The Research Council of Norway

University of Stavanger

Towards symmetric higher order discretization schemes on the lattice

Alexander Rothkopf
Faculty of Science and Technology
Department of Mathematics and Physics
University of Stavanger

based on: A.R. and J. Nordström **arXiv:2205.14028**
motivated by A.R. arXiv:2102.08616

Norwegian Particle, Astroparticle & Cosmology Theory network

NORDIC LATTICE MEETING – AUGUST 22ND 2022 – HELSINKI UNIVERSITY – FINLAND (HYBRID)

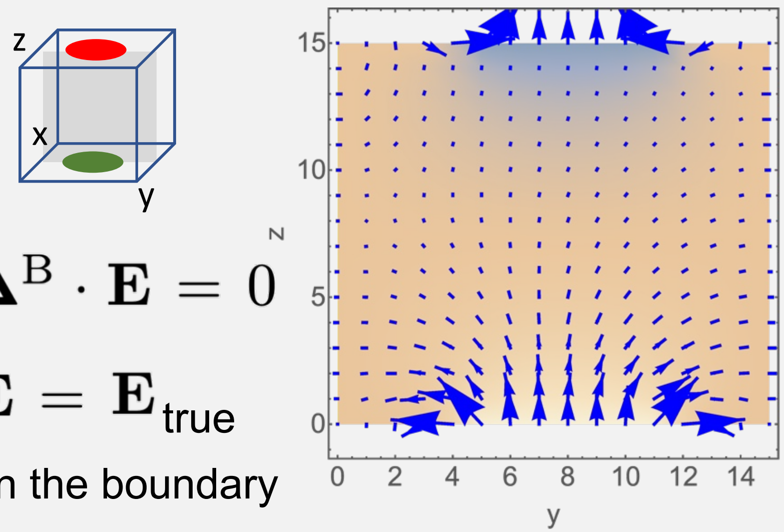
Motivation

University of Stavanger

- Systems without translational invariance: **finite extent** or **presence of sources**
  small system collisions at LHC, strong coupling cavity QED, quarkonium real-time dynamics …
- Classical Wilson action corresponds to a **backward finite difference** Gauss-law

Finite size capacitor

backward finite difference



$$\mathbf{\Delta}^B \cdot \mathbf{E} = 0$$

$$\mathbf{E} = \mathbf{E}_{\text{true}}$$

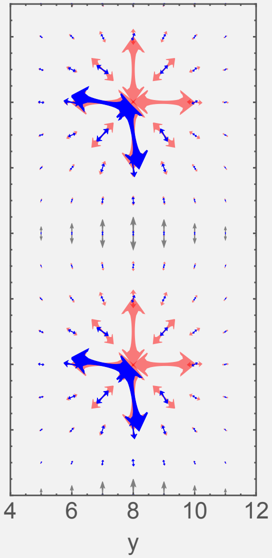
on the boundary

missing field strength close to forward boundary

Abelian examples

Charge-anticharge pair

backward finite difference



$$\mathbf{\Delta}^B \cdot \mathbf{E} = \frac{1}{a_s^3}\left[\delta_{\mathbf{x}\mathbf{x}_0} - \delta_{\mathbf{x}\mathbf{x}_1}\right]$$

force density from stress tensor highly asymmetric

for more details see: A.R. arXiv:2102.08616

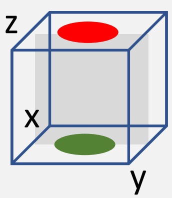
Motivation

University of Stavanger

- Systems without translational invariance: **finite extent** or **presence of sources**
  small system collisions at LHC, strong coupling cavity QED, quarkonium real-time dynamics …
- Classical Wilson action corresponds to a **backward finite difference** Gauss-law

Finite size capacitor

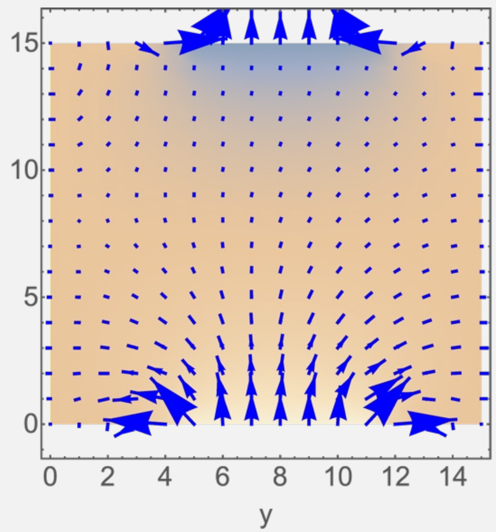
backward finite difference



$$\mathbf{\Delta}^{\mathrm{B}} \cdot \mathbf{E} = 0$$

$$\mathbf{E} = \mathbf{E}_{\text{true}}$$

on the boundary

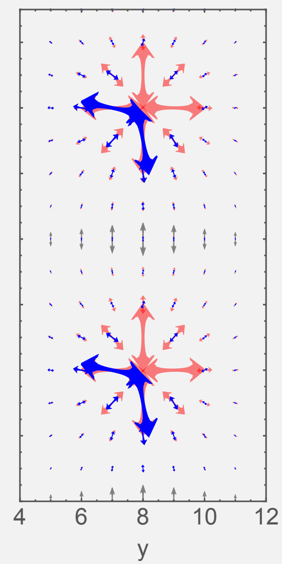


missing field strength close to forward boundary

Abelian examples

Charge-anticharge pair

backward finite difference



$$\mathbf{\Delta}^{\mathrm{B}} \cdot \mathbf{E} = \frac{1}{a_s^3}\left[\delta_{\mathbf{x}\mathbf{x}_0} - \delta_{\mathbf{x}\mathbf{x}_1}\right]$$

force density from stress tensor highly asymmetric

for more details see: A.R. arXiv:2102.08616

- Goal: discretization that accommodate boundaries & is symmetric around charges

Gauss Law is tricky even locally

- Need a symmetric discretization, but naïve central finite differences do not respect the integral form of the Gauss law

$$Q = \int dV\, q = \int dV\, (\nabla \mathbf{E}) = \int_{\partial V} d\mathbf{A} \cdot \mathbf{E}$$

Gauss Law is tricky even locally

University of Stavanger

- Need a symmetric discretization, but naïve central finite differences do not respect the integral form of the Gauss law

$$Q = \int dV\, q = \int dV\, (\nabla \mathbf{E}) \neq \int_{\partial V} d\mathbf{A} \cdot \mathbf{E}$$

Gauss Law is tricky even locally

University of Stavanger

- Need a symmetric discretization, but naïve central finite differences do not respect the integral form of the Gauss law

$$Q = \int dV\, q = \int dV\, (\nabla \mathbf{E}) \neq \int_{\partial V} d\mathbf{A} \cdot \mathbf{E}$$

$$\mathbf{\Delta}^{\mathrm{C}} \cdot \mathbf{E} =$$

$$\frac{1}{a_s^3}\left[\delta_{\mathbf{x}\mathbf{x}_0} - \delta_{\mathbf{x}\mathbf{x}_1}\right]$$

naïve central FD

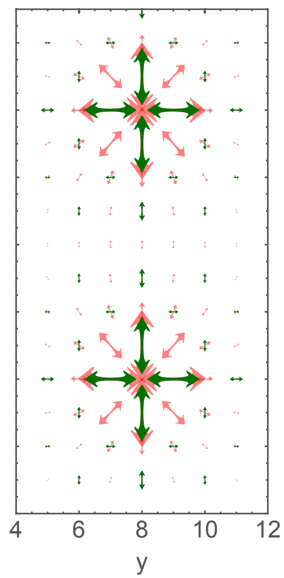
Gauss Law is tricky even locally

University of Stavanger

- Need a symmetric discretization, but naïve central finite differences do not respect the integral form of the Gauss law

$$Q = \int dV\, q = \int dV\, (\nabla \mathbf{E}) \neq \int_{\partial V} d\mathbf{A} \cdot \mathbf{E}$$

$$\boldsymbol{\Delta}^{\mathrm{C}} \cdot \mathbf{E} = \frac{1}{a_s^3}\left[\delta_{\mathbf{x}\mathbf{x}_0} - \delta_{\mathbf{x}\mathbf{x}_1}\right]$$



naïve central FD

Gauss Law is tricky even locally

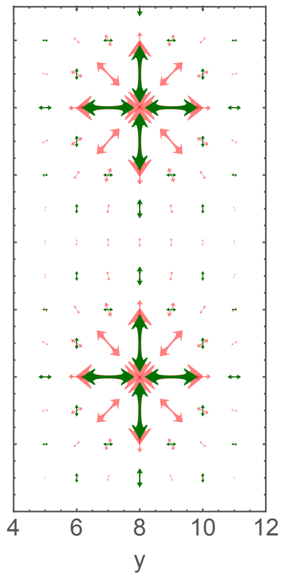
- Need a symmetric discretization, but naïve central finite differences do not respect the integral form of the Gauss law

$$Q = \int dV\, q = \int dV\, (\nabla \mathbf{E}) \neq \int_{\partial V} d\mathbf{A} \cdot \mathbf{E}$$

- Solution known in computational electrodynamics: finite volume discretization

$$\int_{x_{i-1/2}}^{x_{i+1/2}} dx \int_{y_{i-1/2}}^{y_{i+1/2}} dy \int_{z_{i-1/2}}^{z_{i+1/2}} dz \left(\frac{dE_x}{dx} + \frac{dE_y}{dy} + \frac{dE_z}{dz}\right) = \int d^3x\, \delta^{(3)}(\mathbf{x}-\mathbf{x}_0).$$

$$\Delta^{\mathrm{C}} \cdot \mathbf{E} = \frac{1}{a_s^3}\left[\delta_{\mathbf{x}\mathbf{x}_0} - \delta_{\mathbf{x}\mathbf{x}_1}\right]$$



naïve central FD

Gauss Law is tricky even locally

University of Stavanger

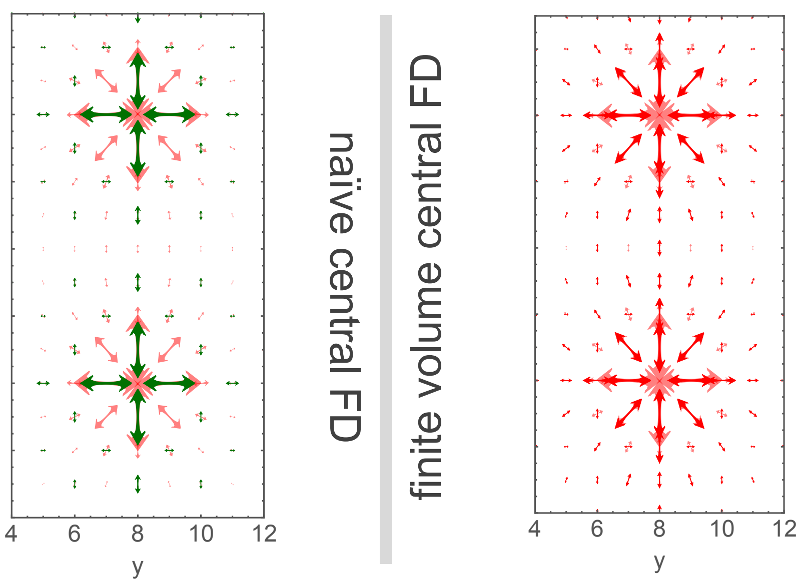
- Need a symmetric discretization, but naïve central finite differences do not respect the integral form of the Gauss law

$$Q = \int dV\, q = \int dV\, (\nabla \mathbf{E}) \neq \int_{\partial V} d\mathbf{A} \cdot \mathbf{E}$$

- Solution known in computational electrodynamics: finite volume discretization

$$\int_{x_{i-1/2}}^{x_{i+1/2}} dx \int_{y_{i-1/2}}^{y_{i+1/2}} dy \int_{z_{i-1/2}}^{z_{i+1/2}} dz \left(\frac{dE_x}{dx} + \frac{dE_y}{dy} + \frac{dE_z}{dz}\right) = \int d^3x\, \delta^{(3)}(\mathbf{x} - \mathbf{x}_0).$$

$$\mathbf{\Delta}^{\mathrm{C}} \cdot \mathbf{E} = \frac{1}{a_s^3}\left[\delta_{\mathbf{x}\mathbf{x}_0} - \delta_{\mathbf{x}\mathbf{x}_1}\right]$$



$$\sum_i \Delta_i^C E_i(\mathbf{x}) = \frac{1}{8a^3}\left[\sum_i \left(\delta_{\mathbf{x}+a\hat{\mathbf{i}},\mathbf{x}_0} + \delta_{\mathbf{x}-a\hat{\mathbf{i}},\mathbf{x}_0}\right) - 2\delta_{\mathbf{x},\mathbf{x}_0}\right]$$

Symanzik's improvement program

University of Stavanger

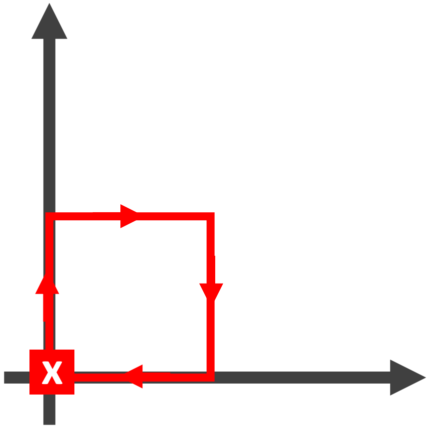
- Starting point is the Wilson plaquette action with forward finite differences

K.G. Wilson, PRD 10, 2445 (1974)

$$P^{1\times1}_{\mu\nu,x} = U_{\mu,x}U_{\nu,x+a_\mu\hat{\mu}}U^\dagger_{\mu,x+a_\nu\hat{\nu}}U^\dagger_{\nu,x} = e^{ia_\mu a_\nu \tilde{F}_{\mu\nu,x}} + \mathcal{O}(a^2)$$

$$\tilde{F}_{\mu\nu} = \Delta^{\rm F}_\mu A_{\nu,x} - \Delta^{\rm F}_\nu A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}].$$

$$\Delta^{\rm F}_\mu \phi(x) = (\phi(x+a_\mu\hat{\mu}) - \phi(x))/a_\mu$$



Symanzik's improvement program

University of Stavanger

- Starting point is the Wilson plaquette action with forward finite differences

K.G. Wilson, PRD 10, 2445 (1974)

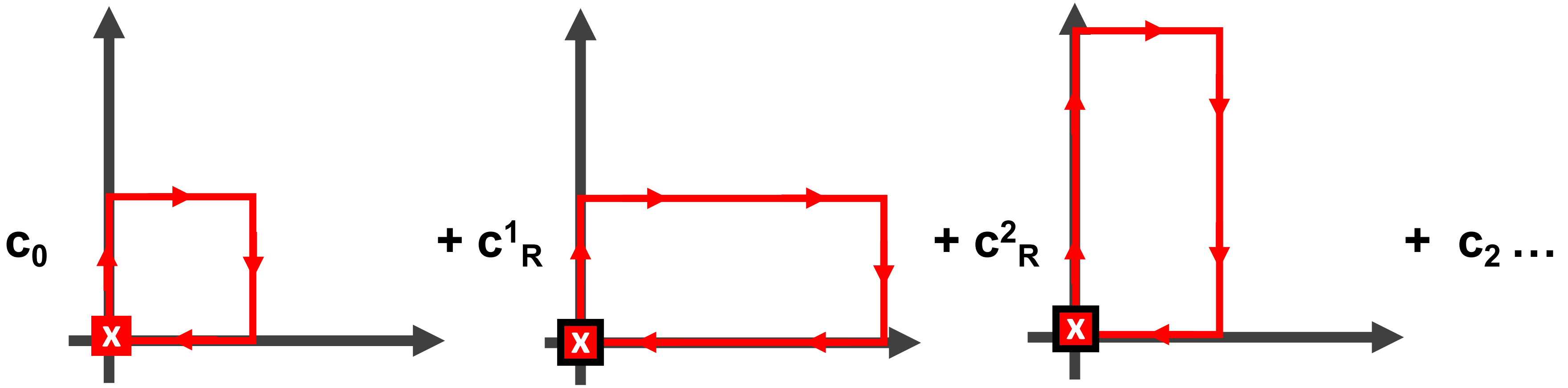
$$P^{1\times1}_{\mu\nu,x} = U_{\mu,x}U_{\nu,x+a_\mu\hat\mu}U^\dagger_{\mu,x+a_\nu\hat\nu}U^\dagger_{\nu,x} = e^{ia_\mu a_\nu \tilde F_{\mu\nu,x}} + \mathcal{O}(a^2)$$

$$\tilde F_{\mu\nu} = \Delta^{\rm F}_\mu A_{\nu,x} - \Delta^{\rm F}_\nu A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}].$$

$$\Delta^{\rm F}_\mu \phi(x) = (\phi(x+a_\mu\hat\mu) - \phi(x))/a_\mu$$

- Improvement deployed in modern actions: higher order forward finite differences

initiated in K. Symanzik, NPBB 226, 187 (1983) & NPB 226, 205 (1983)



Symanzik's improvement program

- Starting point is the Wilson plaquette action with forward finite differences

K.G. Wilson, PRD 10, 2445 (1974)

