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LEARNING OPTIMAL KERNELS FOR REAL-TIME COMPLEX LANGEVIN

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(1st part) with Daniel Alvestad, Rasmus Larsen & Denes Sexty

JHEP 08 (2021) 138, JHEP 04 (2023) 057 & PRD 109 (2024) 3, L031502

(2nd part) with J. Nordström & Will Horowitz

JCP 498 (2024) 112652 and arXiv:2404.18676

NPACT
Norwegian Particle, Astroparticle & Cosmology Theory network

ML MEETS LFT WORKSHOP – JULY 25TH 2024 – SWANSEA UNIVERSITY – UNITED KINGDOM

Outline

- Motivation: Quantum Initial Value Problems
- Part 1: Machine Learning Assisted Complex Langevin
- Part 2: Towards Exact Continuum Symmetries for ML Training
- Summary

Quantum Initial Value Problems

Schwinger-Keldysh Path Integral

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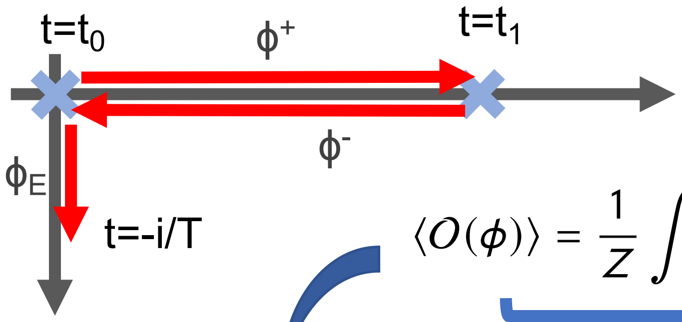


$<O(t_0)O(t_1)> = \mathrm{Tr}[\ \rho\ O(t_0)O(t_1)\ ]$

$$\langle \mathcal{O}(\phi)\rangle = \frac{1}{Z}\int d\phi_1 \int d\phi_2\, \rho(\phi_1,\phi_2) \int_{\phi_2}^{\phi_1} D\phi^+ D\phi^-\ \mathcal{O}(\phi)\ e^{iS[\phi_+]-iS[\phi_-]}$$

sampling over statistically distributed initial conditions

quantum “sum over paths”

$$\langle \mathcal{O}(\phi)\rangle = \frac{1}{Z}\int D\phi_E\, e^{-S_E[\phi_E]} \int_{\phi_E(\beta)}^{\phi_E(0)} D\phi^+ D\phi^-\ \mathcal{O}(\phi)\ e^{iS[\phi_+]-iS[\phi_-]}$$

Real-valued Feynman weight: Monte-Carlo methods applicable

Pure phase Feynman weight implies MC sign problem. One strategy: **Complex Langevin**
see C. Berger et.al. Phys.Rept. 892 (2021)

- Sign problem is NP-hard: **no generic solution** strategy is likely to exist
  Troyer, Wiese PRL 94 170201 (2004)

Stochastic Quantization

- Langevin evolution in fictitious additional time to reproduce quantum fluctuations

for an in-depth review: M. Namiki et.al. Stochastic Quantization (Springer) 1992

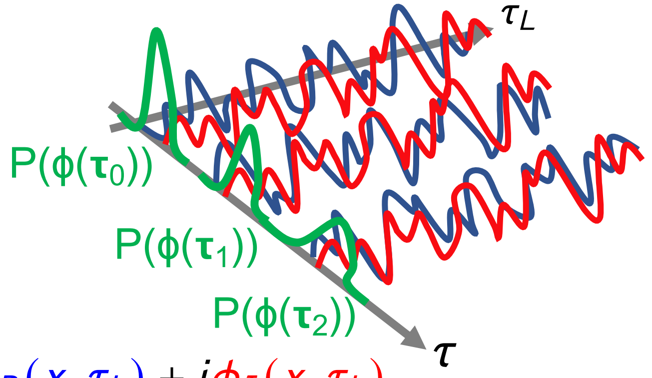
$$\frac{d\phi}{d\tau_L} = -\frac{\delta S_E[\phi]}{\delta\phi(x)} + \eta(x,\tau_L) \quad \text{with} \quad \langle\eta(x,\tau_L)\rangle = 0, \quad \langle\eta(x,\tau_L)\eta(x',\tau_L')\rangle = 2\delta(x-x')\delta(\tau_L-\tau_L')$$

Stochastic partial differential equation (SDE) with Gaussian noise

- Associated Fokker-Planck equation for P[ϕ]

$$\frac{\partial}{\partial\tau_L}\mathcal{P}(\phi) = \nabla_\phi\left[\left(S_E[\phi] + \nabla_\phi\right)\mathcal{P}(\phi)\right]$$

- Proof of convergence: $\lim_{\tau_L\to\infty} P[\phi,\tau_L] = e^{-S_E[\phi]}$



complexification: $-\frac{\delta S_E[\phi]}{\delta\phi(x)} \Rightarrow i\frac{\delta S[\phi]}{\delta\phi(x)}$ $\quad \phi(x,\tau_L) = \phi_R(x,\tau_L) + i\phi_I(x,\tau_L)$

$$\langle O[\phi]\rangle \leftrightarrow \lim_{T\to\infty}\frac{1}{T}\int_0^T d\tau_L O[\phi_R(x,\tau_L) + i\phi_I(x,\tau_L)]$$

Two major challenges for Complex Langevin

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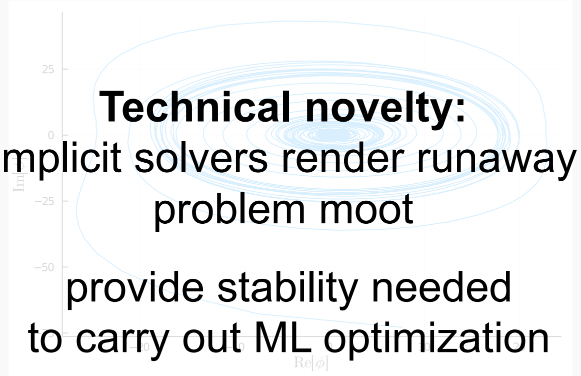
$$\frac{d\phi_R}{d\tau_L} = \mathrm{Re}\left[i\frac{\delta S[\phi]}{\delta\phi(x)}\Big|_{\phi=\phi_R+i\phi_I} \right] + \eta(x,\tau_L), \quad \frac{d\phi_I}{d\tau_L} = \mathrm{Im}\left[i\frac{\delta S[\phi]}{\delta\phi(x)}\Big|_{\phi=\phi_R+i\phi_I} \right]$$

Divergent solutions (runaways)



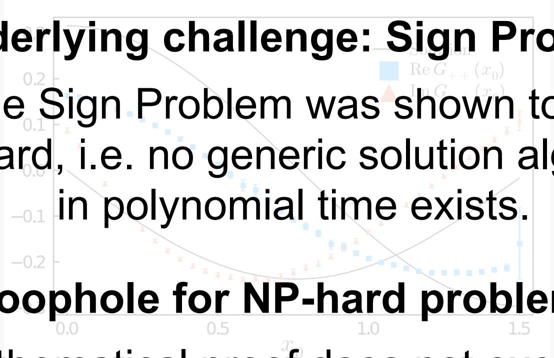
Technical novelty:
Implicit solvers render runaway problem moot

provide stability needed to carry out ML optimization

In practice: use adaptive step size in attempt to keep solution finite

see e.g.: G. Aarts et.al. PLB 687(2-3), 154–159 (2010)

Convergence to incorrect solutions



Underlying challenge: Sign Problem

The Sign Problem was shown to be NP-hard, i.e. no generic solution algorithm in polynomial time exists.

