not* all independent and arbitrary, we can't use the FTCV: progress is difficult

Lagrange Multipliers

- 3) Since

$$\frac{\partial f}{\partial q^i}\,\delta q^i = 0 \quad \Rightarrow \quad \lambda(t)\,\frac{\partial f}{\partial q^i}\left[q^i(t)\right]\delta q^i(t) = 0$$

- We may then add to $\delta S = 0$:

$$\delta S = \int_{t_i}^{t_f} dt \left[\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} + \lambda\frac{\partial f}{\partial q^i}\right]\delta q^i \Bigg|_{f(q^i+\delta q^i,\,t)=0} = 0$$

Independent and Dependent Variables

- Consider one q_D^α as *dependent* on the q_I^j *independent* coordinates
  - – $\delta q_D\alpha$ depend on δq_I^j
- $\lambda(t)$ *is* independent and arbitrary
  - – Choose $\lambda(t)$ such that

$$\frac{\partial L}{\partial q^\alpha} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^\alpha} + \lambda \frac{\partial f}{\partial q^\alpha} = 0$$

Apply FTCV

- Then we have

$$\delta S = \int_{t_i}^{t_f} dt \left[\frac{\partial L}{\partial q^j} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^j} + \lambda \frac{\partial f}{\partial q_j} \right] \delta q^j = 0$$

independent and arbitrary!

  – and thus

$$\frac{\partial L}{\partial q^j} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^j} + \lambda \frac{\partial f}{\partial q_j} = 0$$

Full Solution

- Putting our two sets of equations together:

$$\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} + \lambda \frac{\partial f}{\partial q^i} = 0$$

  - We have solution for *all* coordinates i

Adjoined Lagrangian

- 4) One may directly adjoin

$$\lambda(t)\, f\left[q^i(t)\right]$$

to our original Lagrangian, treat $\lambda(t)$ *and* all the q^i as independent and arbitrary, and use Hamilton's Principle

- One finds same EoM for q^i, plus

$$f = 0$$

Non-holonomic Constraints

- Hard
- Correct EoM derived in 2011 (!)

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} = \lambda \frac{\partial g}{\partial \dot{q}^i}$$

Flannery, J Math Phys 52 (2011)

- Want to understand from a variational principle point of view

Obstructions

- Finding a variational principle is difficult because
  - 1) One *cannot* rely on the transposition rule

$$\delta\left(\frac{d}{dt}q^i(t)\right) = \frac{d}{dt}\left(\delta q^i(t)\right)$$

  - 2) Adjoining the Lagrangian with L mult's leads to spurious forces

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} = \lambda\left(\frac{\partial g}{\partial q^i} - \frac{d}{dt}\frac{\partial g}{\partial \dot{q}^i}\right) - \dot{\lambda}\frac{\partial g}{\partial \dot{q}^i}$$