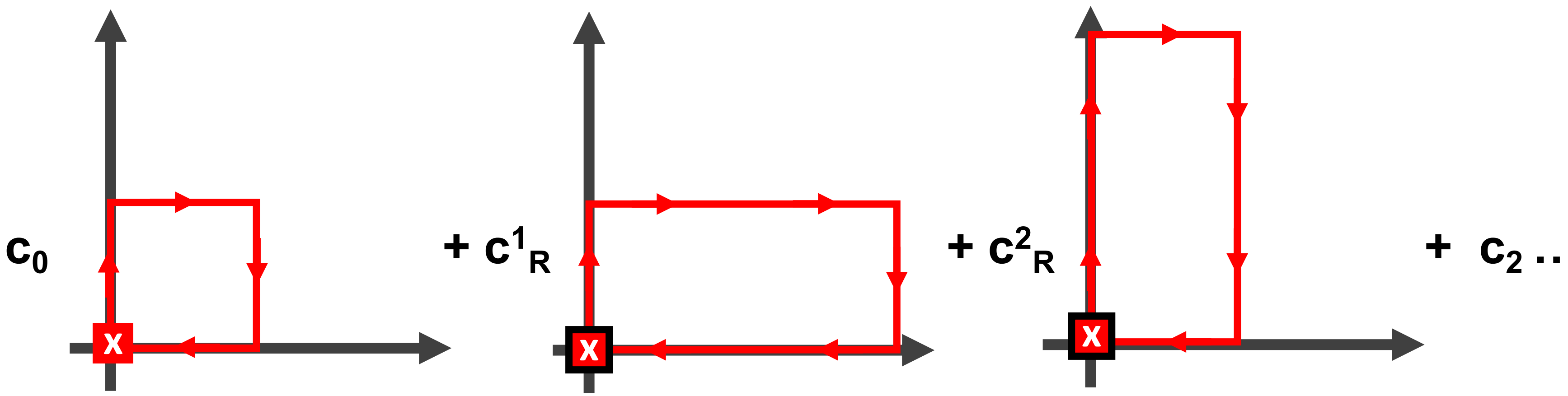
$$P^{1\times1}_{\mu\nu,x} = U_{\mu,x}U_{\nu,x+a_\mu\hat{\mu}}U^\dagger_{\mu,x+a_\nu\hat{\nu}}U^\dagger_{\nu,x} = e^{ia_\mu a_\nu \tilde{F}_{\mu\nu,x}} + \mathcal{O}(a^2)$$

$$\tilde{F}_{\mu\nu} = \Delta^{\rm F}_\mu A_{\nu,x} - \Delta^{\rm F}_\nu A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}].$$

$$\Delta^{\rm F}_\mu \phi(x) = (\phi(x+a_\mu\hat{\mu}) - \phi(x))/a_\mu$$

- Improvement deployed in modern actions: higher order forward finite differences

initiated in K. Symanzik, NPBB 226, 187 (1983) & NPB 226, 205 (1983)

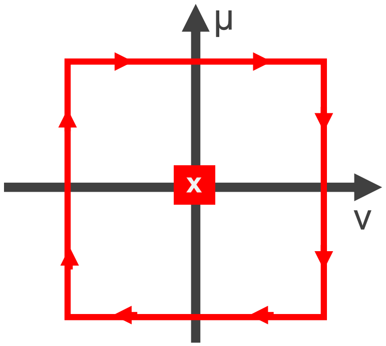


- Does not realize a symmetric discretization of field strength around charges

A naïve symmetric discretization

University of Stavanger

- A stand-alone plaquette for symmetric discretization of the interior (overall O(a²))



see discussion in A.R. arXiv:2102.08616

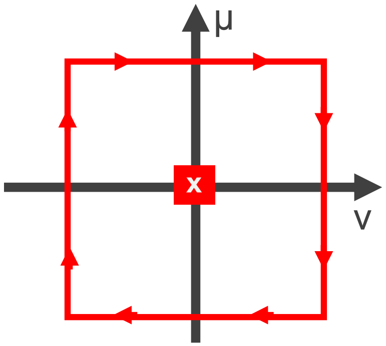
see also [OpenLAT] stabilized Wilson fermions: arXiv:2201.03874

$$\begin{aligned} P^{2\times 2}_{\mu\nu,x} =& \bar{U}_{\mu,x-a\hat{\mu}-a\hat{\nu}}\bar{U}_{\mu,x-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}}\times \\ & \bar{U}^{\dagger}_{\mu,x+a\hat{\nu}}\bar{U}^{\dagger}_{\mu,x-a\hat{\mu}+a\hat{\nu}}\bar{U}^{\dagger}_{\nu,x-a\hat{\mu}}\bar{U}^{\dagger}_{\nu,x-a\hat{\mu}-a\hat{\nu}} \\ =& \exp\left[4iga_\mu a_\nu \bar{F}_{\mu\nu,x}\right] + \mathcal{O}(a^3) \end{aligned}$$

$$\bar{F}_{\mu\nu,x} = \boldsymbol{\Delta}^{\rm C}_{\mu} A_{\nu,x} - \boldsymbol{\Delta}^{\rm C}_{\nu} A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}]$$

A naïve symmetric discretization

- A stand-alone plaquette for symmetric discretization of the interior (overall O(a²))



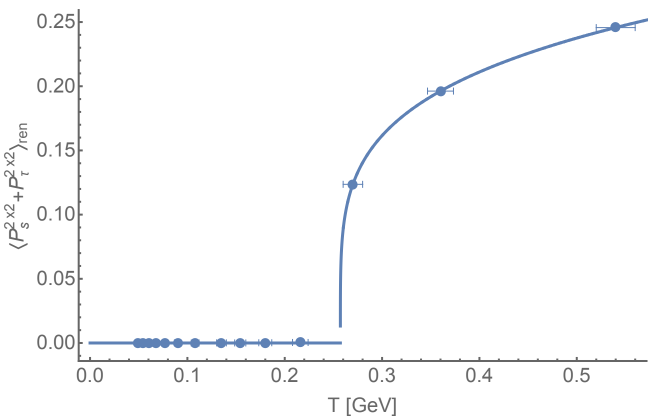
see discussion in A.R. arXiv:2102.08616

see also [OpenLAT] stabilized Wilson fermions: arXiv:2201.03874

$$P^{2\times 2}_{\mu\nu,x} = \bar U_{\mu,x-a\hat\mu-a\hat\nu}\bar U_{\mu,x-a\hat\nu}\bar U_{\nu,x+a\hat\mu-a\hat\nu}\bar U_{\nu,x+a\hat\mu}\times$$
$$\bar U^\dagger_{\mu,x+a\hat\nu}\bar U^\dagger_{\mu,x-a\hat\mu+a\hat\nu}\bar U^\dagger_{\nu,x-a\hat\mu}\bar U^\dagger_{\nu,x-a\hat\mu-a\hat\nu}$$
$$= \exp\left[4iga_\mu a_\nu \bar F_{\mu\nu,x}\right] + \mathcal{O}(a^3)$$

$$\bar F_{\mu\nu,x} = \mathbf{\Delta}^{\rm C}_\mu A_{\nu,x} - \mathbf{\Delta}^{\rm C}_\nu A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}]$$

- Qualitatively consistent but trace anomaly too large

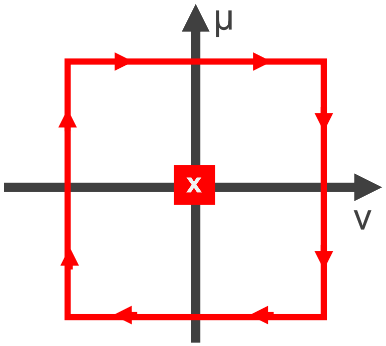


see e.g. A. R. and W.A. Horowitz arXiv:2109.01422

A naïve symmetric discretization

University of Stavanger

- A stand-alone plaquette for symmetric discretization of the interior (overall O(a²))



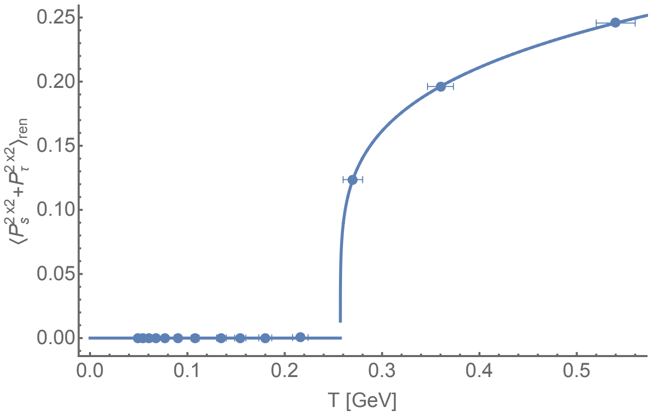
see discussion in
A.R. arXiv:2102.08616

see also [OpenLAT] stabilized
Wilson fermions: arXiv:2201.03874

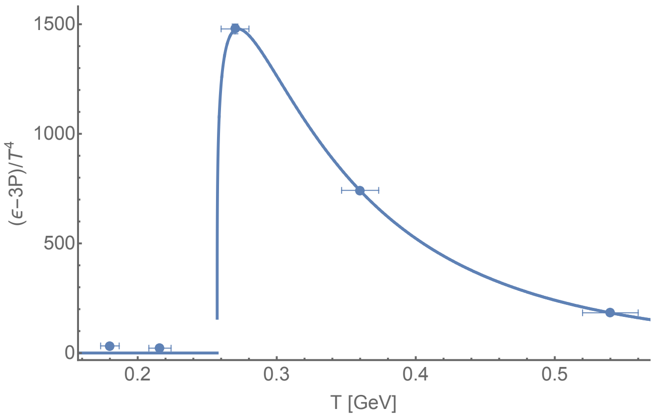
$$P^{2\times 2}_{\mu\nu,x} = \bar U_{\mu,x-a\hat\mu-a\hat\nu}\bar U_{\mu,x-a\hat\nu}\bar U_{\nu,x+a\hat\mu-a\hat\nu}\bar U_{\nu,x+a\hat\mu}\times$$
$$\bar U^\dagger_{\mu,x+a\hat\nu}\bar U^\dagger_{\mu,x-a\hat\mu+a\hat\nu}\bar U^\dagger_{\nu,x-a\hat\mu}\bar U^\dagger_{\nu,x-a\hat\mu-a\hat\nu}$$
$$=\exp\big[4iga_\mu a_\nu \bar F_{\mu\nu,x}\big] + \mathcal{O}(a^3)$$

$$\bar F_{\mu\nu,x} = \mathbf{\Delta}^{\rm C}_\mu A_{\nu,x} - \mathbf{\Delta}^{\rm C}_\nu A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}]$$

- Qualitatively consistent but trace anomaly too large



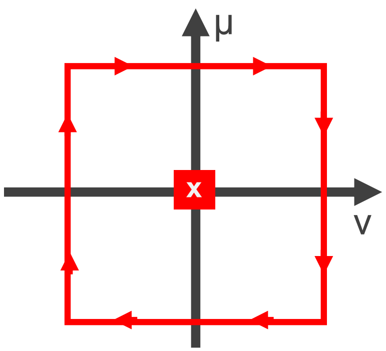
see e.g. A. R. and W.A. Horowitz arXiv:2109.01422



A naïve symmetric discretization

University of Stavanger

- A stand-alone plaquette for symmetric discretization of the interior (overall O(a²))



see discussion in A.R. arXiv:2102.08616

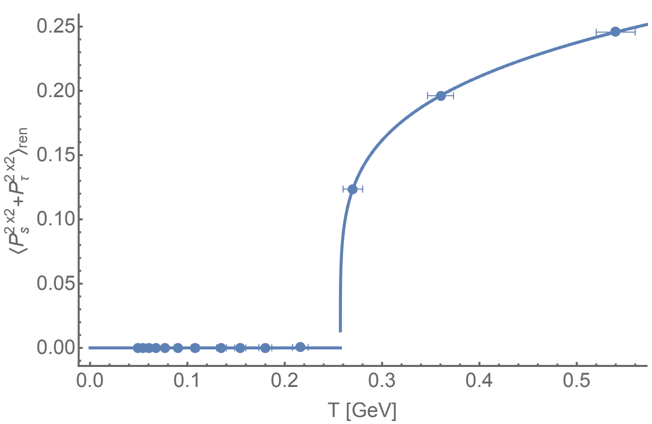
see also [OpenLAT] stabilized Wilson fermions: arXiv:2201.03874

$$P^{2\times2}_{\mu\nu,x} = \bar{U}_{\mu,x-a\hat{\mu}-a\hat{\nu}}\bar{U}_{\mu,x-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}}\times \bar{U}^\dagger_{\mu,x+a\hat{\nu}}\bar{U}^\dagger_{\mu,x-a\hat{\mu}+a\hat{\nu}}\bar{U}^\dagger_{\nu,x-a\hat{\mu}}\bar{U}^\dagger_{\nu,x-a\hat{\mu}-a\hat{\nu}}$$
$$= \exp\left[4iga_\mu a_\nu \bar{F}_{\mu\nu,x}\right] + \mathcal{O}(a^3)$$

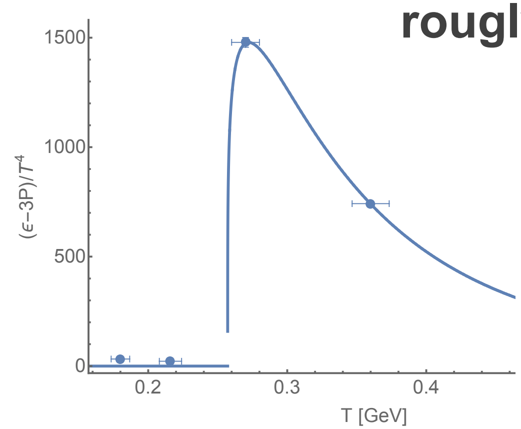
$$\bar{F}_{\mu\nu,x} = \boldsymbol{\Delta}^{\rm C}_\mu A_{\nu,x} - \boldsymbol{\Delta}^{\rm C}_\nu A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}]$$

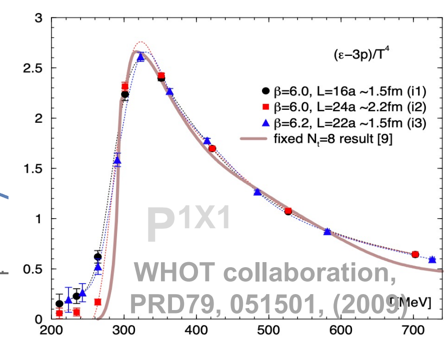
- Qualitatively consistent but trace anomaly too large

rougly factor 4x8x15



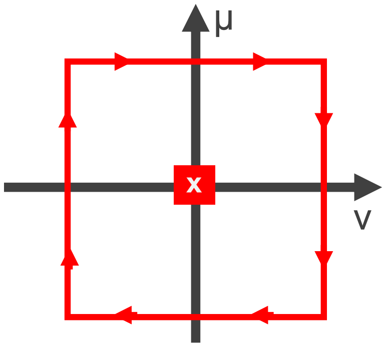
see e.g. A. R. and W.A. Horowitz arXiv:2109.01422





A naïve symmetric discretization

- A stand-alone plaquette for symmetric discretization of the interior (overall $O(a^2)$)



$$P^{2\times 2}_{\mu\nu,x} = \bar{U}_{\mu,x-a\hat{\mu}-a\hat{\nu}}\bar{U}_{\mu,x-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}}\times \bar{U}^{\dagger}_{\mu,x+a\hat{\nu}}\bar{U}^{\dagger}_{\mu,x-a\hat{\mu}+a\hat{\nu}}\bar{U}^{\dagger}_{\nu,x-a\hat{\mu}}\bar{U}^{\dagger}_{\nu,x-a\hat{\mu}-a\hat{\nu}}$$
$$= \exp\left[4iga_\mu a_\nu \bar{F}_{\mu\nu,x}\right] + \mathcal{O}(a^3)$$

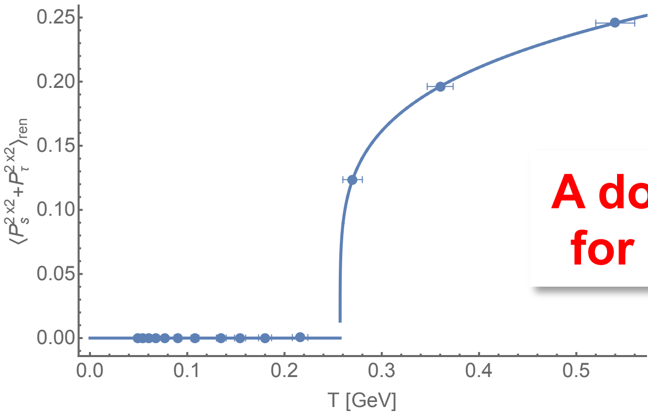
see discussion in
A.R. arXiv:2102.08616

$$\bar{F}_{\mu\nu,x} = \boldsymbol{\Delta}^{\rm C}_{\mu} A_{\nu,x} - \boldsymbol{\Delta}^{\rm C}_{\nu} A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}]$$