A loophole for NP-hard problems:

Mathematical proof does not exclude system specific solution algorithm –

use ML to infuse system specific info

slow decay of tails in histograms

see e.g.: G. Aarts et.al. Eur. Phys. J. C71 (2011) 1756

Part 1: Machine Learning Assisted Complex Langevin

See also talk by Denes Sexty
at Lattice 2024 - 30 Jul 2024, 15:05

Reinforcement learning – a ML success

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- Agent with a set of **predefined actions** [e.g. move left, jump] in an **environment**
  Karakovskiy and Togelius , *IEEE Trans. on Com. Intel. and AI in Games* 4.1 (2012): 55-67

- **Policy/Cost function** that defines **success** [e.g. score on computer screen]

- Need to **encode** choice of actions and evaluate **gradients** to minimize cost Wang, Ziyu, et al. *Int. conf. on machine learning*. PMLR, 2016.

Need to handle **failure state** [e.g. falling into pits]

Improving the score: allow for more actions [e.g. move right]

RL & Quantum simulation – executive summary

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$$\frac{d\phi}{d\tau_L} = iK[\phi]\frac{\partial S}{\partial \phi} + \frac{\partial K[\phi]}{\partial \phi} + \sqrt{K[\phi]}\eta$$

- Environment: **space of distributions** explored by a stochastic process
- **Agent**: controller of the **non-neutral modification** represented by the **kernel K**. Limited actions – keep the kernel field & τ_L independent
- **Cost function**: deviation of late τ_L stationary distribution from **prior knowledge** (symmetries, known cumulants, etc.)
- Use auto differentiation or shadowing analysis to compute **robust gradients** of the inherently **chaotic dynamics**.
- We achieve **convergence to correct stationary distribution** for model systems in parameter regimes **previously inaccessible**.

Manual exploration of kernels

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- Simultaneous modification of drift and noise allows to modify convergence

$$\frac{d\phi}{d\tau_L} = iK[\phi]\frac{\partial S}{\partial \phi} + \frac{\partial K[\phi]}{\partial \phi} + \sqrt{K[\phi]}\eta$$

- Observation in simple models: kernel that renders drift real restores convergence

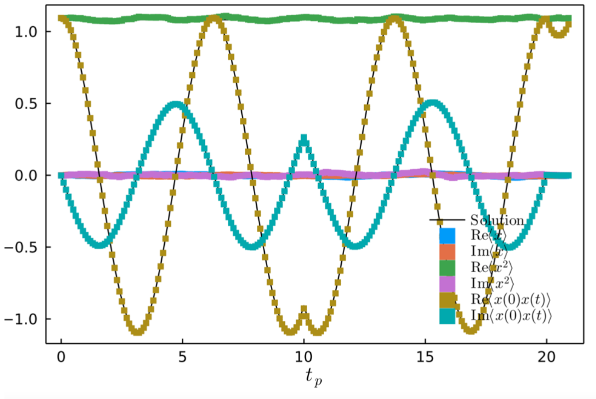
Okamoto, Okano, Schülke, Tanaka, PLB 324 684 (1989)

Free theory in real-time

$$S = \phi^t M \phi \qquad K = iM^{-1}$$

$$iK\frac{dS}{d\phi} = -\phi$$

$$\frac{d\phi}{d\tau_L} = -\phi + \sqrt{iM^{-1}}\eta$$



D. Alvestad, R. Larsen, A.R JHEP 04 (2023) 057

- Stroke-of-genius approach: find bespoke kernel for your system (c.f. reformulation)

Systematic learning of kernels

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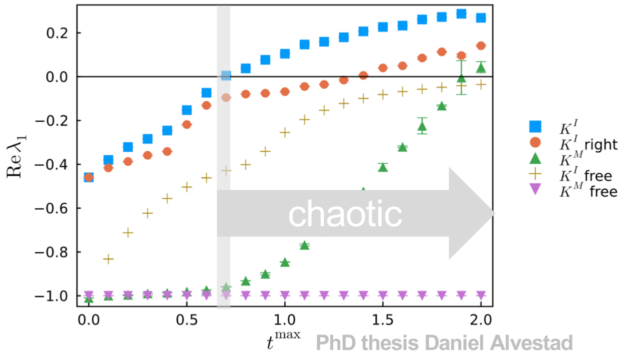
- **Optimal kernels via prior information from continuum theory**

$$L^{\text{sym}} = \sum_t \left\{ \langle \phi_t \rangle^2 + \langle \phi_t^3 \rangle^2 + \left(\langle \phi_t^2 \rangle - \phi^2 \right) \right\}$$

$$L^{\text{bnd}} = \sum_i \sum_k \left\{ \langle L_c[\phi_i] \mathcal{O}_k \rangle_Y \right)^2$$

$$L^{\text{eucl}} = \sum_i \left\{ \left(\langle \phi_0 \phi_i \rangle - D_i^E \right)^2 \right\}$$

CL Lyapunov exponents



PhD thesis Daniel Alvestad

- Auto-differentiation techniques to compute $\dfrac{\partial L^{\text{tot}}}{\partial K_{ij}}$ (derivative of stochastic process)
  [note: deterministic dynamics chaotic]

- In principle possible, in practice slow: cheaper optimization functional instead

$$L^{\text{low cost}} = \frac{1}{N_t} \sum_{i=1}^{N_t} \text{Im}[\phi]^2$$

minimizes drift away from the origin
(similar to dynamic stabilization
but remains holomorphic)

Complex Langevin for 1+1d scalar fields

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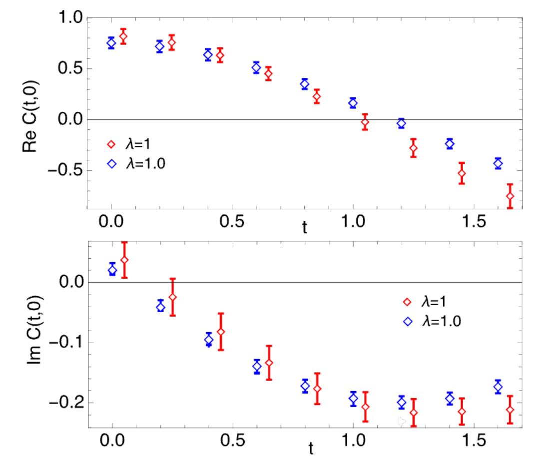
- Using a field independent kernel $K = exp[A + iB]$ with A,B real matrices

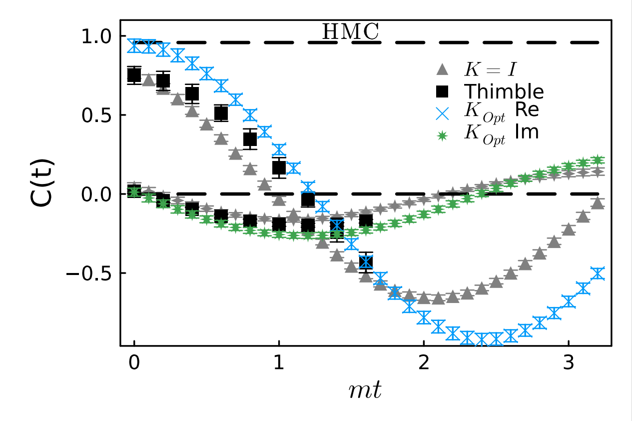
Contour Deformations



A. Alexandru et.al. PRD 95 (2017) 11, 114501

- coarse grid due to high method cost

Optimal learned CL kernels



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- avoid discretization artifacts with finer grids, accessible dur to good scaling