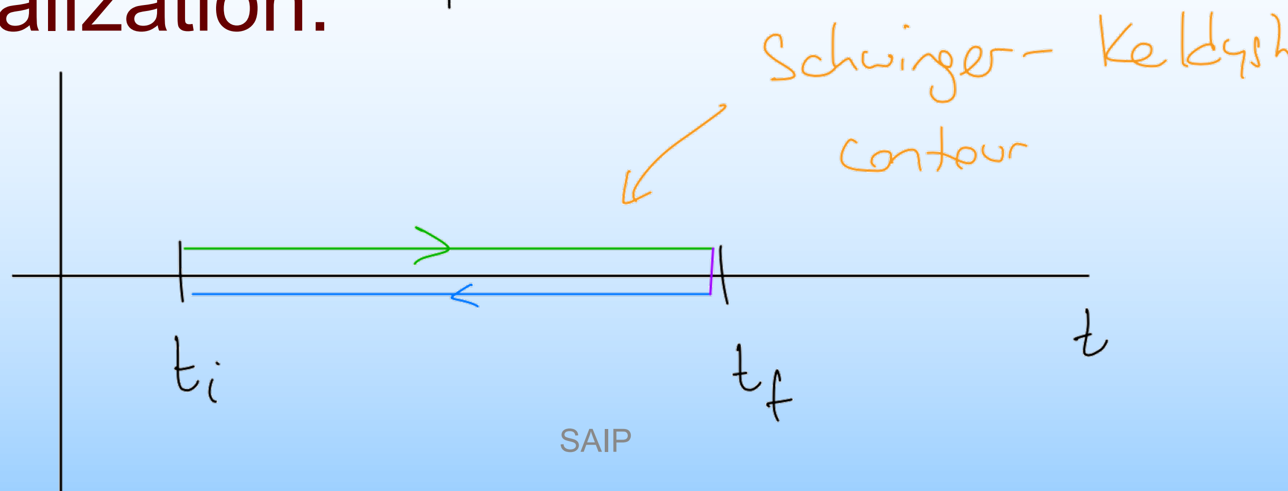
Double the DoF

- Consider the expectation value of an operator in QM

$$\langle \hat{O} \rangle (t_f) = \langle \psi(t_f) | \hat{O}(t_f) | \psi(t_f) \rangle$$

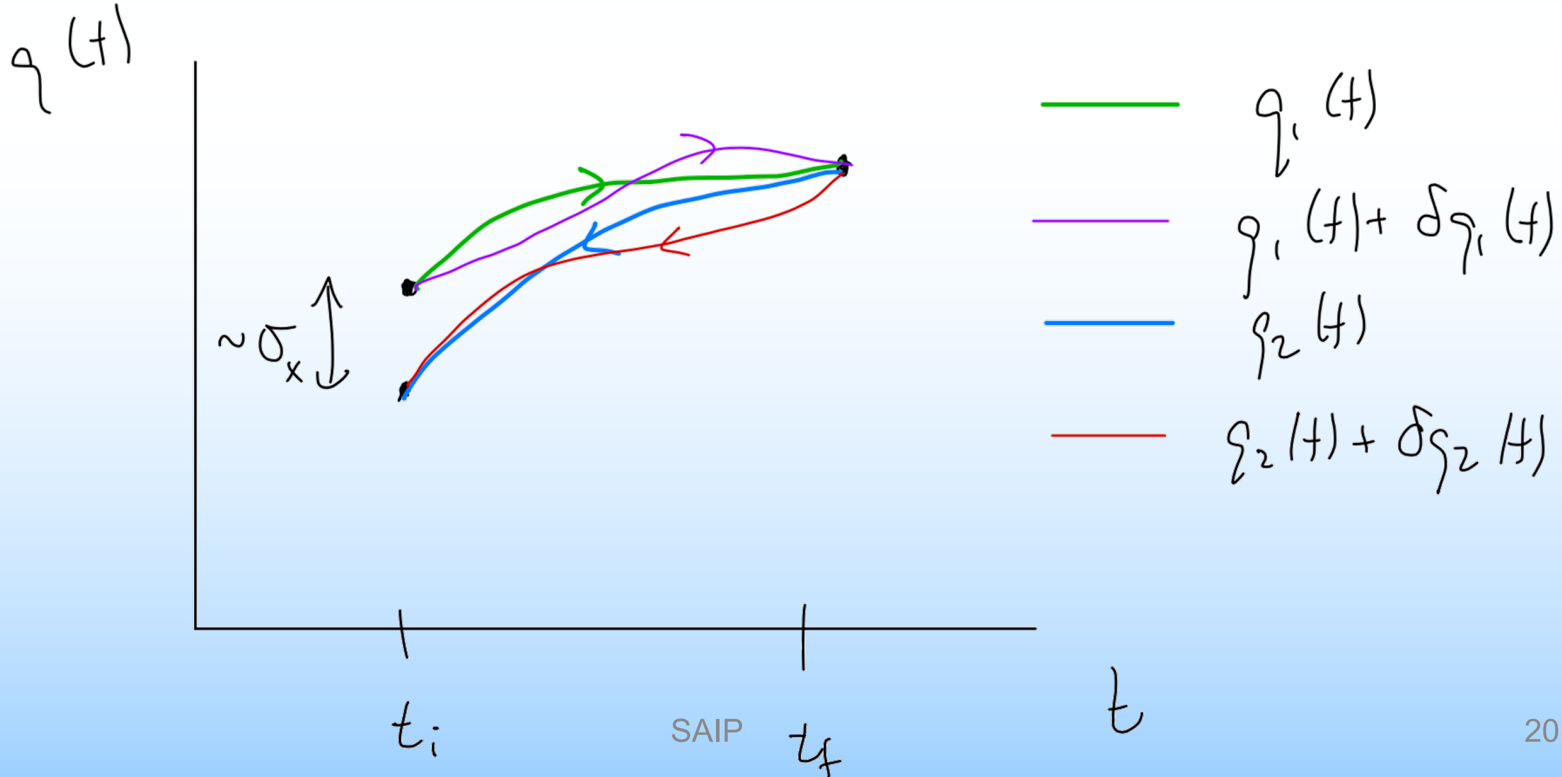
$$= \langle \psi(t_i) | \hat{U}^{\dagger}_{\hat{H}}(t_f, t_i)\, \hat{O}(t_f)\, \hat{U}_{\hat{H}}(t_f, t_i) | \psi(t_i) \rangle$$