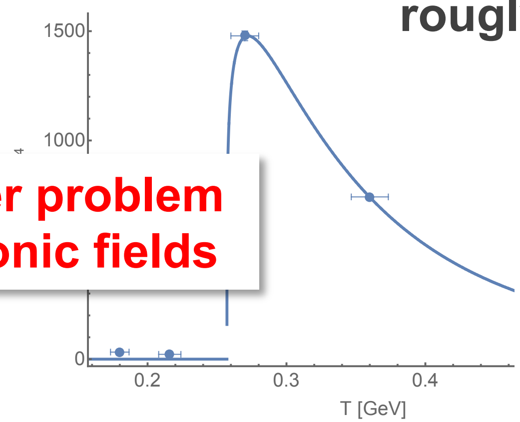
see also [OpenLAT] stabilized
Wilson fermions: arXiv:2201.03874

- Qualitatively consistent but trace anomaly too large

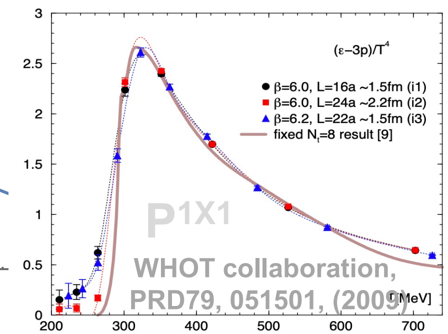
rougly factor 4x8x15



see e.g. A. R. and W.A. Horowitz arXiv:2109.01422



A doubler problem for bosonic fields



Doublers and the Wilson term

University of Stavanger

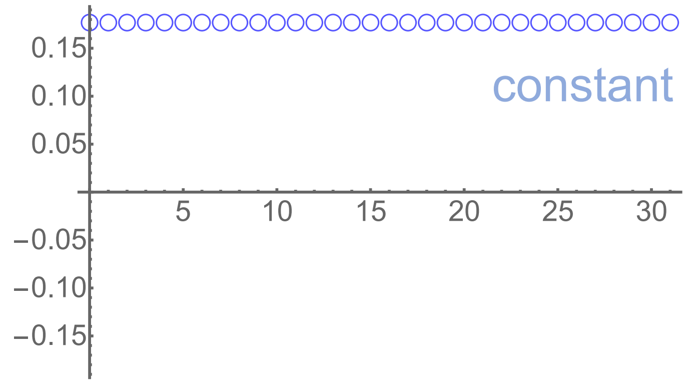
- Problem already apparent in finite difference schemes in one dimension

$$D^{\mathrm{C}} = \frac{1}{\Delta x}\begin{bmatrix} \ddots & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & \ddots \end{bmatrix}$$

Doublers and the Wilson term

- Problem already apparent in finite difference schemes in one dimension

$$D^{\mathrm{C}} = \frac{1}{\Delta x}\begin{bmatrix} \ddots & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & \ddots \end{bmatrix}$$



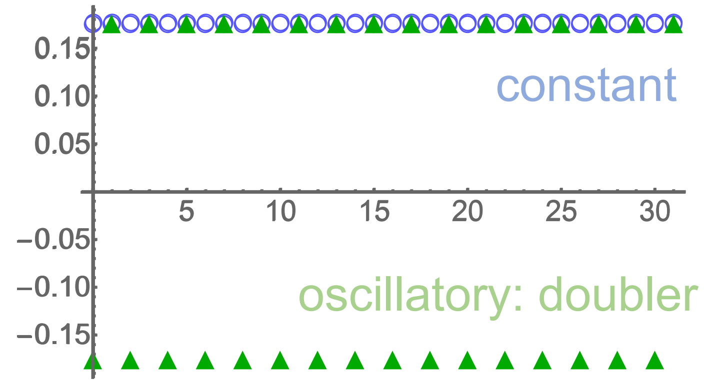
Doublers and the Wilson term

University of Stavanger

- Problem already apparent in finite difference schemes in one dimension

$$D^C = \frac{1}{\Delta x}\begin{bmatrix} \ddots & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & \ddots \end{bmatrix}$$

zero eigenvalue eigenfunctions of D^C and $(D^C)^t$ distinct

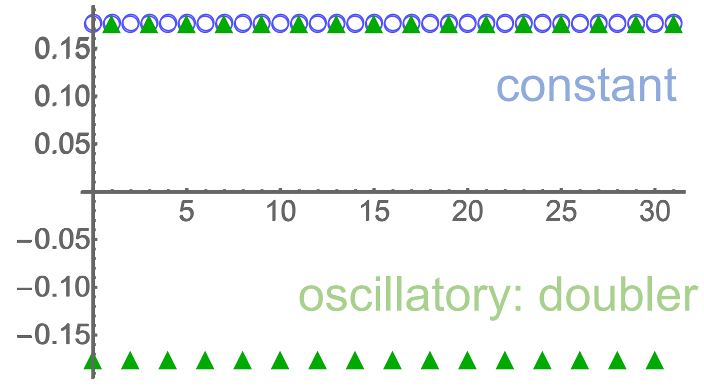


Doublers and the Wilson term

- Problem already apparent in finite difference schemes in one dimension

$$D^C = \frac{1}{\Delta x}\begin{bmatrix} \ddots & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & \ddots \end{bmatrix}$$

zero eigenvalue eigenfunctions of D^C and $(D^C)^t$ distinct



- Modification: add a higher derivative [does not affect **D x^r = r x^{r-1}** for r <= order]

$$\frac{1}{\Delta x}\begin{bmatrix} \ddots & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & \ddots \end{bmatrix} + \frac{\Delta x}{2\Delta x^2}\begin{bmatrix} \ddots & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & \ddots \end{bmatrix} = D^F$$

upwind modification

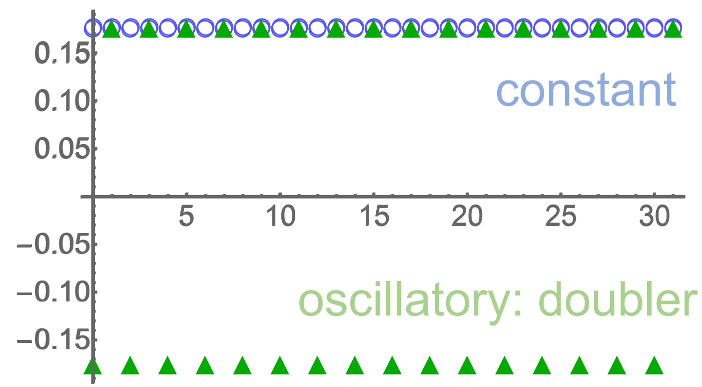
Doublers and the Wilson term

University of Stavanger

- Problem already apparent in finite difference schemes in one dimension

$$D^C = \frac{1}{\Delta x}\begin{bmatrix} \ddots & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & \ddots \end{bmatrix}$$

zero eigenvalue eigenfunctions of D^C and $(D^C)^t$ distinct



- Modification: add a higher derivative [does not affect **D x^r = r x^(r-1)** for r <= order]

$$\frac{1}{\Delta x}\begin{bmatrix} \ddots & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & \ddots \end{bmatrix} + i\,\frac{\Delta x}{2\Delta x^2}\begin{bmatrix} \ddots & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & \ddots \end{bmatrix} = D^W$$

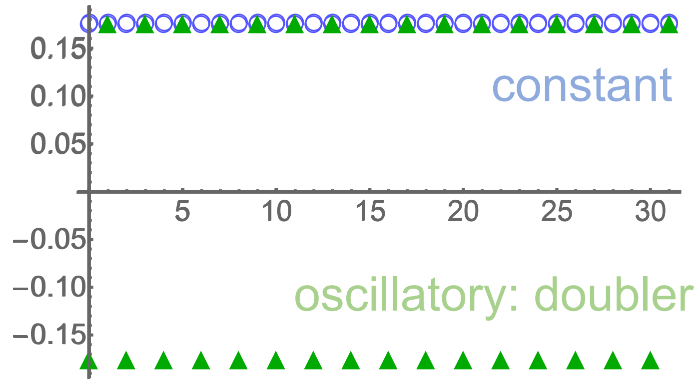
Wilson term

Doublers and the Wilson term

- Problem already apparent in finite difference schemes in one dimension

$$D^C = \frac{1}{\Delta x}\begin{bmatrix} \ddots & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & \ddots \end{bmatrix}$$

zero eigenvalue eigenfunctions of D^C and $(D^C)^t$ distinct



- Modification: add a higher derivative [does not affect $\mathbf{D\, x^r = r\, x^{r-1}}$ for r <= order]

$$\frac{1}{\Delta x}\begin{bmatrix} \ddots & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & \ddots \end{bmatrix} + i\,\frac{\Delta x}{2\Delta x^2}\begin{bmatrix} \ddots & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & \ddots \end{bmatrix} = D^W$$

Wilson term

- Wilson term applicable when acting on complex functions: what to do for real A^μ_a?

Do we have another lever?

- In finite systems boundaries are physical otherwise can be chosen at convenience

Do we have another lever?

University of Stavanger

- In finite systems boundaries are physical otherwise can be chosen at convenience

Weak viewpoint: boundary/initial conditions only as tight as order of approximation

see e.g. Fernandez, D.C.D.R., Hicken, J.E., Zingg, D.W., Comp. & Fluids 95, 171–196 (2014)

Do we have another lever?

University of Stavanger

- In finite systems boundaries are physical otherwise can be chosen at convenience

Weak viewpoint: boundary/initial conditions only as tight as order of approximation

see e.g. Fernandez, D.C.D.R., Hicken, J.E., Zingg, D.W., Comp. & Fluids 95, 171–196 (2014)

- For ODEs / PDEs well established (penalty term from boundary data):

see e.g. Lundquist, T., Nordström J., JCP 270, 86–104 (2014)

Simultaneous Approximation Terms

$$u'(x) = g(x) \quad u(0) = u_0$$

Do we have another lever?

University of Stavanger

- In finite systems boundaries are physical otherwise can be chosen at convenience

Weak viewpoint: boundary/initial conditions only as tight as order of approximation

see e.g. Fernandez, D.C.D.R., Hicken, J.E., Zingg, D.W., Comp. & Fluids 95, 171–196 (2014)

- For ODEs / PDEs well established (penalty term from boundary data):

see e.g. Lundquist, T., Nordström J., JCP 270, 86–104 (2014)

Simultaneous Approximation Terms

$$u'(x) = g(x) \quad u(0) = u_0$$

$$D\mathbf{u} = \mathbf{g} + \frac{1}{a} E_0 \left(\mathbf{u} - \mathbf{u}_0 \right)$$

$$E_0 = \mathrm{diag}[1, 0, \ldots]$$

Do we have another lever?

University of Stavanger

- In finite systems boundaries are physical otherwise can be chosen at convenience

Weak viewpoint: boundary/initial conditions only as tight as order of approximation

see e.g. Fernandez, D.C.D.R., Hicken, J.E., Zingg, D.W., Comp. & Fluids 95, 171–196 (2014)

- For ODEs / PDEs well established (penalty term from boundary data):

see e.g. Lundquist, T., Nordström J., JCP 270, 86–104 (2014)

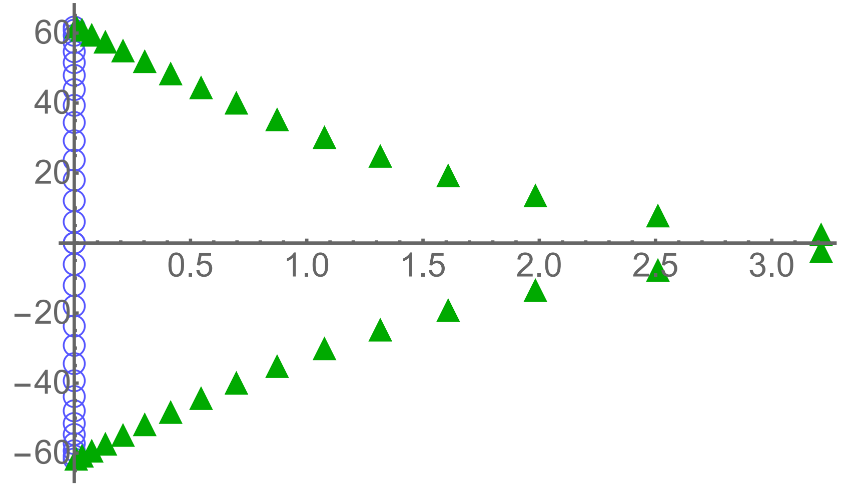
Simultaneous Approximation Terms

$$u'(x) = g(x) \quad u(0) = u_0$$

$$D\mathbf{u} = \mathbf{g} + \frac{1}{a}E_0(\mathbf{u} - \mathbf{u}_0)$$

$$E_0 = \mathrm{diag}[1, 0, \ldots]$$

$$\tilde{D} = D - \frac{1}{a}E_0$$



Do we have another lever?

University of Stavanger

- In finite systems boundaries are physical otherwise can be chosen at convenience

Weak viewpoint: boundary/initial conditions only as tight as order of approximation

see e.g. Fernandez, D.C.D.R., Hicken, J.E., Zingg, D.W., Comp. & Fluids 95, 171–196 (2014)

- For ODEs / PDEs well established (penalty term from boundary data):

see e.g. Lundquist, T., Nordström J., JCP 270, 86–104 (2014)

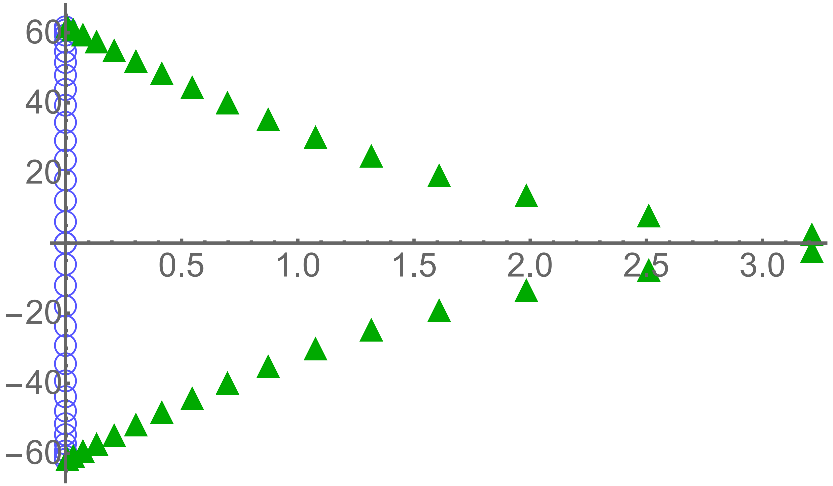
Simultaneous Approximation Terms

$$u'(x) = g(x) \quad u(0) = u_0$$

$$D\mathbf{u} = \mathbf{g} + \frac{1}{a}E_0(\mathbf{u} - \mathbf{u}_0)$$

$$E_0 = \mathrm{diag}[1, 0, \ldots]$$

$$\tilde{D} = D - \frac{1}{a}E_0$$



$$\tilde{D}\mathbf{u} = \mathbf{g} - \frac{1}{a}E_0\mathbf{u}_0$$

invertible $\widetilde{D}$ and modified inhomogeneous RHS

Introducing boundary data in the action

University of Stavanger

- In lattice applications (both classical statistical & path integral) action is central
- In an action we do not have an “=“ sign to move boundary terms around

Introducing boundary data in the action

University of Stavanger

- In lattice applications (both classical statistical & path integral) action is central
- In an action we do not have an "=" sign to move boundary terms around

Affine coordinate formulation

A. Rothkopf, J. Nordström, arXiv:2205.14028

$$S = \int dx \left[u'(x) u'(x) \right] \qquad u(0) = u_0$$

Introducing boundary data in the action

University of Stavanger

- In lattice applications (both classical statistical & path integral) action is central
- In an action we do not have an "=" sign to move boundary terms around

Affine coordinate formulation

A. Rothkopf, J. Nordström, arXiv:2205.14028

$$S = \int dx \left[u'(x)u'(x)\right] \qquad u(0) = u_0$$

$$S \approx (D\mathbf{u})^\dagger H D\mathbf{u} \qquad H = \Delta x \,\mathrm{diag}[\tfrac{1}{2}, 1, \ldots, 1, \tfrac{1}{2}]$$

$$\frac{1}{\Delta x}\begin{bmatrix} -1 & 1 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0-1 & 1 \end{bmatrix}$$

Introducing boundary data in the action

University of Stavanger

- In lattice applications (both classical statistical & path integral) action is central
- In an action we do not have an “=“ sign to move boundary terms around

Affine coordinate formulation

A. Rothkopf, J. Nordström, arXiv:2205.14028

$$S = \int dx \left[u'(x)u'(x)\right] \qquad u(0) = u_0$$

$$S \approx (D\mathbf{u})^\dagger H D\mathbf{u} \qquad H = \Delta x\, \mathrm{diag}[\tfrac{1}{2}, 1, \ldots, 1, \tfrac{1}{2}]$$

$$\tilde{D}\mathbf{u} = D\mathbf{u} + H^{-1}E_0\left(\mathbf{u} - \mathbf{u}_0\right)$$

$$\frac{1}{\Delta x}\begin{bmatrix} -1 & 1 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0-1 & 1 \end{bmatrix}$$

Introducing boundary data in the action

- In lattice applications (both classical statistical & path integral) action is central
- In an action we do not have an "=" sign to move boundary terms around