Learned Kernels

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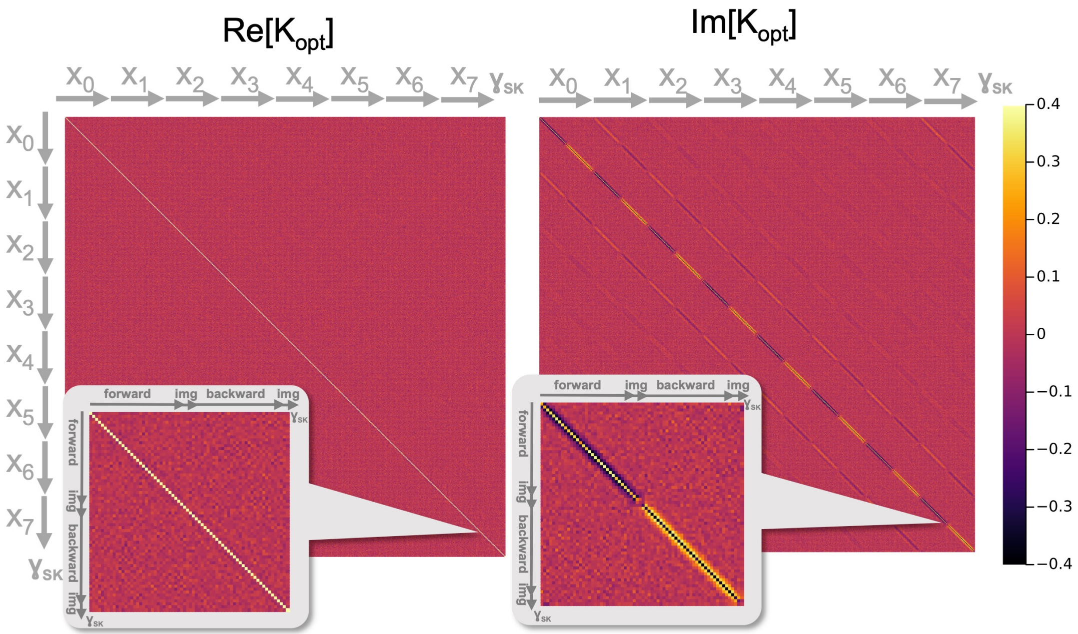
- Optimal learned kernels achieve convergence with minimal modification (sparse)



- ML results as starting point for a better analytic understanding of kernel structure

Limits to our current strategy

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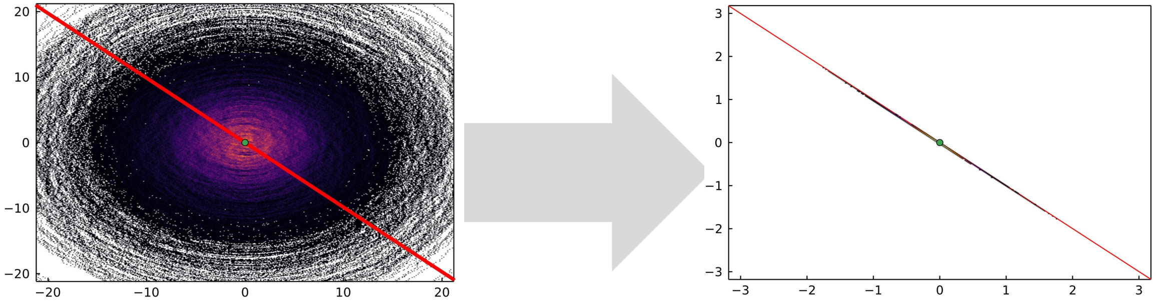
- Constant kernel works well in theories with single critical point at the origin

simple Gaussian model $$S = \frac{1}{2} i x^2$$

Lefschetz thimbles $$\frac{d\phi}{d\tau} = \overline{\frac{dS}{d\phi}}$$

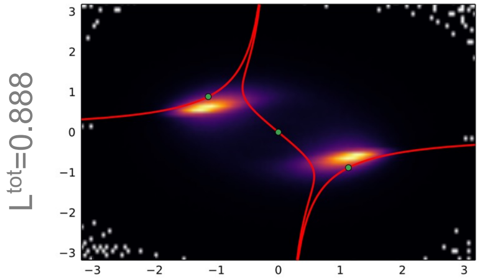
naïve CL

learned kernelled CL

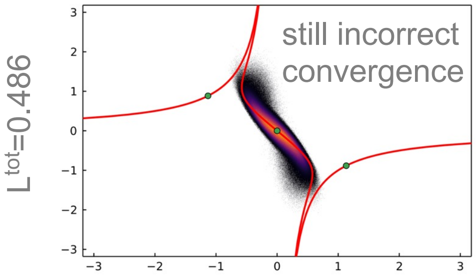


- Multiple critical points may require a field dependent kernel: $S = 2ix^2 + (1/2)x^4$

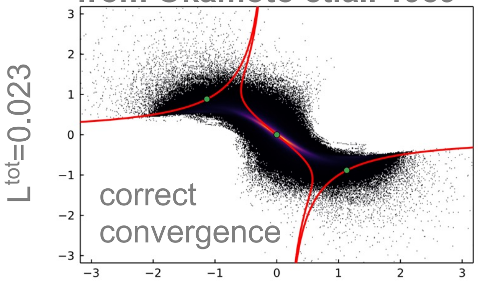
naïve CL



learned const. kernelled CL



field dependent kernel from Okamoto et.al. 1989



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Part 2: Towards Exact Continuum Symmetries for ML Training

The Continuum Symmetry Challenge

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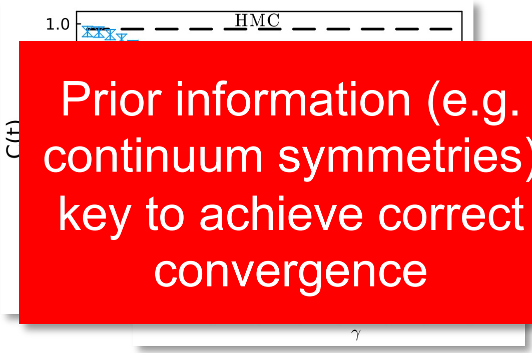
Quantum Initial Value Problems

Complex Langevin



Prior information (e.g. continuum symmetries) key to achieve correct convergence

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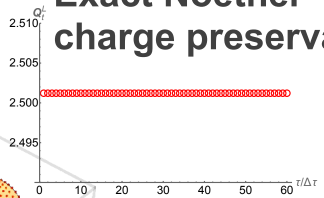
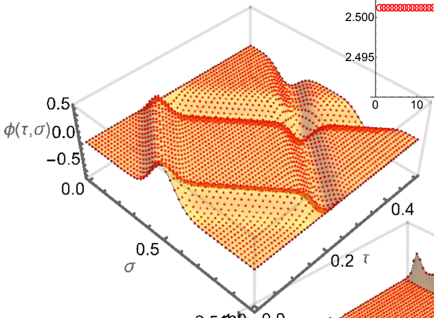
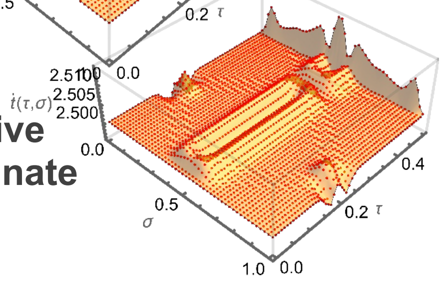
PRD 109 (2024) 3, L031502