- Visualization:



Variation of Paths

- Consider a wavepacket of width σ_x for initial state. Then we have a path out $q_1(t)$ with variations $\delta q_1(t)$ and a path back $q_2(t)$ with variations $\delta q_2(t)$



Plus/minus Paths

- It's often useful to consider a change of variables

$$q_+(t) = \frac{1}{2}\left(q_1(t) + q_2(t)\right)$$

$$q_-(t) = q_1(t) - q_2(t).$$

  – As hbar => 0 limit, $q_+(t)$ is the classical path and $q_-(t)$ are the quantum fluctuations

Action in Doubled DoF

- One may consider an action from the path integral associated with

$$\langle \psi(t_i) | \hat{U}^\dagger_{\hat{H}}(t_f, t_i)\, \hat{O}(t_f)\, \hat{U}_{\hat{H}}(t_f, t_i) | \psi(t_i) \rangle$$

such that

$$S[q_1^i(t), q_2^i(t)] = \int_{t_i}^{t_f} dt \left[L\left(q_1^i(t), \dot{q}_1^i(t), t\right) - L\left(q_2^i(t), \dot{q}_2^i(t), t\right) \right]$$

Lagrange Multipliers Part II

- Since DoF are doubled, we can add Lagrange multipliers in new ways, e.g.:

$$\tilde{S}[q_1^i(t), q_2^i(t)] =$$

$$\int_{t_i}^{t_f} dt \Big[L\big(q_1^i(t), \dot{q}_1^i(t), t\big) - L\big(q_2^i(t), \dot{q}_2^i(t), t\big)$$

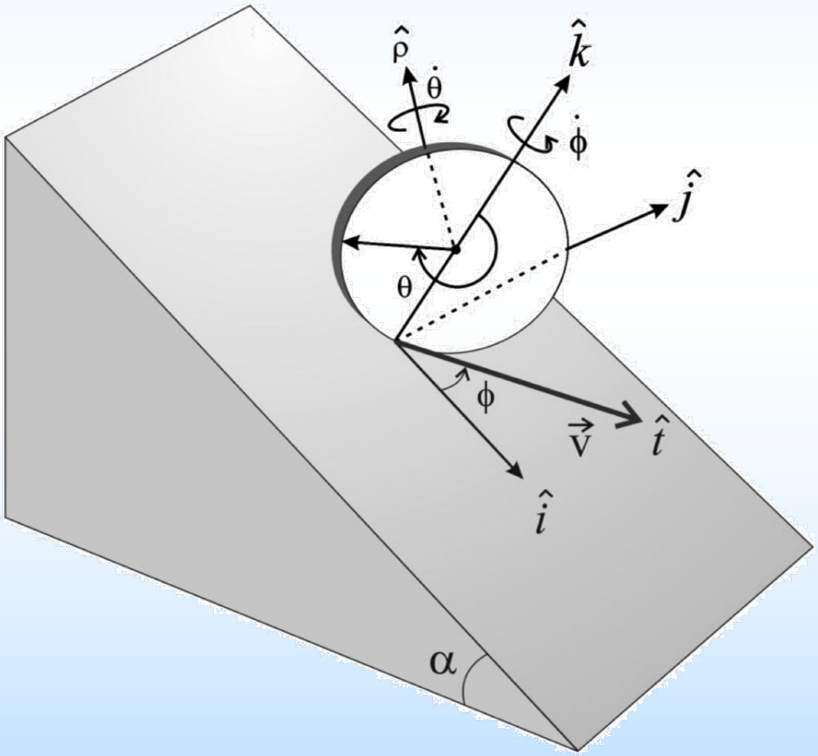
$$+ \lambda_-(t)\, g\big(q_+^i(t), \dot{q}_+^i(t), t\big) - \lambda_+(t)\, q_-^i(t) \frac{\partial g}{\partial q^i}\Big|_{q^i = q_+^i} \Big]$$

Rothkopf and WAH, arXiv:2409.11063

  - Apply Hamilton's Principle => correct EoM!