Affine coordinate formulation

A. Rothkopf, J. Nordström, arXiv:2205.14028

$$S = \int dx \left[u'(x) u'(x) \right] \qquad u(0) = u_0$$

$$S \approx (D\mathbf{u})^\dagger H D\mathbf{u} \qquad H = \Delta x \, \mathrm{diag}[\tfrac{1}{2}, 1, \ldots, 1, \tfrac{1}{2}]$$

$$\tilde{D}\mathbf{u} = D\mathbf{u} + H^{-1} E_0 \left(\mathbf{u} - \mathbf{u}_0 \right)$$

same modification as on the ODE level

$$\frac{1}{\Delta x} \begin{bmatrix} -1 & 1 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0-1 & 1 \end{bmatrix}$$

Introducing boundary data in the action

University of Stavanger

- In lattice applications (both classical statistical & path integral) action is central
- In an action we do not have an "=" sign to move boundary terms around

Affine coordinate formulation

A. Rothkopf, J. Nordström, arXiv:2205.14028

$$S = \int dx \big[u'(x)u'(x)\big] \qquad u(0) = u_0$$

$$S \approx (D\mathbf{u})^\dagger H D\mathbf{u} \qquad H = \Delta x \, \mathrm{diag}[\tfrac{1}{2}, 1, \ldots, 1, \tfrac{1}{2}]$$

$$\tilde{D}\mathbf{u} = D\mathbf{u} + H^{-1}E_0\big(\mathbf{u} - \mathbf{u}_0\big)$$

same modification as on the ODE level (under $H^{-1}E_0$)

constant shift (under $\mathbf{u} - \mathbf{u}_0$)

$$\frac{1}{\Delta x}\begin{bmatrix} -1 & 1 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0-1 & 1 \end{bmatrix}$$

Introducing boundary data in the action

University of Stavanger

- In lattice applications (both classical statistical & path integral) action is central
- In an action we do not have an "=" sign to move boundary terms around

Affine coordinate formulation

A. Rothkopf, J. Nordström, arXiv:2205.14028

$$S = \int dx \left[u'(x)u'(x)\right] \qquad u(0) = u_0$$

$$S \approx (D\mathbf{u})^\dagger H D\mathbf{u} \qquad H = \Delta x\,\mathrm{diag}[\tfrac{1}{2}, 1, \dots, 1, \tfrac{1}{2}]$$

$$\tilde{D}\mathbf{u} = D\mathbf{u} + H^{-1}E_0\big(\mathbf{u} - \mathbf{u}_0\big)$$

$H^{-1}E_0$: same modification as on the ODE level

$(\mathbf{u} - \mathbf{u}_0)$: constant shift

$$\frac{1}{\Delta x}\begin{bmatrix} -1 & 1 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0-1 & 1 \end{bmatrix}$$

↓

$$\frac{1}{\Delta x}\begin{bmatrix} -1+2 & 1 & 0 & 0 & -2u_0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\mathbf{u} = [u(0), u(\Delta x), \dots, u(N_x\Delta x), 1]$$

Introducing boundary data in the action

University of Stavanger

- In lattice applications (both classical statistical & path integral) action is central
- In an action we do not have an "=" sign to move boundary terms around

Affine coordinate formulation

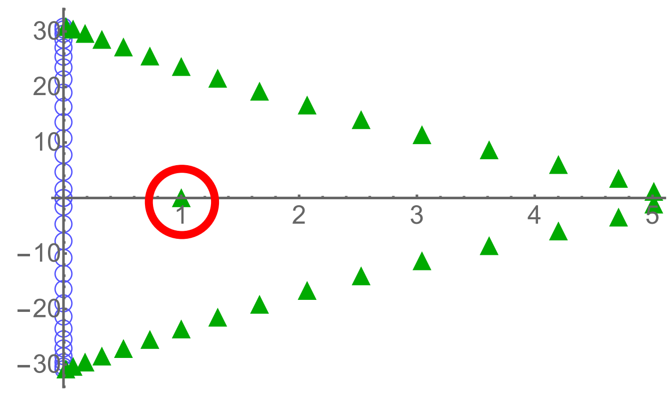
A. Rothkopf, J. Nordström, arXiv:2205.14028

$$S = \int dx \big[u'(x)u'(x)\big] \qquad u(0) = u_0$$

$$S \approx (D\mathbf{u})^\dagger H D\mathbf{u} \qquad H = \Delta x\, \mathrm{diag}[\tfrac{1}{2}, 1, \ldots, 1, \tfrac{1}{2}]$$

$$\tilde{D}\mathbf{u} = D\mathbf{u} + H^{-1}E_0\big(\mathbf{u} - \mathbf{u}_0\big)$$

same modification as on the ODE level ($H^{-1}E_0$) — constant shift ($\mathbf{u}_0$)



+ all zero modes are lifted
+ physical constant mode with correct boundary behavior now as unit EV

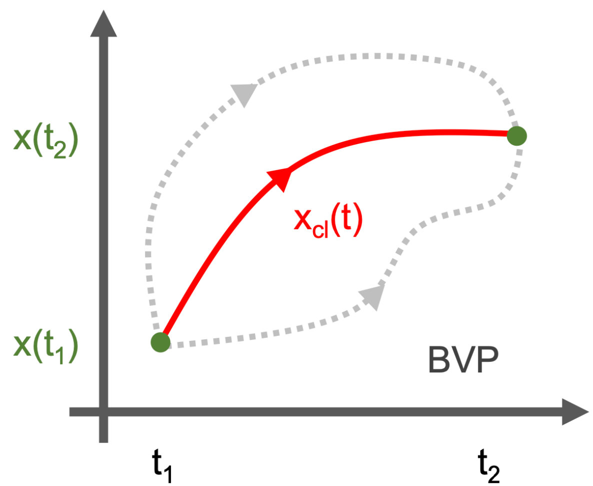
Application to initial value problems (IVP)

University of Stavanger

- Long term goal: gauge invariant real-time quantum dynamics of QCD
- Intermediate goal: gauge invariant real-time dynamics for classical lattice YM
- First modest step: Variational solver for 0+1d classical IVP from the Lagrangian

Application to initial value problems (IVP)

- Long term goal: gauge invariant real-time quantum dynamics of QCD
- Intermediate goal: gauge invariant real-time dynamics for classical lattice YM
- First modest step: Variational solver for 0+1d classical IVP from the Lagrangian



IVP challenge: standard $\delta S[x,v]/\delta x(t)=0$ only as boundary value problem

A variational formulation of IVPs

University of Stavanger

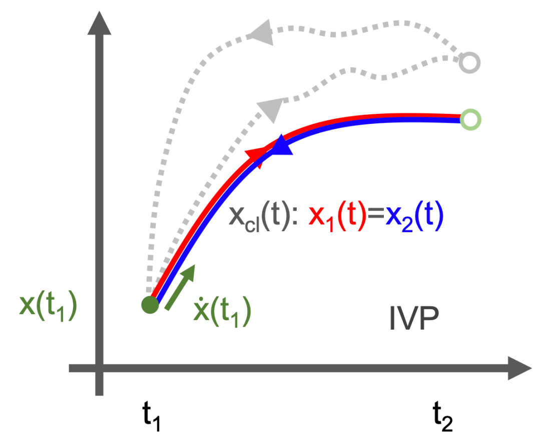
- How to formulate a variational problem with an unknown endpoint at t_2 ?

A variational formulation of IVPs

- How to formulate a variational problem with an unknown endpoint at t_2 ?

- Take inspiration from Schwinger-Keldysh:

Galley, C.R., PRL 110(17), 174301 (2013)



"a double shooting method"

A variational formulation of IVPs

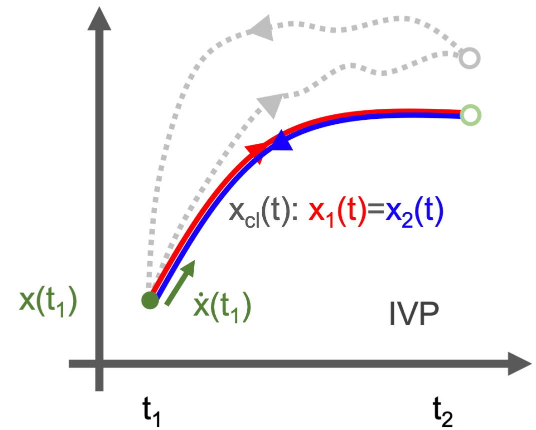
University of Stavanger

- How to formulate a variational problem with an unknown endpoint at t_2 ?

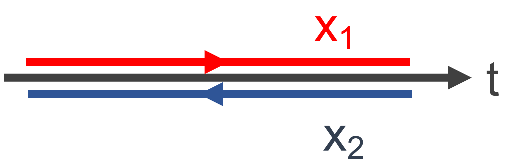
- Take inspiration from Schwinger-Keldysh:

Galley, C.R., PRL 110(17), 174301 (2013)

$$S_{\rm IVP}[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)] = \int_{t_1}^{t_2} dt\Big(\mathcal{L}[x_1(t),\dot{x}_1(t)] - \mathcal{L}[x_2(t),\dot{x}_2(t)]\Big)$$



"a double shooting method"



A variational formulation of IVPs

University of Stavanger

- How to formulate a variational problem with an unknown endpoint at t_2 ?

- Take inspiration from Schwinger-Keldysh:

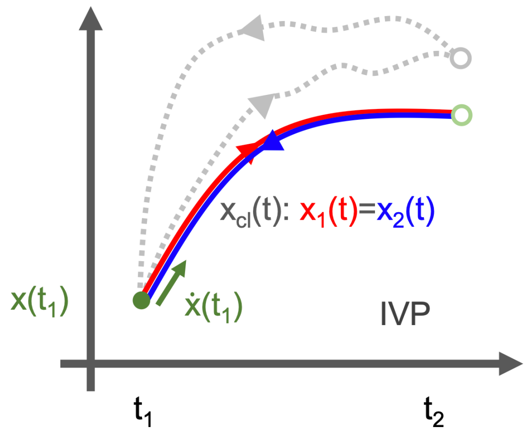
Galley, C.R., PRL 110(17), 174301 (2013)

$$S_{\rm IVP}[x_1(t),\dot x_1(t),x_2(t),\dot x_2(t)] = \int_{t_1}^{t_2} dt\Big(\mathcal{L}[x_1(t),\dot x_1(t)] - \mathcal{L}[x_2(t),\dot x_2(t)]\Big)$$

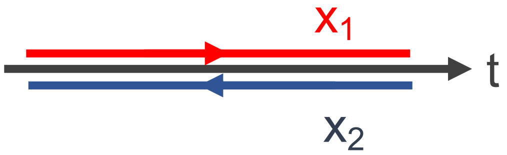
$x_+ = (x_1+x_2)/2$

$x_- = x_1-x_2$

$$\delta\mathcal{S}_{\rm IVP} = \int dt\Big(\Big\{\frac{\partial {\rm L}}{\partial x_+} - \frac{d}{dt}\frac{\partial {\rm L}}{\partial \dot x_+}\Big\}\delta x_+ + \Big\{\frac{\partial {\rm L}}{\partial x_-} - \frac{d}{dt}\frac{\partial {\rm L}}{\partial \dot x_-}\Big\}\delta x_-\Big) + \Big[\frac{\delta {\rm L}}{\delta \dot x_+}\delta x_+ + \frac{\delta {\rm L}}{\delta \dot x_-}\delta x_-\Big]\Big|_{t_1}^{t_2}.$$



"a double shooting method"



A variational formulation of IVPs

University of Stavanger

- How to formulate a variational problem with an unknown endpoint at t_2 ?

- Take inspiration from Schwinger-Keldysh:

Galley, C.R., PRL 110(17), 174301 (2013)

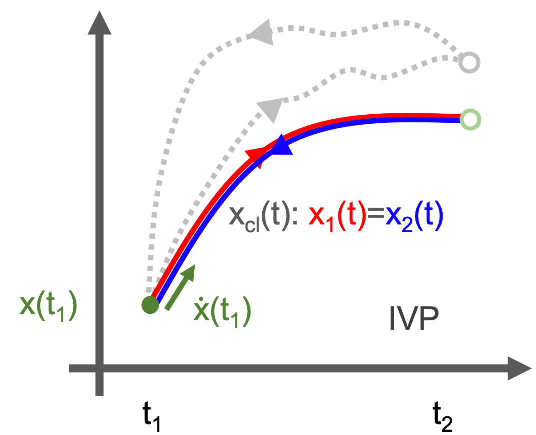
$$S_{\rm IVP}[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)] = \int_{t_1}^{t_2} dt\Big(\mathcal{L}[x_1(t),\dot{x}_1(t)] - \mathcal{L}[x_2(t),\dot{x}_2(t)]\Big)$$

$x_+ = (x_1+x_2)/2$

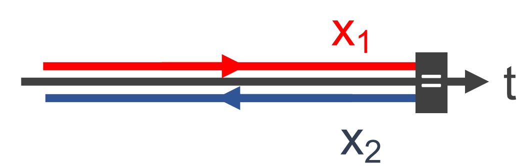
$x_- = x_1 - x_2$

$$\delta\mathcal{S}_{\rm IVP} = \int dt\Big(\Big\{\frac{\partial L}{\partial x_+} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}_+}\Big\}\delta x_+ + \Big\{\frac{\partial L}{\partial x_-} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}_-}\Big\}\delta x_-\Big)$$
$$+ \Big[\frac{\delta L}{\delta \dot{x}_+}\delta x_+ + \frac{\delta L}{\delta \dot{x}_-}\delta x_-\Big]\Big|_{t_1}^{t_2}.$$

To make **boundary terms vanish**:
$x_1(t_2) = x_2(t_2)$ & $\dot{x}_1(t_2) = \dot{x}_2(t_2)$
do not need to know values at t_2



"a double shooting method"



A variational formulation of IVPs

University of Stavanger

- How to formulate a variational problem with an unknown endpoint at t_2 ?

- Take inspiration from Schwinger-Keldysh:

Galley, C.R., PRL 110(17), 174301 (2013)

$$S_{\rm IVP}[x_1(t),\dot x_1(t),x_2(t),\dot x_2(t)] = \int_{t_1}^{t_2} dt\Big(\mathcal{L}[x_1(t),\dot x_1(t)] - \mathcal{L}[x_2(t),\dot x_2(t)]\Big)$$

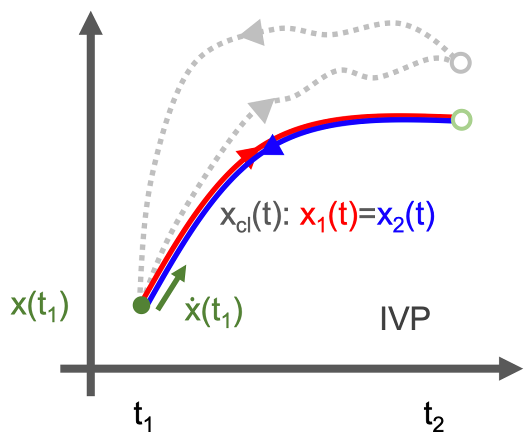
$x_+ = (x_1+x_2)/2$

$x_- = x_1 - x_2$

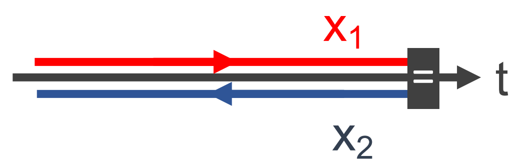
$$\delta \mathcal{S}_{\rm IVP} = \int dt\Big(\Big\{\frac{\partial L}{\partial x_+} - \frac{d}{dt}\frac{\partial L}{\partial \dot x_+}\Big\}\delta x_+ + \Big\{\frac{\partial L}{\partial x_-} - \frac{d}{dt}\frac{\partial L}{\partial \dot x_-}\Big\}\delta x_-\Big) + \Big[\frac{\delta L}{\delta \dot x_+}\delta x_+ + \frac{\delta L}{\delta \dot x_-}\delta x_-\Big]\Big|_{t_1}^{t_2}.$$

To make **boundary terms vanish**:
$x_1(t_2) = x_2(t_2)$ & $\dot x_1(t_2) = \dot x_2(t_2)$
do not need to know values at t_2

$$\frac{\delta S_{\rm IVP}[x_\pm]}{\delta x_-}\Big|_{x_-=0,\,x_+=x_{\rm class}} = 0$$



“a double shooting method”



Initial values as time boundary

- Correct implementation of boundary conditions in FD: **summation by parts**
- Discretization of integration and differentiation must be **compatible**

$$\int_{t_1}^{t_2} dt f(t) g(t) \approx \mathbf{f}^t H \mathbf{g} = (\mathbf{f}, \mathbf{g}) \qquad \mathbb{H}^{[2,1]} = \Delta t \begin{bmatrix} 1/2 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & 1/2 \end{bmatrix} \qquad \mathbb{D}^{[2,1]} = \frac{1}{2\Delta t} \begin{bmatrix} -2 & 2 & & & \\ -1 & 0 & 1 & & \\ & & \ddots & & \\ & & -1 & 0 & 1 \\ & & & -2 & 2 \end{bmatrix}$$

$$(\Delta^{\mathrm{SBP}} \mathbf{f}, \mathbf{g}) \stackrel{!}{=} -(\mathbf{f}, \Delta^{\mathrm{SBP}} \mathbf{g}) + f_N g_N - f_1 g_1 \qquad \Delta^{\mathrm{SBP}} = H^{-1} Q, \quad Q^t + Q = \mathrm{diag}[-1, 0, \ldots, 0, 1]$$