Exact Noether charge preservation







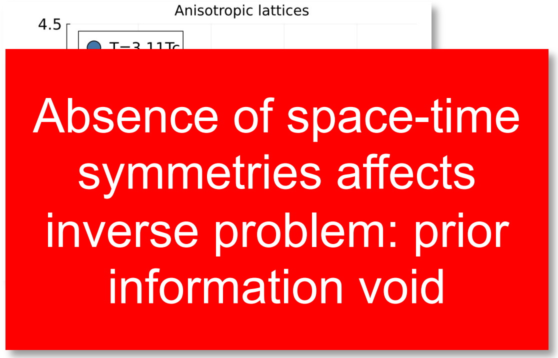
Adaptive coordinate maps

Novel SCL action

Classical Initial Value Problems

Quantum Boundary Value Problems

Euclidean Lattice QCD



Absence of space-time symmetries affects inverse problem: prior information void

R. Larsen, G. Parkar, A.R. J. Weber
arXiv:2402.10819

R. Larsen, A.R. & HotQCD
PRD 109 (2024) 7, 074504

Worldline Formalism in GR

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- Relativistic point particle motion: ”shortest path in given space-time” = geodesic
- Equal treatment of space & time as **dynamic coordinate maps**:
  from trajectory to world line [both t(ɣ) and x(ɣ) evolve dynamically]

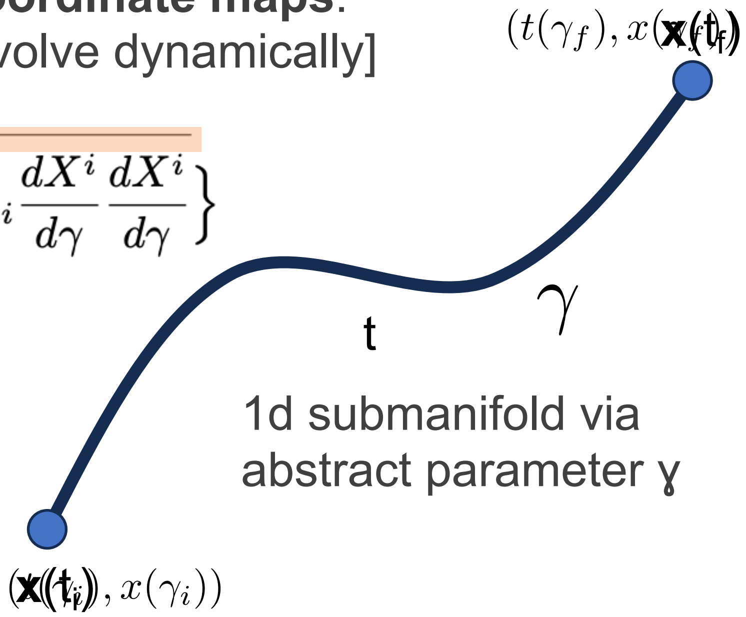
$$S_{\rm geo} = \int d\gamma\,(-mc)\Big\{\sqrt{\Big(G_{00} + \frac{V(\vec{x})}{2mc^2}\Big)\frac{dX^0}{d\gamma}\frac{dX^0}{d\gamma} + G_{ii}\frac{dX^i}{d\gamma}\frac{dX^i}{d\gamma}}\Big\}$$

$$V(\vec{x})/2mc^2 \ll 1$$

$$\frac{d|\vec{x}|/d\gamma}{dt/d\gamma}/c = v/c \ll 1$$

$$X^\mu = (t, \vec{x})^\mu$$

$$S_{\rm nr} = \int dt\,\Big\{-mc^2 + \frac{1}{2}m\dot{\vec{x}}^2(t) - V\big(\vec{x}(t)\big)\Big\}$$



- mc denotes scale where motion through space and time becomes inseparable

Advantages of the worldline formalism

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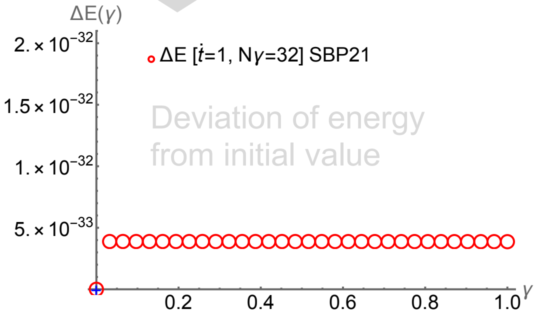
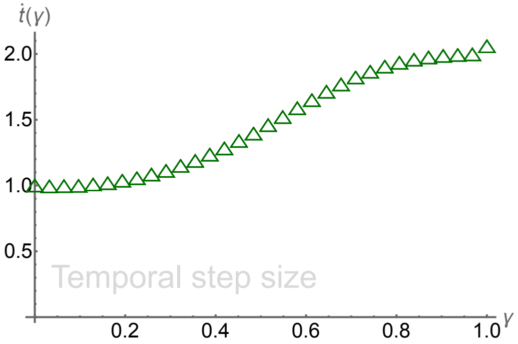
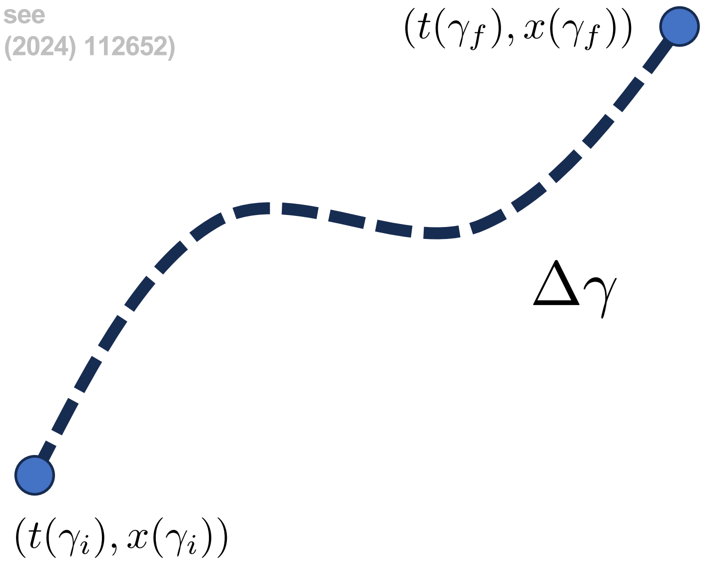
- Discretizing the action in γ leaves space-time coordinates $X^\mu = (t, \vec{x})^\mu$ continuous
- Discretized world-line action invariant under infinitesimal coordinate transforms: Noether's theorem holds! (for a detailed study of point mechanics see A.R., J. Nordström, J.Comput.Phys. 498 (2024) 112652)



Energy of the system preserved *exactly* at its *continuum* value



Resolution of the time grid *adapts* to dynamics of particle



A Field Theory Counterpart?