Examples: Rolling without Slipping

- Setup and constraints:



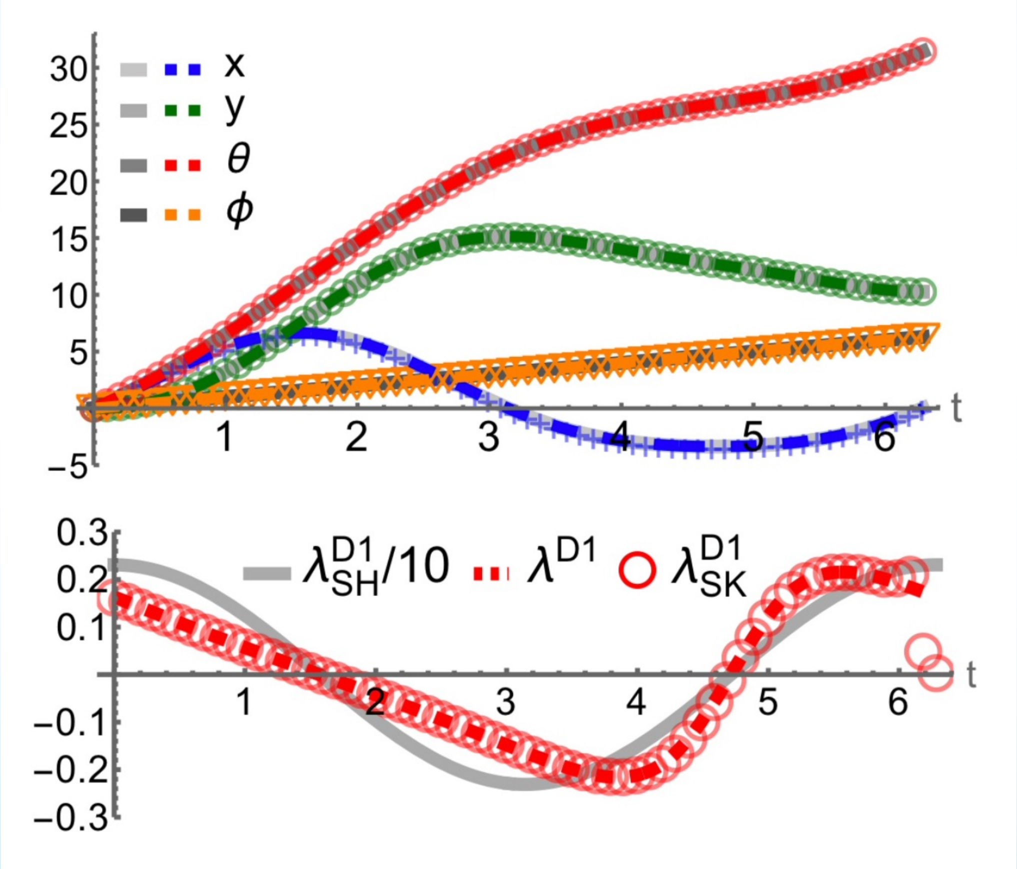
=>

$$\dot{x}^2 + \dot{y}^2 - R^2\dot{\theta}^2 = 0$$

$$\dot{x}\sin\phi - \dot{y}\cos\phi = 0$$

Rolling w/o Slipping Results

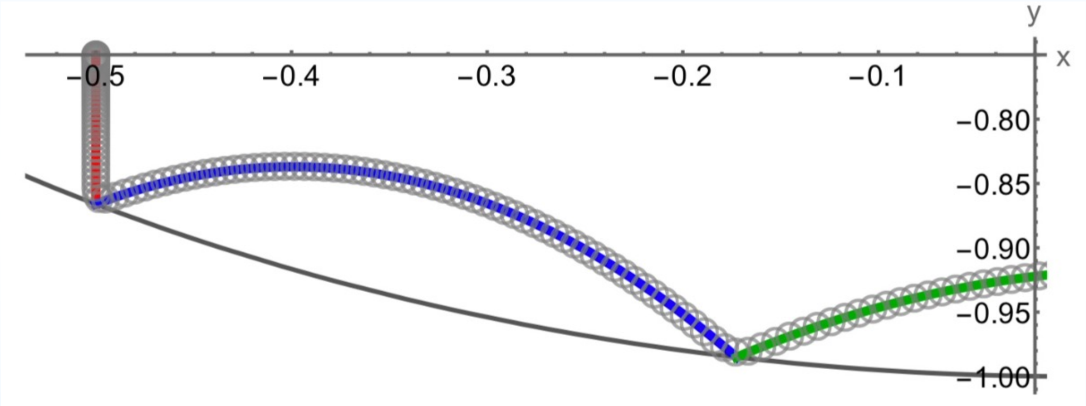
- Novel action yields correct motion!



Rothkopf and WAH, arXiv:2409.11063

Inequality Constraints

- Inequality constraints, such as falling inside a drum, can also be handled:

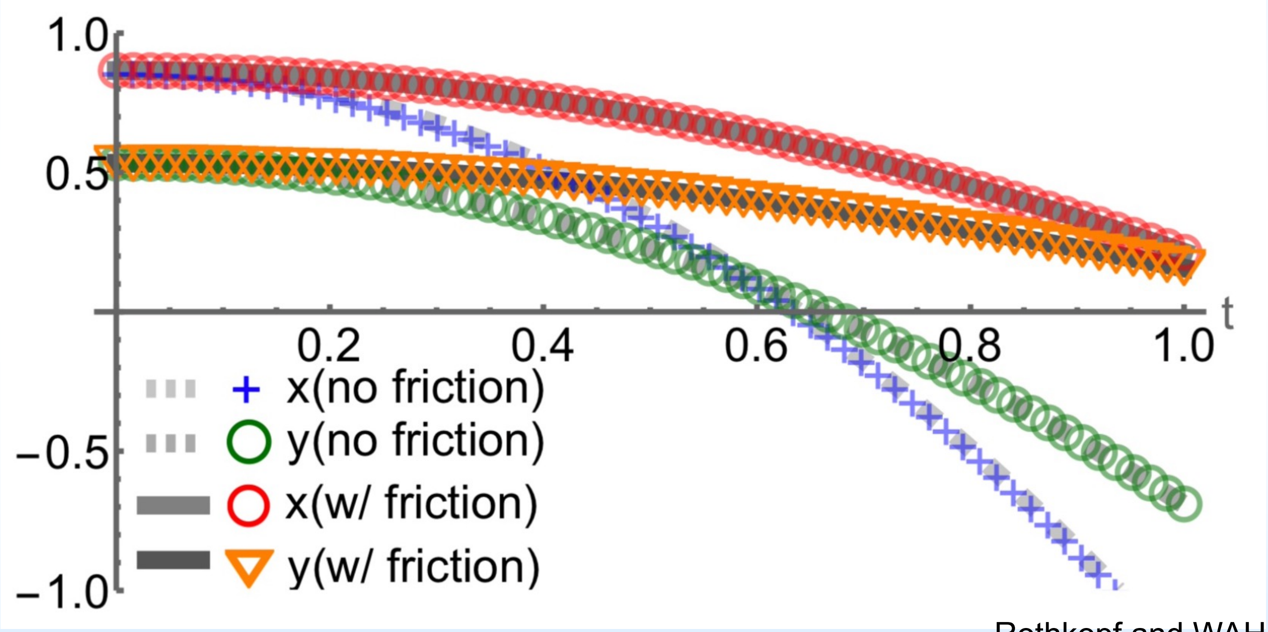


Rothkopf and WAH, arXiv:2409.11063

  – NB: path is *globally* determined
    - No need to locally find where particle collides with boundary

Dissipative Systems

- Novel action also handles dissipative systems



Rothkopf and WAH, arXiv:2409.11063

  – Cannot be formulated in a single path action principle

Conclusions and Outlook

- Found action principle for non-holonomic constraints
  - First time in 180 years of searching
- Doubled DoF can handle
  - Non-holonomic constraints (e.g. rolling w/o slipping)
  - Inequality constraints
  - Dissipative forces
- Future work:
  - Use our action in a path integral to compute quantum mechanics of non-holonomic constraints for the first time
  - Derive the action from first principles