- Straight forward extension to higher orders using $\mathbf{\Delta^{SBP} x^r = r\, x^{r-1}}$ for r <= order

$$\mathbb{H}^{[4,2]} = \Delta t \begin{bmatrix} \frac{17}{48} & & & & & \\ & \frac{59}{48} & & & & \\ & & \frac{43}{48} & & & \\ & & & \frac{49}{48} & & \\ & & & & 1 & \\ & & & & & \ddots \end{bmatrix} \qquad \mathbb{D}^{[4,2]} = \frac{1}{\Delta t} \begin{bmatrix} -\frac{24}{17} & \frac{59}{34} & -\frac{4}{17} & -\frac{3}{34} & & & & \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 & & & & \\ \frac{4}{43} & -\frac{59}{86} & 0 & \frac{59}{86} & -\frac{4}{43} & & & \\ \frac{3}{98} & 0 & -\frac{59}{86} & 0 & \frac{32}{49} & -\frac{4}{49} & & \\ & & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} & \\ & & & & & & & \ddots \end{bmatrix}$$

Implementation with Lagrange multipliers

University of Stavanger

- Simple mechanical model: $\mathcal{S} = \int dt \left(\frac{1}{2} m\dot{x}^2(t) - mgx(t)\right)$ $\quad x(0) = 1, \dot{x}(0) = 0.3$

Naïve discretization

$$\mathbb{S}_{\mathrm{IVP}} = \left\{\frac{1}{2}(\mathbb{D}\mathbf{x}_1)^{\mathrm{T}}\mathbb{H}(\mathbb{D}\mathbf{x}_1) - g\mathbb{1}^{\mathrm{T}}\mathbb{H}\mathbf{x}_1\right\} - \left\{\frac{1}{2}(\mathbb{D}\mathbf{x}_2)^{\mathrm{T}}\mathbb{H}(\mathbb{D}\mathbf{x}_2) - g\mathbb{1}^{\mathrm{T}}\mathbb{H}\mathbf{x}_2\right\}$$
$$+ \lambda_1(x_1(0) - x_i) + \lambda_2((\mathbb{D}\mathbf{x}_1)(0) - \dot{x}_i)$$
$$+ \lambda_3(x_1(N_t) - x_2(N_t)) + \lambda_4((\mathbb{D}\mathbf{x}_1)(N_t) - (\mathbb{D}\mathbf{x}_2)(N_t)).$$

A. Rothkopf, J. Nordström, arXiv:2205.14028

Implementation with Lagrange multipliers

University of Stavanger

- Simple mechanical model: $\mathcal{S} = \int dt \left(\frac{1}{2}m\dot{x}^2(t) - mgx(t)\right)$ $\quad x(0) = 1, \dot{x}(0) = 0.3$

Naïve discretization

$$\mathbb{S}_{\rm IVP} = \left\{\frac{1}{2}(\mathbb{D}\mathbf{x}_1)^{\rm T}\mathbb{H}(\mathbb{D}\mathbf{x}_1) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_1\right\} - \left\{\frac{1}{2}(\mathbb{D}\mathbf{x}_2)^{\rm T}\mathbb{H}(\mathbb{D}\mathbf{x}_2) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_2\right\}$$
$$+ \lambda_1(x_1(0) - x_i) + \lambda_2((\mathbb{D}\mathbf{x}_1)(0) - \dot{x}_i)$$
$$+ \lambda_3(x_1(N_t) - x_2(N_t)) + \lambda_4((\mathbb{D}\mathbf{x}_1)(N_t) - (\mathbb{D}\mathbf{x}_2)(N_t)).$$

Global minimization for x_1,x_2, λ_1, λ_2 (initial cond.), λ_3, λ_4 (path identification) amounts to fully implicit scheme

A. Rothkopf, J. Nordström, arXiv:2205.14028

Implementation with Lagrange multipliers

University of Stavanger

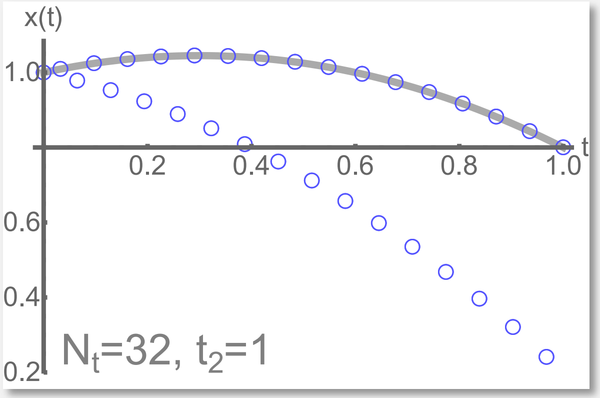
- Simple mechanical model: $\mathcal{S} = \int dt \left(\frac{1}{2}m\dot{x}^2(t) - mgx(t)\right)$ $x(0) = 1, \dot{x}(0) = 0.3$

Naïve discretization

$$\mathbb{S}_{\mathrm{IVP}} = \left\{\frac{1}{2}(\mathbb{D}\mathbf{x}_1)^{\mathrm{T}}\mathbb{H}(\mathbb{D}\mathbf{x}_1) - g\mathbb{1}^{\mathrm{T}}\mathbb{H}\mathbf{x}_1\right\} - \left\{\frac{1}{2}(\mathbb{D}\mathbf{x}_2)^{\mathrm{T}}\mathbb{H}(\mathbb{D}\mathbf{x}_2) - g\mathbb{1}^{\mathrm{T}}\mathbb{H}\mathbf{x}_2\right\}$$
$$+ \lambda_1(x_1(0) - x_i) + \lambda_2((\mathbb{D}\mathbf{x}_1)(0) - \dot{x}_i)$$
$$+ \lambda_3(x_1(N_t) - x_2(N_t)) + \lambda_4((\mathbb{D}\mathbf{x}_1)(N_t) - (\mathbb{D}\mathbf{x}_2)(N_t)).$$

Global minimization for x_1,x_2, λ_1, λ_2 (initial cond.), λ_3, λ_4 (path identification) amounts to fully implicit scheme

solution shows $x_1=x_2$ but contaminated by doublers



Implementation with Lagrange multipliers

University of Stavanger

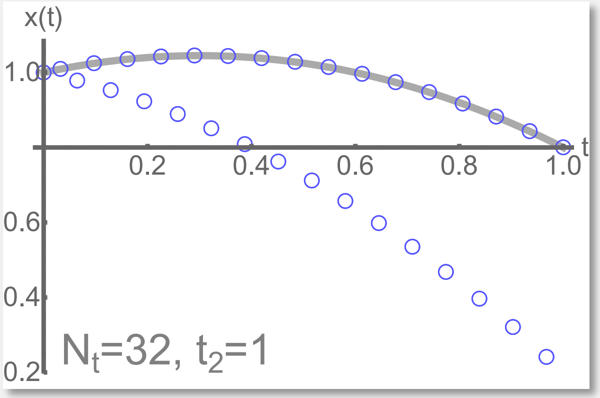
- Simple mechanical model: $\mathcal{S} = \int dt \left(\frac{1}{2} m\dot{x}^2(t) - mgx(t)\right)$ $\quad x(0) = 1, \dot{x}(0) = 0.3$

Naïve discretization

$$\mathbb{S}_{\rm IVP} = \left\{\frac{1}{2}(\mathbb{D}\mathbf{x}_1)^{\rm T}\mathbb{H}(\mathbb{D}\mathbf{x}_1) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_1\right\} - \left\{\frac{1}{2}(\mathbb{D}\mathbf{x}_2)^{\rm T}\mathbb{H}(\mathbb{D}\mathbf{x}_2) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_2\right\}$$
$$+ \lambda_1(x_1(0) - x_i) + \lambda_2((\mathbb{D}\mathbf{x}_1)(0) - \dot{x}_i)$$
$$+ \lambda_3(x_1(N_t) - x_2(N_t)) + \lambda_4((\mathbb{D}\mathbf{x}_1)(N_t) - (\mathbb{D}\mathbf{x}_2)(N_t)).$$

Global minimization for x_1,x_2, λ_1, λ_2 (initial cond.), λ_3, λ_4 (path identification) amounts to fully implicit scheme

solution shows x_1=x_2 but contaminated by doublers



Regularization with initial value data

$$\mathbb{S}_{\rm IVP} = \left\{\frac{1}{2}(\bar{\mathbb{D}}\bar{\mathbf{x}}_1)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}\bar{\mathbf{x}}_1) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_1\right\} - \left\{\frac{1}{2}(\bar{\mathbb{D}}\bar{\mathbf{x}}_2)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}\bar{\mathbf{x}}_2) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_2\right\}$$
$$+ \lambda_1(x_1(0) - x_i) + \lambda_2((\mathbb{D}\mathbf{x}_1)(0) - \dot{x}_i)$$
$$+ \lambda_3(x_1(N_t) - x_2(N_t)) + \lambda_4((\mathbb{D}\mathbf{x}_1)(N_t) - (\mathbb{D}\mathbf{x}_2)(N_t)).$$

$\bar{D}$ finite difference operator in affine coordinates

$\bar{H}$ quadrature matrix w/ one more row & column of 0s

A. Rothkopf, J. Nordström, arXiv:2205.14028

Implementation with Lagrange multipliers

University of Stavanger

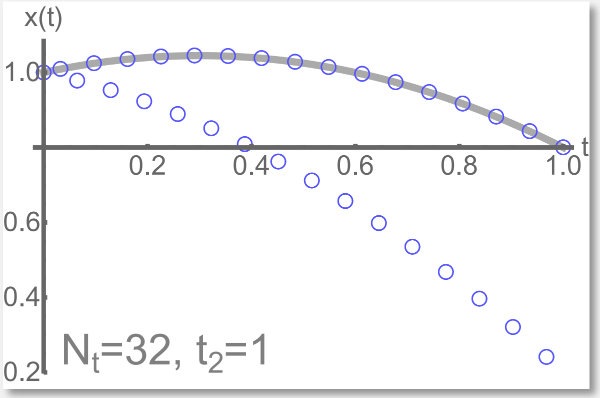
- Simple mechanical model: $\mathcal{S} = \int dt \left(\frac{1}{2} m\dot{x}^2(t) - mgx(t)\right)$ $\quad x(0) = 1, \dot{x}(0) = 0.3$

Naïve discretization

$$\mathbb{S}_{\rm IVP} = \left\{\frac{1}{2}(\mathbb{D}\mathbf{x}_1)^{\rm T}\mathbb{H}(\mathbb{D}\mathbf{x}_1) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_1\right\} - \left\{\frac{1}{2}(\mathbb{D}\mathbf{x}_2)^{\rm T}\mathbb{H}(\mathbb{D}\mathbf{x}_2) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_2\right\}$$
$$+ \lambda_1(x_1(0) - x_i) + \lambda_2((\mathbb{D}\mathbf{x}_1)(0) - \dot{x}_i)$$
$$+ \lambda_3(x_1(N_t) - x_2(N_t)) + \lambda_4((\mathbb{D}\mathbf{x}_1)(N_t) - (\mathbb{D}\mathbf{x}_2)(N_t)).$$

Global minimization for x_1,x_2, λ_1, λ_2 (initial cond.), λ_3, λ_4 (path identification) amounts to fully implicit scheme

solution shows x_1=x_2 but contaminated by doublers

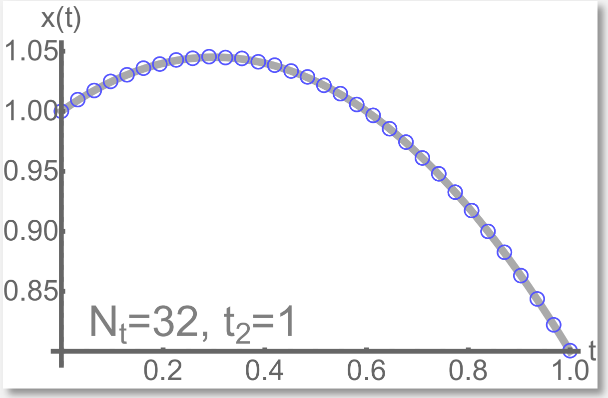


Regularization with initial value data

$$\mathbb{S}_{\rm IVP} = \left\{\frac{1}{2}(\bar{\mathbb{D}}\bar{\mathbf{x}}_1)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}\bar{\mathbf{x}}_1) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_1\right\} - \left\{\frac{1}{2}(\bar{\mathbb{D}}\bar{\mathbf{x}}_2)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}\bar{\mathbf{x}}_2) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_2\right\}$$
$$+ \lambda_1(x_1(0) - x_i) + \lambda_2((\mathbb{D}\mathbf{x}_1)(0) - \dot{x}_i)$$
$$+ \lambda_3(x_1(N_t) - x_2(N_t)) + \lambda_4((\mathbb{D}\mathbf{x}_1)(N_t) - (\mathbb{D}\mathbf{x}_2)(N_t)).$$

$\bar{D}$ finite difference operator in affine coordinates

$\bar{H}$ quadrature matrix w/ one more row & column of 0s



A. Rothkopf, J. Nordström, arXiv:2205.14028

Implementation with Lagrange multipliers

University of Stavanger

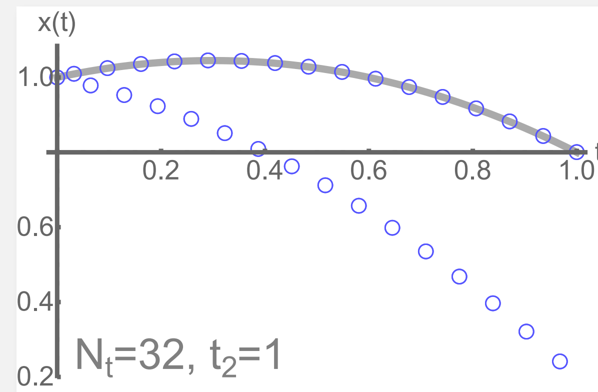
- Simple mechanical model: $\mathcal{S} = \int dt \left(\frac{1}{2} m\dot{x}^2(t) - mgx(t)\right)$ $\quad x(0) = 1, \dot{x}(0) = 0.3$

Naïve discretization

$$\mathbb{S}_{\rm IVP} = \left\{\frac{1}{2}(\mathbb{D}\mathbf{x}_1)^{\rm T}\mathbb{H}(\mathbb{D}\mathbf{x}_1) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_1\right\} - \left\{\frac{1}{2}(\mathbb{D}\mathbf{x}_2)^{\rm T}\mathbb{H}(\mathbb{D}\mathbf{x}_2) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_2\right\}$$
$$+ \lambda_1(x_1(0) - x_i) + \lambda_2((\mathbb{D}\mathbf{x}_1)(0) - \dot{x}_i)$$
$$+ \lambda_3(x_1(N_t) - x_2(N_t)) + \lambda_4((\mathbb{D}\mathbf{x}_1)(N_t) - (\mathbb{D}\mathbf{x}_2)(N_t)).$$

Global minimization for x_1,x_2, λ_1, λ_2 (initial cond.), λ_3, λ_4 (path identification) amounts to fully implicit scheme

solution shows x_1=x_2 but contaminated by doublers

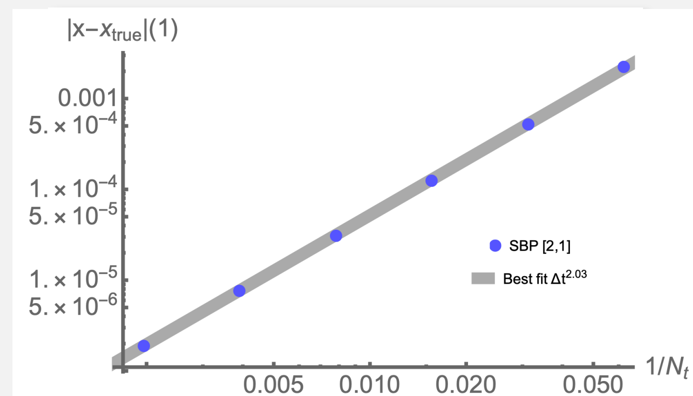


Regularization with initial value data

$$\mathbb{S}_{\rm IVP} = \left\{\frac{1}{2}(\bar{\mathbb{D}}\bar{\mathbf{x}}_1)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}\bar{\mathbf{x}}_1) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_1\right\} - \left\{\frac{1}{2}(\bar{\mathbb{D}}\bar{\mathbf{x}}_2)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}\bar{\mathbf{x}}_2) - g\mathbb{1}^{\rm T}\mathbb{H}\mathbf{x}_2\right\}$$
$$+ \lambda_1(x_1(0) - x_i) + \lambda_2((\mathbb{D}\mathbf{x}_1)(0) - \dot{x}_i)$$
$$+ \lambda_3(x_1(N_t) - x_2(N_t)) + \lambda_4((\mathbb{D}\mathbf{x}_1)(N_t) - (\mathbb{D}\mathbf{x}_2)(N_t)).$$

$\bar{D}$ finite difference operator in affine coordinates

$\bar{H}$ quadrature matrix w/ one more row & column of 0s



A. Rothkopf, J. Nordström, arXiv:2205.14028

Added bonus: dissipative systems

University of Stavanger

- Inspiration from path integrals: doubled paths accommodate 1st order e.o.m.

$$S_{\rm IVP}[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)] = \int_{t_1}^{t_2} dt\Big(\mathcal{L}[x_1(t),\dot{x}_1(t)] - \mathcal{L}[x_2(t),\dot{x}_2(t)] + \Lambda[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)]\Big)$$