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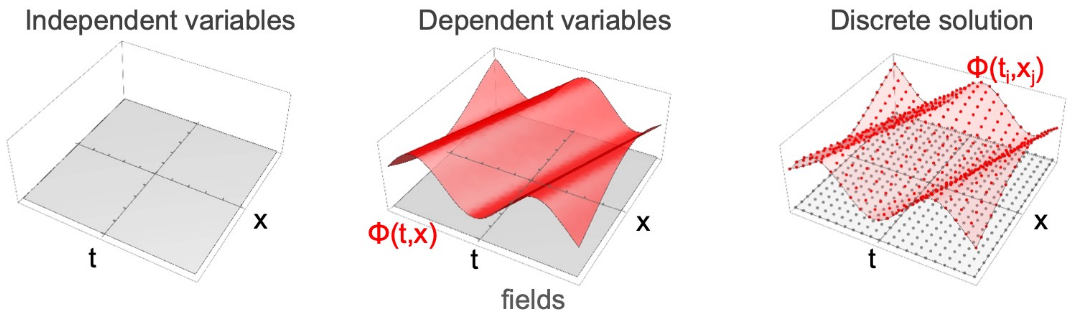
Conventional field theory



Spacetime symmetries broken by Δt and Δx

Field theory with dynamic coordinate maps

Spacetime symmetries unaffected by Δτ and Δσ?

YES!

A world ”volume” action for fields?

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- Starting point is the standard reparameterization invariant action

$$S = \int d^{(d+1)}X \sqrt{-\det[G]}\frac{1}{2}\Big(G^{\mu\nu}\partial_\mu\phi(X)\partial_\nu\phi(X) - V(\phi)\Big)$$

- Are we perhaps overlooking a constant term, just as in the non-relativistic action?

$$S = \int d^{(d+1)}X \sqrt{-\det[G]}\Big\{-T + \frac{1}{2}\Big(G^{\mu\nu}\partial_\mu\phi(X)\partial_\nu\phi(X) - V(\phi)\Big)\Big\}.$$

- Consider as low energy limit of another more general action (κ = action density/T)

$$\mathcal{S}_{\rm BVP} \equiv \int d^{(d+1)}X \sqrt{-\det[G]}(-T)\Big\{1 - \frac{1}{2T}\Big(G^{\mu\nu}\partial_\mu\phi(X)\partial_\nu\phi(X) - V(\phi)\Big)\Big\} + \mathcal{O}(\kappa^2)$$

—

Towards the SCL action

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- Crucial next step: elevate spacetime coordinates to dynamical coordinate maps

worldline: $t \to t(\gamma)$ here: $X^\mu \to X^\mu(\Sigma)$ $\Sigma^a = (\tau, \vec{\sigma})^a = (\tau, \sigma_1, \ldots, \sigma_d)^a$

$$\mathcal{S}_{\rm BVP} = \int d^{(d+1)}\Sigma \, (-T)\sqrt{\Big(\frac{1}{T}V(\phi) - 1\Big)\det[g] + \frac{1}{T}\partial_a\phi(\Sigma)\partial_b\phi(\Sigma)\text{adj}[g]_{ab}}.$$

$$\text{adj}[g] = g^{-1}\det[g]$$

- Can absorb the Jacobian into new *induced metric g* on the space of parameters

$$\sqrt{-\det[J]\det[G]\det[J]} = \sqrt{-\det[J^T]\det[G]\det[J]} = \sqrt{-\det[J^T G J]} = \sqrt{-\det[g]}$$

- The scale T denotes where field and coordinate dynamics become inseparable

Proof-of-principle in (1+1)d

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- Scalar wave propagation is numerically challenging (stability, accuracy)

$$\mathcal{S}_{\rm BVP} = \int d\tau d\sigma \, (-T)\sqrt{\quad -\det[g] + \frac{1}{T}\partial_a\phi(\Sigma)\partial_b\phi(\Sigma){\rm adj}[g]_{ab}}$$
$$= \int d\tau d\sigma \, (-T)\Big\{c^2(\dot{t}x' - \dot{x}t')^2$$
$$+\frac{1}{T}\Big(\dot{\phi}^2(c^2(t')^2 - (x')^2) + 2\dot{\phi}\phi'(\dot{x}x' - c^2\dot{t}t') + (\phi')^2(c^2\dot{t}^2 - \dot{x}^2)\Big)\Big\}^{1/2}$$

- Simplify by considering only time as dynamical mapping (trivial x[τ,σ]= σ)

$$\mathcal{E}_{\rm BVP} \overset{x=\sigma}{\equiv} \int d\tau d\sigma \, \frac{1}{2}\Big\{(\dot{t})^2 + \frac{1}{T}\Big(\dot{\phi}^2((t')^2 - 1) - 2\dot{\phi}\phi'\dot{t}t' + (\phi')^2(\dot{t}^2)\Big)\Big\}$$

Summation-by-parts finite differences

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- Derivation of Noether theorem or governing equations rely on integration by parts
- Mimetic discretization needed to preserve IBP in discrete setting:

for a review see D. Fernández, J. E. Hicken, and D. W. Zingg, Comp. & Fluids 95 171 (2014)

$$\int_{t_i}^{t_f} dt\, u(t)\, v(t) \approx \mathbf{u}^t\, \mathbb{H}\, \mathbf{v}$$

quadrature rule

$$\mathbb{D} = \mathbb{H}^{-1}\mathbb{Q}$$

finite difference stencil

$$\mathbb{Q} + \mathbb{Q}^t = \mathbb{E}_N - \mathbb{E}_0$$

$$= \mathrm{diag}[-1, 0, \ldots, 0, 1]$$

$$(\mathbb{D}\mathbf{u})^t\, \mathbb{H}\, \mathbf{v} = -\mathbf{u}^t\, \mathbb{H}\, \mathbb{D}\mathbf{v} + \mathbf{u}_N \mathbf{v}_N - \mathbf{u}_0 \mathbf{v}_0$$

Δt

For more details on the discretization strategy

Lattice 2024 - 29 July 2024, 11:35

for SBP operator as momentum operator for particle in a finite box see S.Kim, A.R. 2403.13558

Classical wave propagation in (1+1)d

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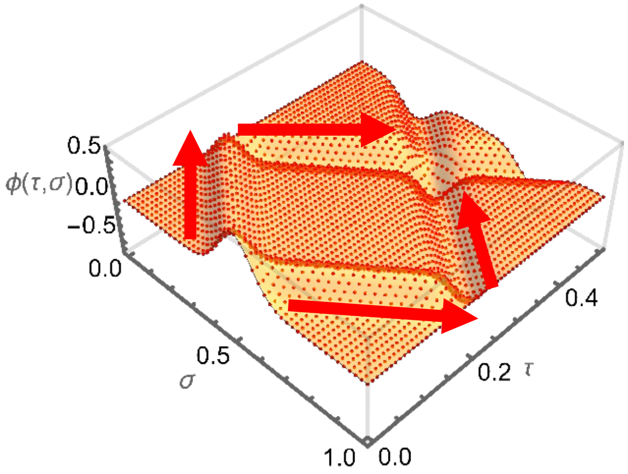
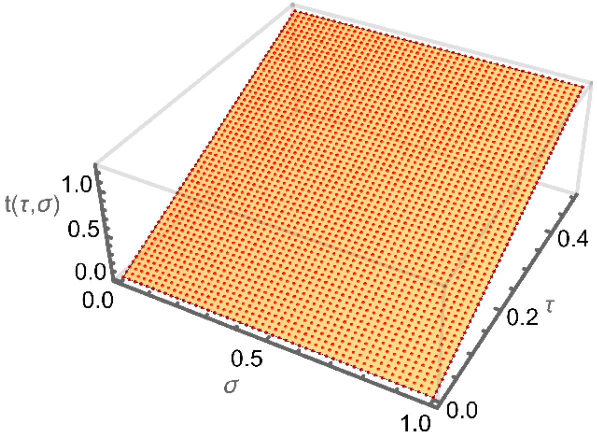
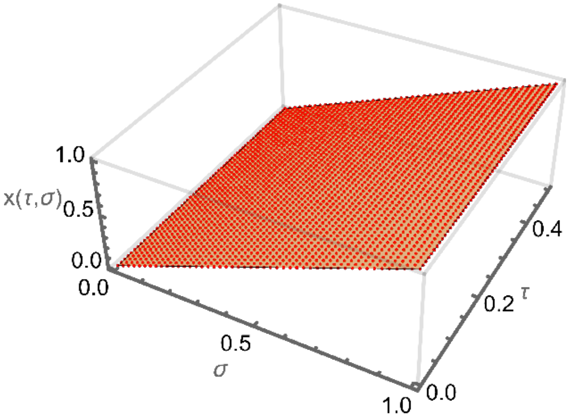
- Numerical search for critical point ($\phi_{cl}[\tau,\sigma]$, $t_{cl}[\tau,\sigma]$) of the classical action



field evolution $\phi[\tau,\sigma]$



temporal map $t[\tau,\sigma]$



trivial spatial map $x[\tau,\sigma]= \sigma$

- Here T=10.000, choice to obtain effects on the coordinate maps on percent level

Coordinate maps adjust to dynamics

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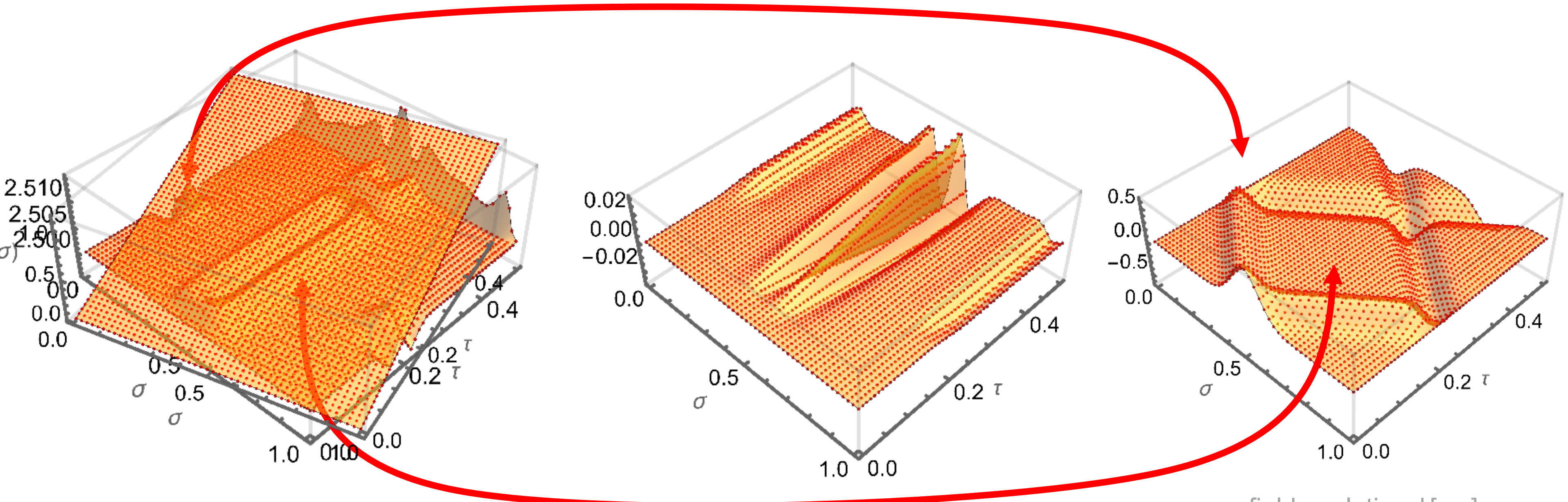

τ derivative of t[τ,σ]

σ derivative of t[τ,σ]

field evolution ϕ[τ,σ]

- Temporal map automatically adapts resolution according to wave dynamics

Noether Charge – Time Translations

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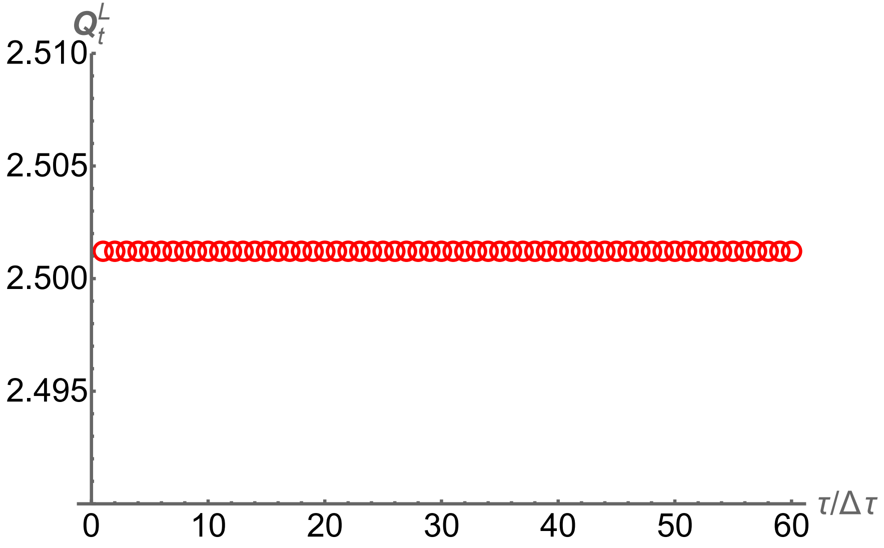
- Due to mimetic SBP discretization: continuum expression with

for more details see A.R., W.A. Horowitz, J. Nordström arXiv:2404.18676

$$Q_t^{\mathrm{L}} = \mathbb{H}_\sigma \underbrace{\left\{(\mathbb{D}_\tau \boldsymbol{t}_1) + \frac{1}{T}\Big((\mathbb{D}_\sigma \boldsymbol{\phi}_1)^2 \circ (\mathbb{D}_\tau \boldsymbol{t}_1) - (\mathbb{D}_\tau \boldsymbol{\phi}_1) \circ (\mathbb{D}_\sigma \boldsymbol{\phi}_1) \circ (\mathbb{D}_\sigma \boldsymbol{t}_1)\Big)\right\}}_{\boldsymbol{J}^0 \in \mathbb{R}^{N_\tau \times N_\sigma}}$$

$$+ \underbrace{\left\{(\boldsymbol{h}_\sigma^T \tilde{\boldsymbol{\lambda}}^t)\mathfrak{d}^\tau[0] + (\boldsymbol{h}_\sigma^T \tilde{\boldsymbol{\gamma}}^t)\mathfrak{d}^\tau[N_\tau]\right\}}_{\text{Lagr. mult. contrib.}},$$

- **Exact conservation** of the Noether charge associated with time translations: vital **prior information** for future use in machine learning context.