Added bonus: dissipative systems

University of Stavanger

- Inspiration from path integrals: doubled paths accommodate 1st order e.o.m.

$$S_{\rm IVP}[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)] = \int_{t_1}^{t_2} dt\Big(\mathcal{L}[x_1(t),\dot{x}_1(t)] - \mathcal{L}[x_2(t),\dot{x}_2(t)] + \Lambda[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)]\Big)$$

Similar to Feynman-Vernon influence functional: terms that do not factorize into Lagrangians

Added bonus: dissipative systems

- Inspiration from path integrals: doubled paths accommodate 1st order e.o.m.

$$S_{\rm IVP}[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)] = \int_{t_1}^{t_2} dt \Big(\mathcal{L}[x_1(t),\dot{x}_1(t)] - \mathcal{L}[x_2(t),\dot{x}_2(t)] + \Lambda[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)]\Big)$$

Similar to Feynman-Vernon influence functional: terms that do not factorize into Lagrangians

- Damped Harmonic oscillator: $\mathcal{L} = \frac{1}{2} m x^2(t) - \kappa x^2$ $\quad \Lambda = -\xi \dot{x}_+(t) x_-(t)$

Added bonus: dissipative systems

University of Stavanger

- Inspiration from path integrals: doubled paths accommodate 1st order e.o.m.

$$S_{\rm IVP}[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)] = \int_{t_1}^{t_2} dt\Big(\mathcal{L}[x_1(t),\dot{x}_1(t)] - \mathcal{L}[x_2(t),\dot{x}_2(t)] + \Lambda[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)]\Big)$$

Similar to Feynman-Vernon influence functional: terms that do not factorize into Lagrangians

- Damped Harmonic oscillator: $\mathcal{L} = \frac{1}{2}m\dot{x}^2(t) - \kappa x^2 \qquad \Lambda = -\xi\dot{x}_+(t)x_-(t)$

$$S_{\rm IVP} = \int_{t_1}^{t_2} dt\Big(m\dot{x}_+(t)\dot{x}_-(t) - 2\kappa x_+(t)x_-(t) - \xi\dot{x}_+(t)x_-(t)\Big)$$

Added bonus: dissipative systems

University of Stavanger

- Inspiration from path integrals: doubled paths accommodate 1st order e.o.m.

$$S_{\rm IVP}[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)] = \int_{t_1}^{t_2} dt \Big(\mathcal{L}[x_1(t),\dot{x}_1(t)] - \mathcal{L}[x_2(t),\dot{x}_2(t)] + \Lambda[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)] \Big)$$

Similar to Feynman-Vernon influence functional: terms that do not factorize into Lagrangians

- Damped Harmonic oscillator: $\mathcal{L} = \frac{1}{2} m x^2(t) - \kappa x^2 \qquad \Lambda = -\xi \dot{x}_+(t) x_-(t)$

$$S_{\rm IVP} = \int_{t_1}^{t_2} dt \big(m\dot{x}_+(t)\dot{x}_-(t) - 2\kappa x_+(t)x_-(t) - \xi\dot{x}_+(t)x_-(t) \big)$$

Regularized with initial values

$$\begin{aligned} \mathbb{S}_{\rm GIVP} = &\Big\{\frac{1}{2}\mu(\bar{\mathbb{D}}\bar{\mathbf{x}}_1)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}\bar{\mathbf{x}}_1) - \frac{1}{2}\kappa(\mathbf{x}_1)^{\rm T}\mathbb{H}\mathbf{x}_1\Big\} - \Big\{\frac{1}{2}\mu(\bar{\mathbb{D}}\bar{\mathbf{x}}_2)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}\bar{\mathbf{x}}_2) - \frac{1}{2}\kappa(\mathbf{x}_2)^{\rm T}\mathbb{H}\mathbf{x}_2\Big\} \\ &- \xi\frac{1}{2}\Big(\bar{\mathbb{D}}(\bar{\mathbf{x}}_1+\bar{\mathbf{x}}_2)\Big)^{\rm T}\bar{\mathbb{H}}(\mathbf{x}_1-\mathbf{x}_2) + \lambda_1(x_1(0)-x_i) + \lambda_2((\mathbb{D}\mathbf{x}_1)(0)-\dot{x}_i) \\ &+ \lambda_3(x_1(N_t)-x_2(N_t)) + \lambda_4((\mathbb{D}\mathbf{x}_1)(N_t)-(\mathbb{D}\mathbf{x}_2)(N_t)) \end{aligned}$$

Global minimization for x_1,x_2, λ_1, λ_2 (initial cond.), λ_3, λ_4 (path identification) amounts to fully implicit scheme

$\overline{D}$ finite difference operator in affine coordinates

$\overline{H}$ quadrature matrix w/ one more row & column of 0s

Added bonus: dissipative systems

University of Stavanger

- Inspiration from path integrals: doubled paths accommodate 1st order e.o.m.

$$S_{\rm IVP}[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)] = \int_{t_1}^{t_2} dt\Big(\mathcal{L}[x_1(t),\dot{x}_1(t)] - \mathcal{L}[x_2(t),\dot{x}_2(t)] + \Lambda[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)]\Big)$$

Similar to Feynman-Vernon influence functional: terms that do not factorize into Lagrangians

- Damped Harmonic oscillator: $\mathcal{L} = \frac{1}{2}m x^2(t) - \kappa x^2 \qquad \Lambda = -\xi \dot{x}_+(t)x_-(t)$

$$S_{\rm IVP} = \int_{t_1}^{t_2} dt\big(m\dot{x}_+(t)\dot{x}_-(t) - 2\kappa x_+(t)x_-(t) - \xi\dot{x}_+(t)x_-(t)\big)$$

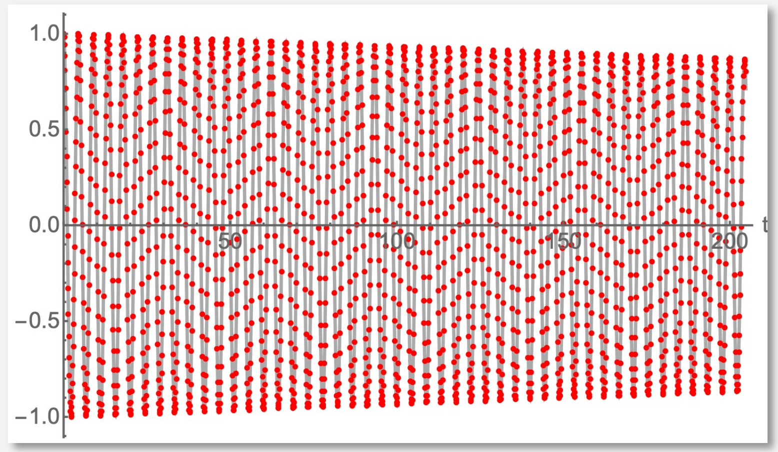
Regularized with initial values

$$\mathbb{S}_{\rm GIVP} = \Big\{\frac{1}{2}\mu(\bar{\mathbb{D}}\bar{\mathbf{x}}_1)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}\bar{\mathbf{x}}_1) - \frac{1}{2}\kappa(\mathbf{x}_1)^{\rm T}\mathbb{H}\mathbf{x}_1\Big\} - \Big\{\frac{1}{2}\mu(\bar{\mathbb{D}}\bar{\mathbf{x}}_2)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}\bar{\mathbf{x}}_2) - \frac{1}{2}\kappa(\mathbf{x}_2)^{\rm T}\mathbb{H}\mathbf{x}_2\Big\}$$
$$- \xi\frac{1}{2}\Big(\bar{\mathbb{D}}(\bar{\mathbf{x}}_1+\bar{\mathbf{x}}_2)\Big)^{\rm T}\bar{\mathbb{H}}(\mathbf{x}_1-\mathbf{x}_2) + \lambda_1(x_1(0)-x_i) + \lambda_2((\mathbb{D}\mathbf{x}_1)(0)-\dot{x}_i)$$
$$+ \lambda_3(x_1(N_t)-x_2(N_t)) + \lambda_4((\mathbb{D}\mathbf{x}_1)(N_t)-(\mathbb{D}\mathbf{x}_2)(N_t))$$

Global minimization for x_1,x_2, λ_1, λ_2 (initial cond.), λ_3, λ_4 (path identification) amounts to fully implicit scheme

$\bar{D}$ finite difference operator in affine coordinates

$\bar{H}$ quadrature matrix w/ one more row & column of 0s



Added bonus: dissipative systems

University of Stavanger

- Inspiration from path integrals: doubled paths accommodate 1st order e.o.m.

$$S_{\rm IVP}[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)] = \int_{t_1}^{t_2} dt\Big(\mathcal{L}[x_1(t),\dot{x}_1(t)] - \mathcal{L}[x_2(t),\dot{x}_2(t)] + \Lambda[x_1(t),\dot{x}_1(t),x_2(t),\dot{x}_2(t)]\Big)$$

Similar to Feynman-Vernon influence functional: terms that do not factorize into Lagrangians

- Damped Harmonic oscillator: $\mathcal{L} = \frac{1}{2}mx^2(t) - \kappa x^2$ $\quad \Lambda = -\xi\dot{x}_+(t)x_-(t)$

$$S_{\rm IVP} = \int_{t_1}^{t_2} dt\big(m\dot{x}_+(t)\dot{x}_-(t) - 2\kappa x_+(t)x_-(t) - \xi\dot{x}_+(t)x_-(t)\big)$$

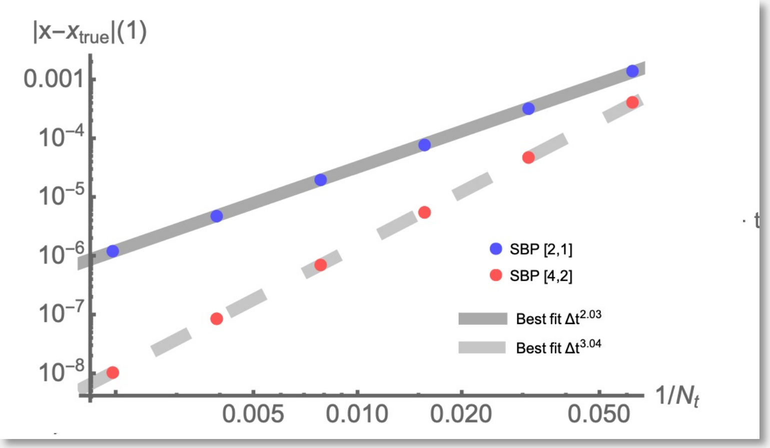
Regularized with initial values

$$\mathbb{S}_{\rm GIVP} = \Big\{\frac{1}{2}\mu(\bar{\mathbb{D}}\bar{\mathbf{x}}_1)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}\bar{\mathbf{x}}_1) - \frac{1}{2}\kappa(\mathbf{x}_1)^{\rm T}\mathbb{H}\mathbf{x}_1\Big\} - \Big\{\frac{1}{2}\mu(\bar{\mathbb{D}}\bar{\mathbf{x}}_2)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}\bar{\mathbf{x}}_2) - \frac{1}{2}\kappa(\mathbf{x}_2)^{\rm T}\mathbb{H}\mathbf{x}_2\Big\}$$
$$-\xi\frac{1}{2}\Big(\bar{\mathbb{D}}(\bar{\mathbf{x}}_1+\bar{\mathbf{x}}_2)\Big)^{\rm T}\bar{\mathbb{H}}(\mathbf{x}_1-\mathbf{x}_2) + \lambda_1(x_1(0)-x_i) + \lambda_2((\mathbb{D}\mathbf{x}_1)(0)-\dot{x}_i)$$
$$+\lambda_3(x_1(N_t)-x_2(N_t)) + \lambda_4((\mathbb{D}\mathbf{x}_1)(N_t)-(\mathbb{D}\mathbf{x}_2)(N_t))$$

Global minimization for x_1,x_2, λ_1, λ_2 (initial cond.), λ_3, λ_4 (path identification) amounts to fully implicit scheme

$\bar{D}$ finite difference operator in affine coordinates

$\bar{H}$ quadrature matrix w/ one more row & column of 0s



late time stability and accuracy

Conclusion & Outlook

University of Stavanger

- Accurate treatment of constraints suggests use of symmetric discretization schemes
- Symmetric finite differences suffer from well known doubling problem but Wilson term not applicable to real-valued bosonic fields
- By exploiting the **weak imposition of boundary / initial values,** unphysical zero modes of finite difference operators can be lifted
- **Affine coordinate formulation: new regularization on the level of the action**
- Affine formulation directly applicable to **higher order discretization schemes**
- Promising results in solving classical equations of motion of various simple models

- Extension of the formalism to higher dimensions is work in progress
- Here we focus on bosons but method also applicable to fermions: alternative regularization for spatial directions of Dirac operator.

Backup slides

Solving Challenge I (Abelian theory)

University of Stavanger

- Correct implementation of boundary conditions in FD: **summation by parts**

$$\int_0^L dx f(x)g(x) \approx \mathcal{T}_0^N[f_x g_x]$$

$$\mathcal{T}_0^N[(\Delta^{\rm SBP} f_x)g_x] \stackrel{!}{=} -\mathcal{T}_0^N[f_x(\Delta^{\rm SBP} g_x)] + f_N g_N - f_0 g_0.$$

Solving Challenge I (Abelian theory)

University of Stavanger

- Correct implementation of boundary conditions in FD: **summation by parts**

$$\int_0^L dx\, f(x)g(x) \approx \mathcal{T}_0^N[f_x g_x] \qquad \mathsf{H} = \Delta x \begin{bmatrix} \frac{1}{2} & & & \\ & 1 & & \\ & & 1 & \\ & & & \frac{1}{2} \end{bmatrix}$$

$$\mathcal{T}_0^N[(\Delta^{\rm SBP} f_x)g_x] \overset{!}{=} -\mathcal{T}_0^N[f_x(\Delta^{\rm SBP} g_x)] + f_N g_N - f_0 g_0.$$

Solving Challenge I (Abelian theory)

University of Stavanger

- Correct implementation of boundary conditions in FD: **summation by parts**

$$\int_0^L dx f(x)g(x) \approx \mathcal{T}_0^N[f_x g_x] \qquad \mathsf{H} = \Delta x \begin{bmatrix} \frac{1}{2} & & & \\ & 1 & & \\ & & 1 & \\ & & & \frac{1}{2} \end{bmatrix} \quad \mathsf{D}_1 = \frac{1}{\Delta x}\begin{bmatrix} -1 & 1 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -1 & 1 \end{bmatrix}$$

$$\mathcal{T}_0^N[(\Delta^{\rm SBP} f_x)g_x] \stackrel{!}{=} -\mathcal{T}_0^N[f_x(\Delta^{\rm SBP} g_x)] + f_N g_N - f_0 g_0.$$

Solving Challenge I (Abelian theory)

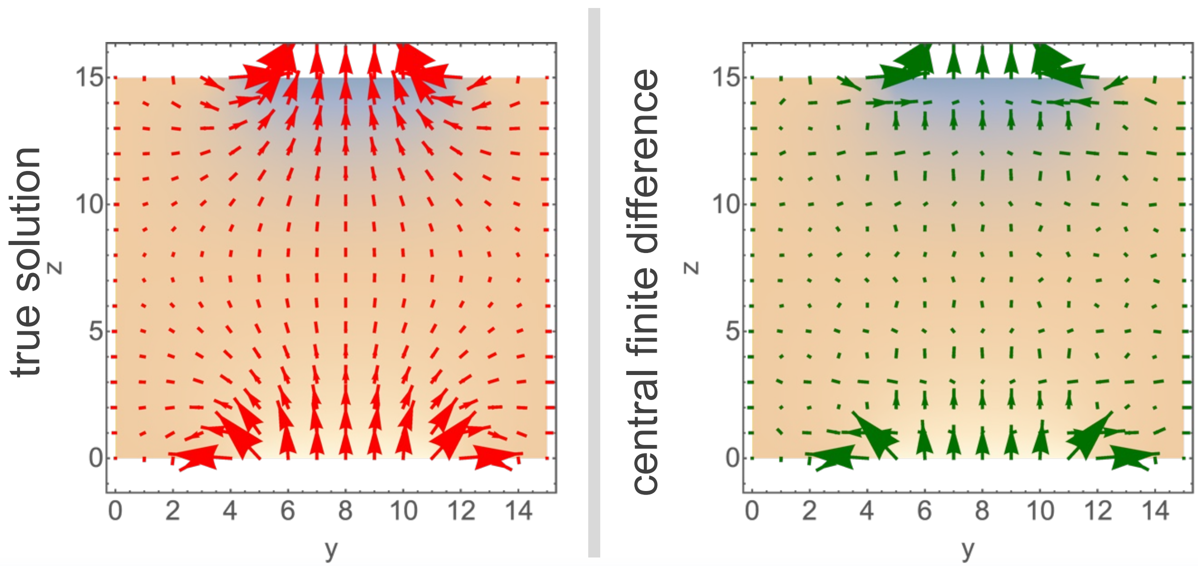
University of Stavanger

- Correct implementation of boundary conditions in FD: **summation by parts**

$$\int_0^L dx\, f(x) g(x) \approx \mathcal{T}_0^N[f_x g_x] \qquad \mathsf{H} = \Delta x \begin{bmatrix} \frac{1}{2} & & & \\ & 1 & & \\ & & 1 & \\ & & & \frac{1}{2} \end{bmatrix} \quad \mathsf{D}_1 = \frac{1}{\Delta x}\begin{bmatrix} -1 & 1 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -1 & 1 \end{bmatrix}$$

$$\mathcal{T}_0^N[(\Delta^{\rm SBP} f_x) g_x] \stackrel{!}{=} -\mathcal{T}_0^N[f_x(\Delta^{\rm SBP} g_x)] + f_N g_N - f_0 g_0.$$