Summary

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- Real-time dynamics of quantum fields challenging due to NP-hard sign problem. **Complex Langevin** one promising path forward.
- **ML strategy**: systematically incorporate **system specific prior information** (symmetries, Euclidean correlators, etc.) in CL simulation via learned optimal **kernels**

Learned optimal field independent kernels

- Optimal **kernels in 1+1d**: new benchmark in accuracy & real-time extent (~2x)

- For effective machine learning **prior knowledge** (training data) plays crucial rule and continuum space-time symmetries are among the most powerful
- Recent progress by developing a novel classical action for scalars with dynamical coordinate maps that **retains continuum space-time symmetries** after discretization

Discretizing the Worldline

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- We discretize in the world-line parameter, not in the time variable:

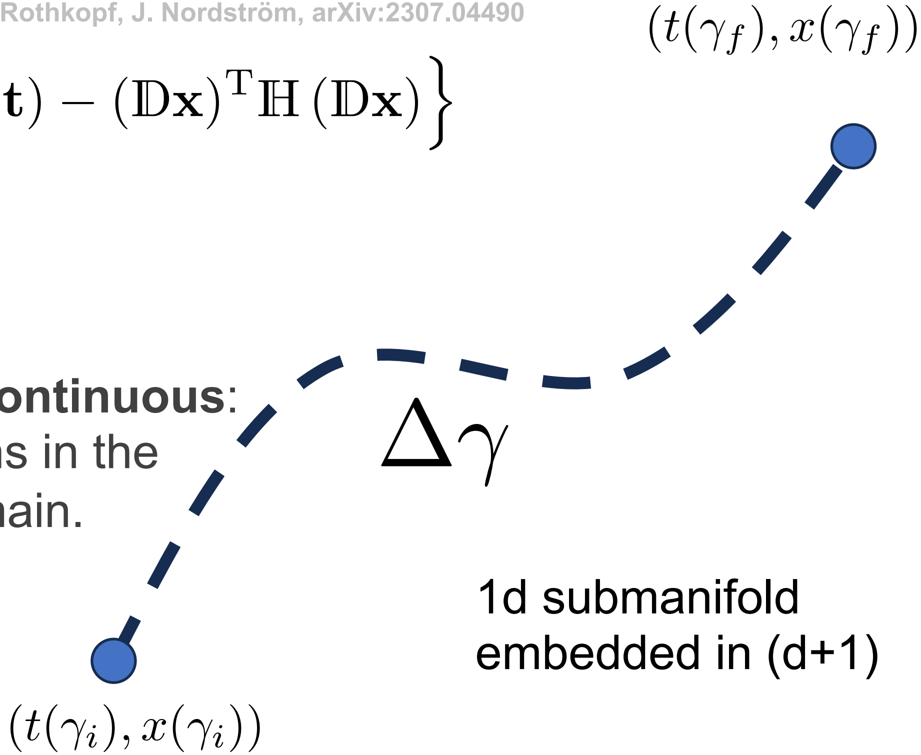
A. Rothkopf, J. Nordström, arXiv:2307.04490

$$\mathbb{E}_{\rm BVP} = \frac{1}{2}\Big\{\Big(\big(c^2 + \frac{2V(\mathbf{x})}{m}\big)\circ \mathbb{D}\mathbf{t}\Big)^{\rm T}\mathbb{H}\,(\mathbb{D}\mathbf{t}) - (\mathbb{D}\mathbf{x})^{\rm T}\mathbb{H}\,(\mathbb{D}\mathbf{x})\Big\}$$
$$+\lambda_1(\mathbf{t}[1]-t_i)+\lambda_2(\mathbf{t}[N_\gamma]-t_f)$$
$$+\lambda_3(\mathbf{x}[1]-t_i)+\lambda_4(\mathbf{x}[N_\gamma]-x_f)$$

- Note that the values of **t** and **x** remain **continuous**: explicit invariance under time translations in the discrete setting. No issue with finite domain.

- Noether charge:

$$\mathbb{Q}_{\mathbf{t}} = 2(\mathbb{D}\mathbf{t})\circ(\mathbf{1}+2\mathbf{V}(\mathbf{x})/m)$$



Now reformulate as IVP

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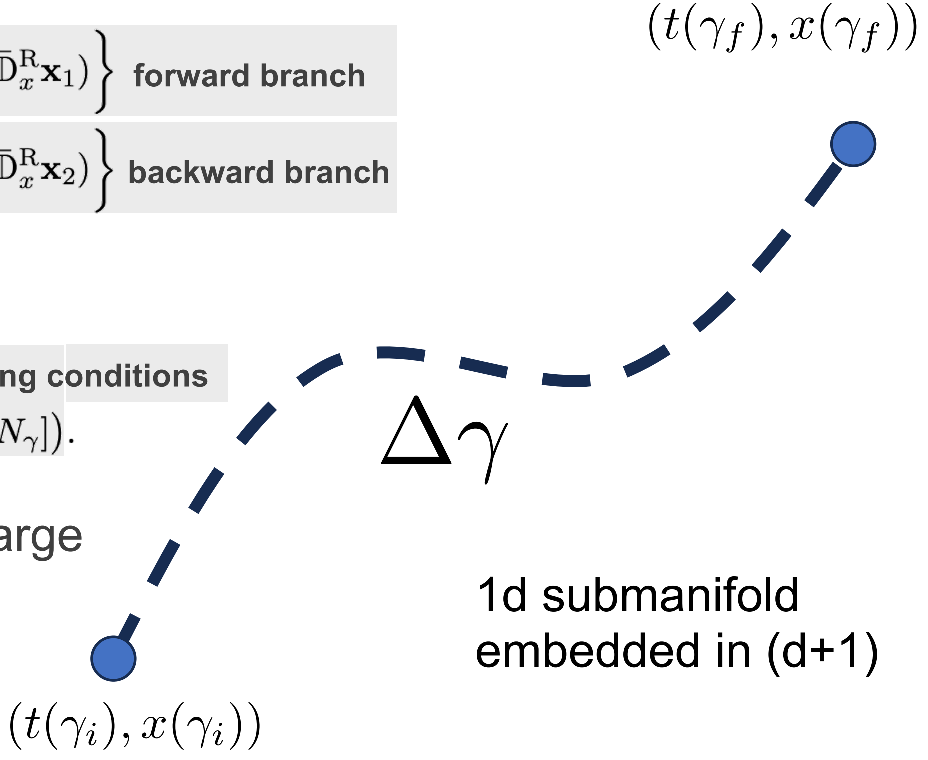
- Forward-backward construction for both time and space coordinate

$$
\begin{aligned}
\mathbb{E}_{\rm IVP} =& \frac{1}{2}\left\{(\bar{\mathbb{D}}_t^{\rm R}\mathbf{t}_1)^{\rm T}\mathbb{d}\left[c^2+\frac{2\mathbf{V}(\mathbf{x}_1)}{m}\right]\bar{\mathbb{H}}(\bar{\mathbb{D}}_t^{\rm R}\mathbf{t}_1)-(\bar{\mathbb{D}}_x^{\rm R}\mathbf{x}_1)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}_x^{\rm R}\mathbf{x}_1)\right\} \quad \text{forward branch}\\
&-\frac{1}{2}\left\{(\bar{\mathbb{D}}_t^{\rm R}\mathbf{t}_2)^{\rm T}\mathbb{d}\left[c^2+\frac{2\mathbf{V}(\mathbf{x}_2)}{m}\right]\bar{\mathbb{H}}(\bar{\mathbb{D}}_t^{\rm R}\mathbf{t}_2)-(\bar{\mathbb{D}}_x^{\rm R}\mathbf{x}_2)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}_x^{\rm R}\mathbf{x}_2)\right\} \quad \text{backward branch}\\
&+\lambda_1\big(\mathbf{t}_1[1]-t_i\big)+\lambda_2\big((\mathbb{D}\mathbf{t}_1)[1]-\dot{t}_i\big)+\lambda_3\big(\mathbf{x}_1[1]-x_i\big)\\
&+\lambda_4\big((\mathbb{D}\mathbf{x}_1)[1]-\dot{x}_i\big) \quad \text{initial conditions}\\
&+\lambda_5\big(\mathbf{t}_1[N_\gamma]-\mathbf{t}_2[N_\gamma]\big)+\lambda_6\big(\mathbf{x}_1[N_\gamma]-\mathbf{x}_2[N_\gamma]\big) \quad \text{connecting conditions}\\
&+\lambda_7\big((\mathbb{D}\mathbf{t}_1)[N_\gamma]-(\mathbb{D}\mathbf{t}_2)[N_\gamma]\big)+\lambda_8\big((\mathbb{D}\mathbf{x}_1)[N_\gamma]-(\mathbb{D}\mathbf{x}_2)[N_\gamma]\big).
\end{aligned}
$$

- Lagrange multipliers modify Noether charge

$$
\mathbb{Q}_{\mathbf{t}} = 2(\mathbb{D}\mathbf{t})\circ(\mathbf{1}+2\mathbf{V}(\mathbf{x})/m) + \lambda_2\delta(\gamma-\gamma_i)+\lambda_7\delta(\gamma-\gamma_f)
$$



Discretized Schwinger-Keldysh action

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- Introduce forward and backward branch (classical Schwinger-Keldysh)

$$
\begin{aligned}
\mathbb{E}^{\rm L}_{\rm IBVP} = & \frac{1}{2}\Big\{(\bar{\mathbb{D}}^t_\tau \boldsymbol{t}_1)^2 + \frac{1}{T}\Big((\bar{\mathbb{D}}^\phi_\tau \boldsymbol{\phi}_1)^2 \circ \big((\mathbb{D}_\sigma \boldsymbol{t}_1)^2 - 1\big) \\
& \quad - 2(\bar{\mathbb{D}}^\phi_\sigma \boldsymbol{\phi}_1) \circ (\bar{\mathbb{D}}^\phi_\tau \boldsymbol{\phi}_1) \circ (\bar{\mathbb{D}}^t_\tau \boldsymbol{t}_1) \circ (\mathbb{D}^t_\sigma \boldsymbol{t}_1) + (\bar{\mathbb{D}}^\phi_\sigma \boldsymbol{\phi}_1)^2 \circ (\bar{\mathbb{D}}^t_\tau \boldsymbol{t}_1)^2\Big)\Big\}^T \boldsymbol{h} \\
& - \frac{1}{2}\Big\{(\bar{\mathbb{D}}^t_\tau \boldsymbol{t}_2)^2 + \frac{1}{T}\Big((\bar{\mathbb{D}}^\phi_\tau \boldsymbol{\phi}_2)^2 \circ \big((\mathbb{D}_\sigma \boldsymbol{t}_2)^2 - 1\big) \\
& \quad - 2(\bar{\mathbb{D}}^\phi_\sigma \boldsymbol{\phi}_2) \circ (\bar{\mathbb{D}}^\phi_\tau \boldsymbol{\phi}_2) \circ (\bar{\mathbb{D}}^t_\tau \boldsymbol{t}_2) \circ (\mathbb{D}^t_\sigma \boldsymbol{t}_2) + (\bar{\mathbb{D}}^\phi_\sigma \boldsymbol{\phi}_2)^2 \circ (\bar{\mathbb{D}}^t_\tau \boldsymbol{t}_2)^2\Big)\Big\}^T \boldsymbol{h}
\end{aligned}
$$

- Enforce initial (temporal), Dirichlet boundary (spatial) and connecting conditions

$$
\begin{aligned}
&+(\boldsymbol{\lambda}^t)^T \mathbb{h}_\sigma\big(\mathbb{P}^0_\tau[\boldsymbol{t}_1] - \boldsymbol{t}_{\rm IC}\big) + (\boldsymbol{\lambda}^\phi)^T \mathbb{h}_\sigma\big(\mathbb{P}^0_\tau[\boldsymbol{\phi}_1] - \boldsymbol{\phi}_{\rm IC}\big) \\
&+(\tilde{\boldsymbol{\lambda}}^t)^T \mathbb{h}_\sigma\big(\mathbb{P}^0_\tau[(\mathbb{D}_\tau \boldsymbol{t}_1)] - \dot{\boldsymbol{t}}_{\rm IC}\big) + (\tilde{\boldsymbol{\lambda}}^\phi)^T \mathbb{h}_\sigma\big(\mathbb{P}^0_\tau[(\mathbb{D}_\tau \boldsymbol{\phi}_1)] - \dot{\boldsymbol{\phi}}_{\rm IC}\big) \\
&+(\boldsymbol{\gamma}^t)^T \mathbb{h}_\sigma\big(\mathbb{P}^{N_\tau}_\tau[\boldsymbol{t}_1] - \mathbb{P}^{N_\tau}_\tau[\boldsymbol{t}_2]\big) + (\boldsymbol{\gamma}^\phi)^T \mathbb{h}_\sigma\big(\mathbb{P}^{N_\tau}_\tau[\boldsymbol{\phi}_1] - \mathbb{P}^{N_\tau}_\tau[\boldsymbol{\phi}_2]\big)
\end{aligned}
$$

$$
\begin{aligned}
&+(\tilde{\boldsymbol{\gamma}}^t)^T \mathbb{h}_\sigma\big(\mathbb{P}^{N_\tau}_\tau[(\mathbb{D}_\tau \boldsymbol{t}_1)] - \mathbb{P}^{N_\tau}_\tau[(\mathbb{D}_\tau \boldsymbol{t}_2)]\big) \\
&+(\tilde{\boldsymbol{\gamma}}^\phi)^T \mathbb{h}_\sigma\big(\mathbb{P}^{N_\tau}_\tau[(\mathbb{D}_\tau \boldsymbol{\phi}_1)] - \mathbb{P}^{N_\tau}_\tau[(\mathbb{D}_\tau \boldsymbol{\phi}_2)]\big) \\
&+(\boldsymbol{\kappa}^\phi)^T \mathbb{h}_\tau\big(\mathbb{P}^0_\sigma[\boldsymbol{\phi}_1] - \boldsymbol{0}\big) + (\tilde{\boldsymbol{\kappa}}^\phi)^T \mathbb{h}_\tau\big(\mathbb{P}^{N_\sigma}_\sigma[\boldsymbol{\phi}_1] - \boldsymbol{0}\big) \\
&+(\boldsymbol{\xi}^\phi)^T \mathbb{h}_\tau\big(\mathbb{P}^0_\sigma[\boldsymbol{\phi}_2] - \boldsymbol{0}\big) + (\tilde{\boldsymbol{\xi}}^\phi)^T \mathbb{h}_\tau\big(\mathbb{P}^{N_\sigma}_\sigma[\boldsymbol{\phi}_2] - \boldsymbol{0}\big).
\end{aligned}
$$

- Locate extremum via numerical optimization (Interior Point Optimization)