- Central finite difference on interior not enough, need genuine SBP form of FD



Solving Challenge I (Abelian theory)

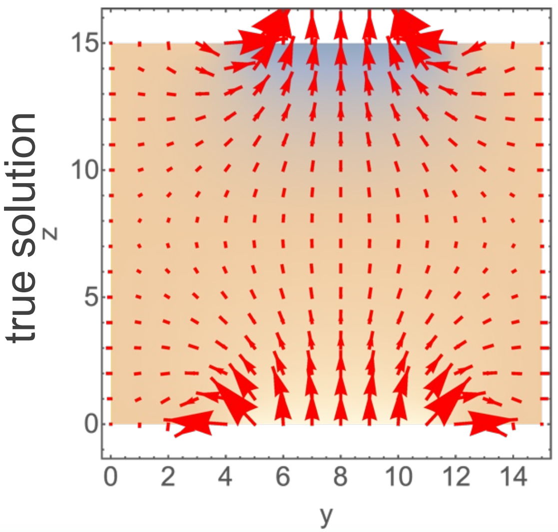
University of Stavanger

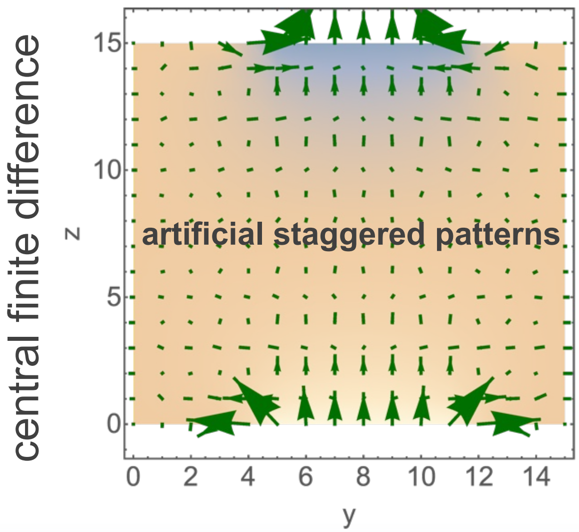
- Correct implementation of boundary conditions in FD: **summation by parts**

$$\int_0^L dx f(x)g(x) \approx \mathcal{T}_0^N[f_x g_x] \qquad \mathsf{H} = \Delta x \begin{bmatrix} \frac{1}{2} & & & \\ & 1 & & \\ & & 1 & \\ & & & \frac{1}{2} \end{bmatrix} \quad \mathsf{D}_1 = \frac{1}{\Delta x}\begin{bmatrix} -1 & 1 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -1 & 1 \end{bmatrix}$$

$$\mathcal{T}_0^N[(\Delta^{\rm SBP} f_x) g_x] \stackrel{!}{=} -\mathcal{T}_0^N[f_x(\Delta^{\rm SBP} g_x)] + f_N g_N - f_0 g_0.$$

- Central finite difference on interior not enough, need genuine SBP form of FD





Solving Challenge I (Abelian theory)

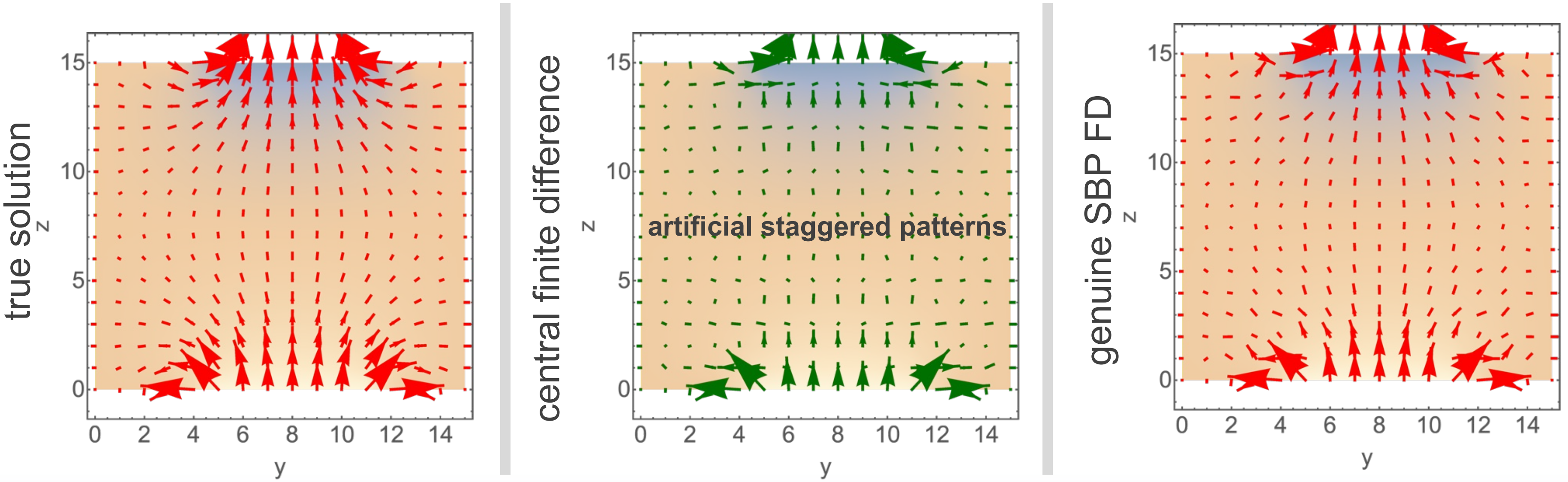
University of Stavanger

- Correct implementation of boundary conditions in FD: **summation by parts**

$$\int_0^L dx\, f(x)g(x) \approx \mathcal{T}_0^N[f_x g_x] \qquad \mathsf{H} = \Delta x \begin{bmatrix} \frac{1}{2} & & & \\ & 1 & & \\ & & 1 & \\ & & & \frac{1}{2} \end{bmatrix} \quad \mathsf{D}_1 = \frac{1}{\Delta x}\begin{bmatrix} -1 & 1 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -1 & 1 \end{bmatrix}$$

$$\mathcal{T}_0^N[(\Delta^{\mathrm{SBP}} f_x)g_x] \stackrel{!}{=} -\mathcal{T}_0^N[f_x(\Delta^{\mathrm{SBP}} g_x)] + f_N g_N - f_0 g_0.$$

- Central finite difference on interior not enough, need genuine SBP form of FD



Challenge II

- Discretization crucial for gauge invariant force field lines via stress tensor

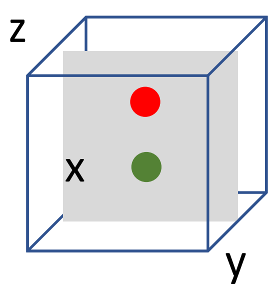
$$\Theta^{ij} = \frac{1}{4\pi}\left(g^{i\mu}F_{\mu\lambda}F^{\lambda j} + \frac{1}{4}g^{ij}F_{\mu\lambda}F^{\mu\lambda}\right) \qquad \mathbf{f} = \nabla \cdot \mathbf{\Theta} + \partial \mathbf{S}/\partial t$$

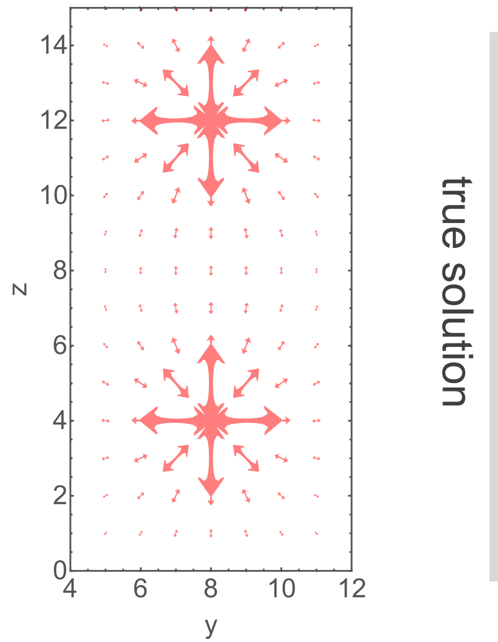
Challenge II

- Discretization crucial for gauge invariant force field lines via stress tensor

$$\Theta^{ij} = \frac{1}{4\pi}\left(g^{i\mu}F_{\mu\lambda}F^{\lambda j} + \frac{1}{4}g^{ij}F_{\mu\lambda}F^{\mu\lambda}\right) \qquad \mathbf{f} = \nabla\cdot\boldsymbol{\Theta} + \partial\mathbf{S}/\partial t$$

- Eigenvectors of Θ encode direction of force field lines (positive eigenvalue)



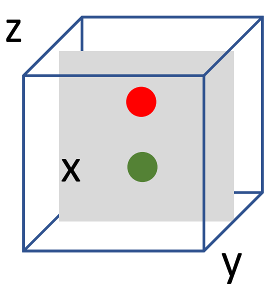


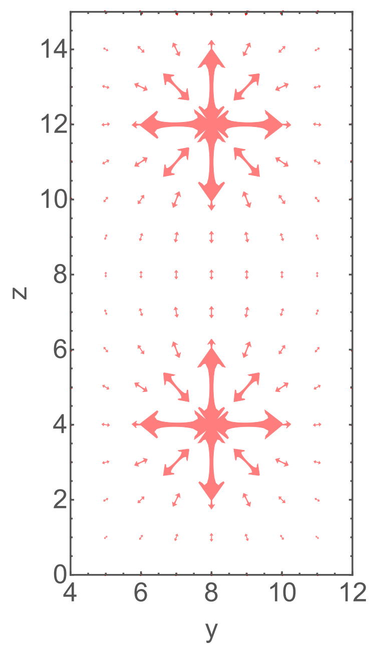
Challenge II

- Discretization crucial for gauge invariant force field lines via stress tensor

$$\Theta^{ij} = \frac{1}{4\pi}\left(g^{i\mu}F_{\mu\lambda}F^{\lambda j} + \frac{1}{4}g^{ij}F_{\mu\lambda}F^{\mu\lambda}\right) \qquad \mathbf{f} = \nabla\cdot\mathbf{\Theta} + \partial\mathbf{S}/\partial t$$

- Eigenvectors of Θ encode direction of force field lines (positive eigenvalue)





true solution

backward finite difference

$$\mathbf{\Delta}^{\mathrm{B}}\cdot\mathbf{E} =$$
$$\frac{1}{a_s^3}\left[\delta_{\mathbf{x}\mathbf{x}_0} - \delta_{\mathbf{x}\mathbf{x}_1}\right]$$

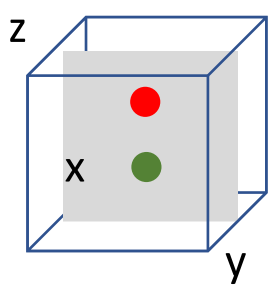
Challenge II

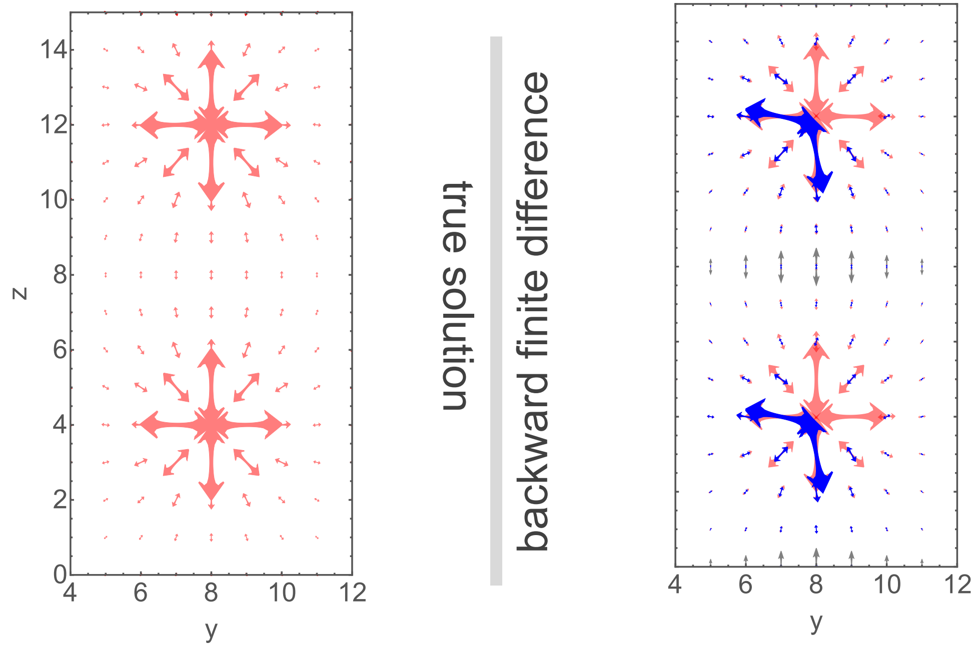
University of Stavanger

- Discretization crucial for gauge invariant force field lines via stress tensor

$$\Theta^{ij} = \frac{1}{4\pi}\left(g^{i\mu}F_{\mu\lambda}F^{\lambda j} + \frac{1}{4}g^{ij}F_{\mu\lambda}F^{\mu\lambda}\right) \qquad \mathbf{f} = \nabla\cdot\mathbf{\Theta} + \partial\mathbf{S}/\partial t$$

- Eigenvectors of Θ encode direction of force field lines (positive eigenvalue)





$$\mathbf{\Delta}^{\mathrm{B}}\cdot\mathbf{E} = \frac{1}{a_s^3}\left[\delta_{\mathbf{x}\mathbf{x}_0} - \delta_{\mathbf{x}\mathbf{x}_1}\right]$$

Solving Challenge I (non-Abelian)

University of Stavanger

- Need a central finite difference discretization for the interior (overall $O(a^2)$)

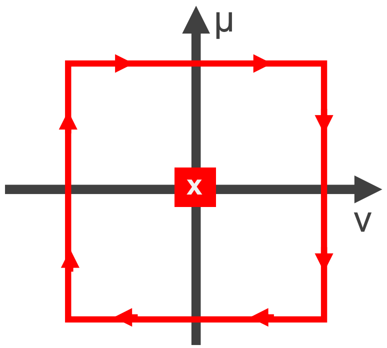
$$\bar{U}_{\mu,x} = \exp\big[ia_\mu A_{\mu,x+\frac{1}{2}a\hat{\mu}}\big] = \exp\big[ia_\mu \tfrac{1}{2}\big(A_{\mu,x} + A_{\mu,x+a\hat{\mu}}\big)\big] + \mathcal{O}(a^2)$$

Solving Challenge I (non-Abelian)

- Need a central finite difference discretization for the interior (overall O(a²))

$$\bar{U}_{\mu,x} = \exp\left[ia_\mu A_{\mu,x+\frac{1}{2}a\hat{\mu}}\right] = \exp\left[ia_\mu \tfrac{1}{2}\left(A_{\mu,x} + A_{\mu,x+a\hat{\mu}}\right)\right] + \mathcal{O}(a^2)$$

$$\begin{aligned} P^{2\times2}_{\mu\nu,x} =& \bar{U}_{\mu,x-a\hat{\mu}-a\hat{\nu}}\bar{U}_{\mu,x-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}}\times \\ & \bar{U}^\dagger_{\mu,x+a\hat{\nu}}\bar{U}^\dagger_{\mu,x-a\hat{\mu}+a\hat{\nu}}\bar{U}^\dagger_{\nu,x-a\hat{\mu}}\bar{U}^\dagger_{\nu,x-a\hat{\mu}-a\hat{\nu}} \\ =& \exp\left[4iga_\mu a_\nu \bar{F}_{\mu\nu,x}\right] + \mathcal{O}(a^3) \\ \bar{F}_{\mu\nu,x} =& \boldsymbol{\Delta}^{\mathrm{C}}_\mu A_{\nu,x} - \boldsymbol{\Delta}^{\mathrm{C}}_\nu A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}] \end{aligned}$$



this study

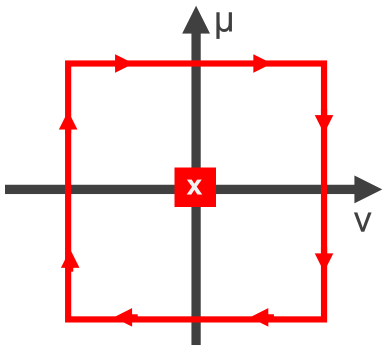
Solving Challenge I (non-Abelian)

University of Stavanger

- Need a central finite difference discretization for the interior (overall O(a²))

$$\bar{U}_{\mu,x} = \exp\left[ia_\mu A_{\mu,x+\frac{1}{2}a\hat{\mu}}\right] = \exp\left[ia_\mu \tfrac{1}{2}\left(A_{\mu,x} + A_{\mu,x+a\hat{\mu}}\right)\right] + \mathcal{O}(a^2)$$

$$\begin{aligned} P^{2\times 2}_{\mu\nu,x} =& \bar{U}_{\mu,x-a\hat{\mu}-a\hat{\nu}}\bar{U}_{\mu,x-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}}\times \\ & \bar{U}^\dagger_{\mu,x+a\hat{\nu}}\bar{U}^\dagger_{\mu,x-a\hat{\mu}+a\hat{\nu}}\bar{U}^\dagger_{\nu,x-a\hat{\mu}}\bar{U}^\dagger_{\nu,x-a\hat{\mu}-a\hat{\nu}} \\ =& \exp\left[4iga_\mu a_\nu \bar{F}_{\mu\nu,x}\right] + \mathcal{O}(a^3) \\ \bar{F}_{\mu\nu,x} =& \boldsymbol{\Delta}^{\rm C}_\mu A_{\nu,x} - \boldsymbol{\Delta}^{\rm C}_\nu A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}] \end{aligned}$$



this study

"sum the exponents not the exponential" (c.f. clover leaf)

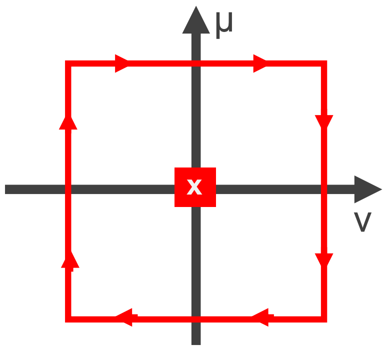
Solving Challenge I (non-Abelian)

University of Stavanger

- Need a central finite difference discretization for the interior (overall O(a²))

$$\bar{U}_{\mu,x} = \exp\big[ia_\mu A_{\mu,x+\frac{1}{2}a\hat{\mu}}\big] = \exp\big[ia_\mu \tfrac{1}{2}\big(A_{\mu,x} + A_{\mu,x+a\hat{\mu}}\big)\big] + \mathcal{O}(a^2)$$

$$\begin{aligned} P^{2\times2}_{\mu\nu,x} =& \bar{U}_{\mu,x-a\hat{\mu}-a\hat{\nu}}\bar{U}_{\mu,x-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}}\times \\ & \bar{U}^\dagger_{\mu,x+a\hat{\nu}}\bar{U}^\dagger_{\mu,x-a\hat{\mu}+a\hat{\nu}}\bar{U}^\dagger_{\nu,x-a\hat{\mu}}\bar{U}^\dagger_{\nu,x-a\hat{\mu}-a\hat{\nu}} \\ =& \exp\big[4iga_\mu a_\nu \bar{F}_{\mu\nu,x}\big] + \mathcal{O}(a^3) \\ \bar{F}_{\mu\nu,x} =& \mathbf{\Delta}^{\rm C}_\mu A_{\nu,x} - \mathbf{\Delta}^{\rm C}_\nu A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}] \end{aligned}$$



this study

”sum the exponents not the exponential” (c.f. clover leaf)

$$S^{2\times2} = \frac{1}{g^2}\sum_{x\notin\partial V} a_t a_s^3 \Big[\frac{2}{16a_t^2a_s^2}\sum_i {\rm ReTr}\big[1 - P^{2\times2}_{0i,x}\big] - \frac{1}{16a_s^4}\sum_{ij}{\rm ReTr}\big[1 - P^{2\times2}_{ij,x}\big]\Big]$$

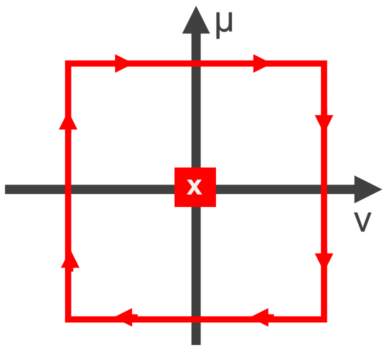
Solving Challenge I (non-Abelian)

University of Stavanger

- Need a central finite difference discretization for the interior (overall O(a²))

$$\bar{U}_{\mu,x} = \exp\big[ia_\mu A_{\mu,x+\frac{1}{2}a\hat{\mu}}\big] = \exp\big[ia_\mu \tfrac{1}{2}\big(A_{\mu,x} + A_{\mu,x+a\hat{\mu}}\big)\big] + \mathcal{O}(a^2)$$

$$\begin{aligned}P^{2\times2}_{\mu\nu,x} =& \bar{U}_{\mu,x-a\hat{\mu}-a\hat{\nu}}\bar{U}_{\mu,x-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}}\times \\ & \bar{U}^\dagger_{\mu,x+a\hat{\nu}}\bar{U}^\dagger_{\mu,x-a\hat{\mu}+a\hat{\nu}}\bar{U}^\dagger_{\nu,x-a\hat{\mu}}\bar{U}^\dagger_{\nu,x-a\hat{\mu}-a\hat{\nu}} \\ =& \exp\big[4iga_\mu a_\nu \bar{F}_{\mu\nu,x}\big] + \mathcal{O}(a^3) \\ \bar{F}_{\mu\nu,x} =& \mathbf{\Delta}^{\rm C}_\mu A_{\nu,x} - \mathbf{\Delta}^{\rm C}_\nu A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}]\end{aligned}$$



this study

"sum the exponents not the exponential" (c.f. clover leaf)

$$S^{2\times2} = \frac{1}{g^2}\sum_{x\notin\partial V} a_t a_s^3\Big[\frac{2}{16a_t^2a_s^2}\sum_i {\rm ReTr}\big[1 - P^{2\times2}_{0i,x}\big] - \frac{1}{16a_s^4}\sum_{ij}{\rm ReTr}\big[1 - P^{2\times2}_{ij,x}\big]\Big]$$

- Combine with forward and backward Wilson plaquettes on the boundary:

$$\tilde{F}_{\mu\nu,x} = \mathbf{\Delta}^{\rm SBP}_\mu A_{\nu,x} - \mathbf{\Delta}^{\rm SBP}_\nu A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}]$$

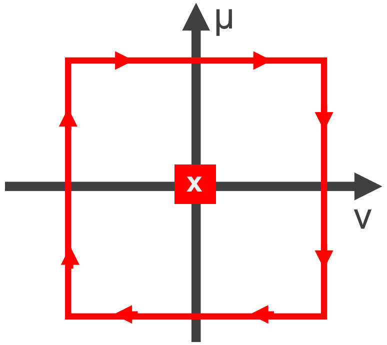
Solving Challenge I (non-Abelian)

University of Stavanger

- Need a central finite difference discretization for the interior (overall O(a²))

$$\bar{U}_{\mu,x} = \exp\big[ia_\mu A_{\mu,x+\frac{1}{2}a\hat{\mu}}\big] = \exp\big[ia_\mu \tfrac{1}{2}\big(A_{\mu,x} + A_{\mu,x+a\hat{\mu}}\big)\big] + \mathcal{O}(a^2)$$

$$\begin{aligned} P^{2\times 2}_{\mu\nu,x} =& \bar{U}_{\mu,x-a\hat{\mu}-a\hat{\nu}}\bar{U}_{\mu,x-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}-a\hat{\nu}}\bar{U}_{\nu,x+a\hat{\mu}}\times \\ & \bar{U}^\dagger_{\mu,x+a\hat{\nu}}\bar{U}^\dagger_{\mu,x-a\hat{\mu}+a\hat{\nu}}\bar{U}^\dagger_{\nu,x-a\hat{\mu}}\bar{U}^\dagger_{\nu,x-a\hat{\mu}-a\hat{\nu}} \\ =& \exp\big[4iga_\mu a_\nu \bar{F}_{\mu\nu,x}\big] + \mathcal{O}(a^3) \\ \bar{F}_{\mu\nu,x} =& \mathbf{\Delta}^{\rm C}_\mu A_{\nu,x} - \mathbf{\Delta}^{\rm C}_\nu A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}] \end{aligned}$$



this study

Szymanzik program:
$P^{1x1}+P^{1x2}+P^{2x2}+\ldots$ (not SBP)

M. Garcia Perez, et.al. NPB 413, 535 (1994). B. Beinlich, et.al., NPB 462, 415 (1996), P. de Forcrand et.al., NPB 499, 409 (1997), J. R. Snippe, NPB 498, 347 (1997), S. O. Bilson-Thompson et.al., Annals Phys. 304, 1 (2003), K. Langfeld, (2004), arXiv:hep-lat/0403018.

"sum the exponents not the exponential" (c.f. clover leaf)

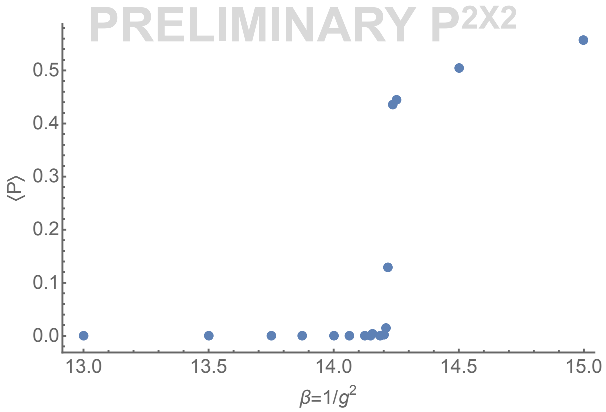
$$S^{2\times 2} = \frac{1}{g^2}\sum_{x\notin\partial V} a_t a_s^3 \Big[\frac{2}{16a_t^2a_s^2}\sum_i {\rm ReTr}\big[1 - P^{2\times 2}_{0i,x}\big] - \frac{1}{16a_s^4}\sum_{ij}{\rm ReTr}\big[1 - P^{2\times 2}_{ij,x}\big]\Big]$$

- Combine with forward and backward Wilson plaquettes on the boundary:

$$\tilde{F}_{\mu\nu,x} = \mathbf{\Delta}^{\rm SBP}_\mu A_{\nu,x} - \mathbf{\Delta}^{\rm SBP}_\nu A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}]$$

First steps towards quantization

- P^{2x2} action in a standard PBC Langevin MC: rough scale setting & beta function

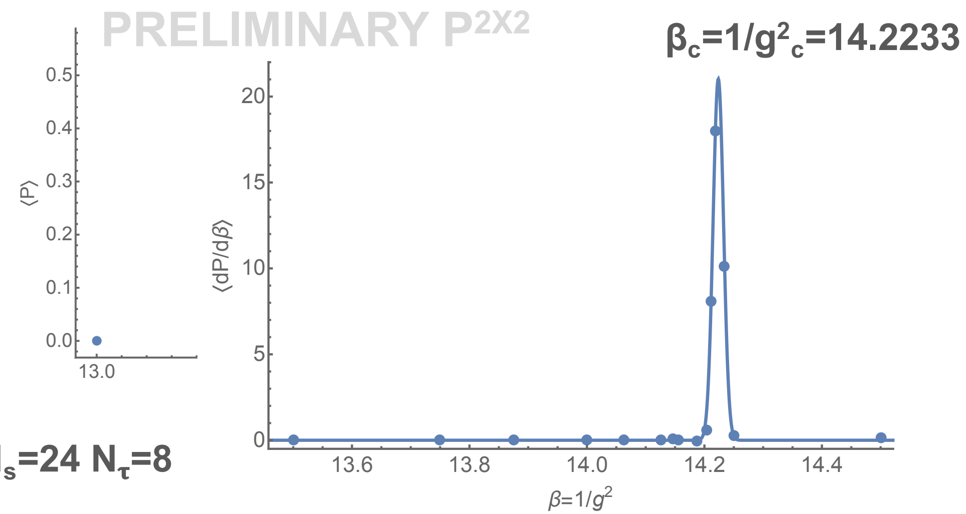


N_s=24 N_τ=8

First steps towards quantization

University of Stavanger

- P^{2x2} action in a standard PBC Langevin MC: rough scale setting & beta function

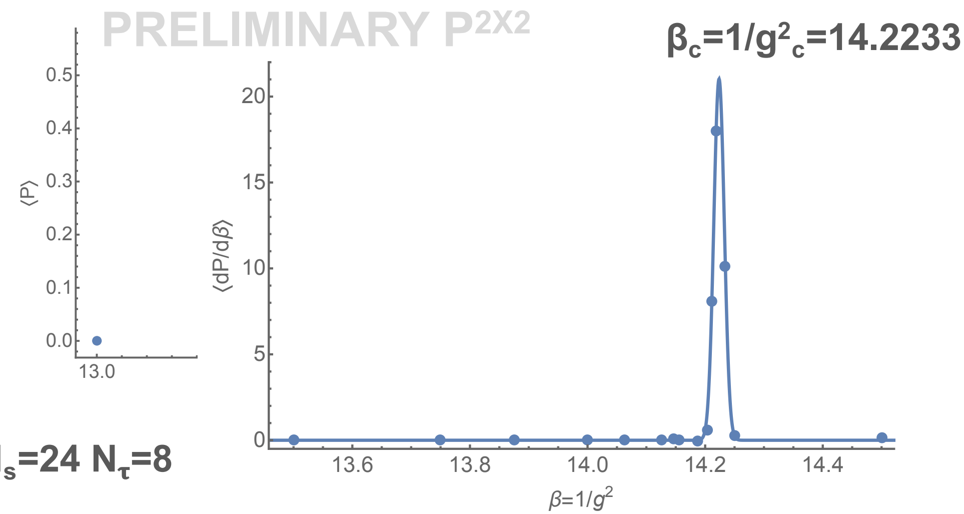


N_s=24 N_τ=8

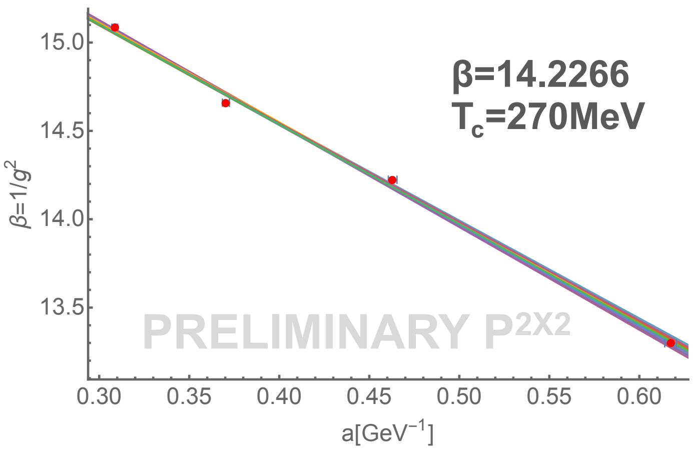
First steps towards quantization

University of Stavanger

- P^{2x2} action in a standard PBC Langevin MC: rough scale setting & beta function



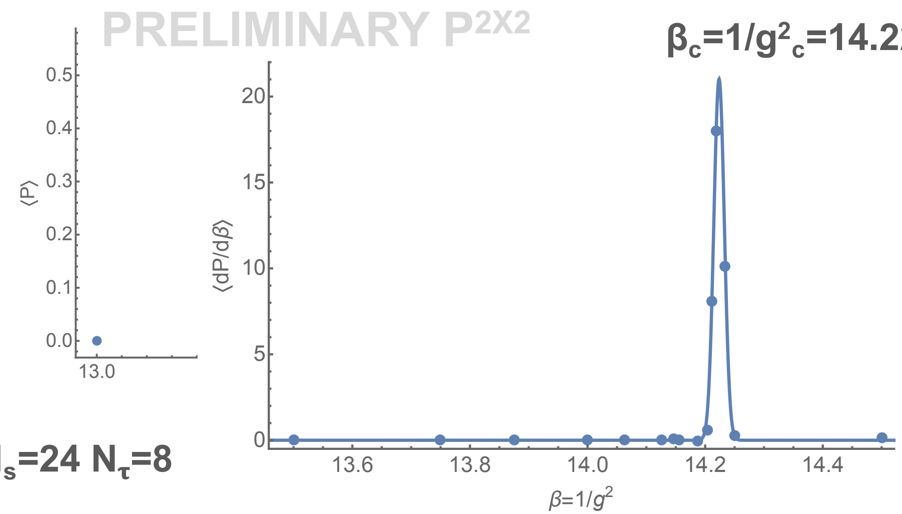
$N_s=24\ N_\tau=8$



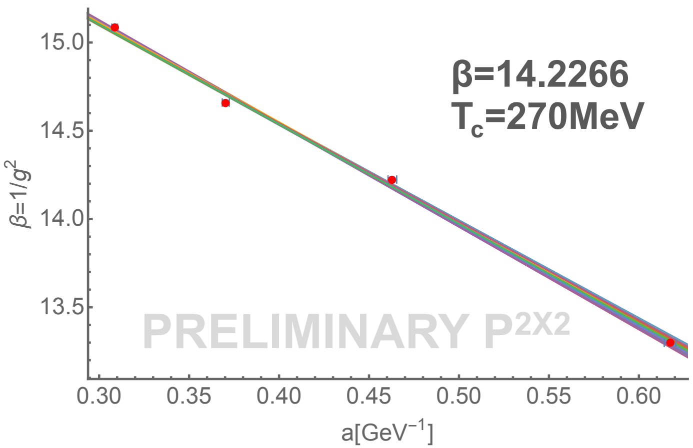
First steps towards quantization

University of Stavanger

- P^{2x2} action in a standard PBC Langevin MC: rough scale setting & beta function



$N_s=24$ $N_\tau=8$

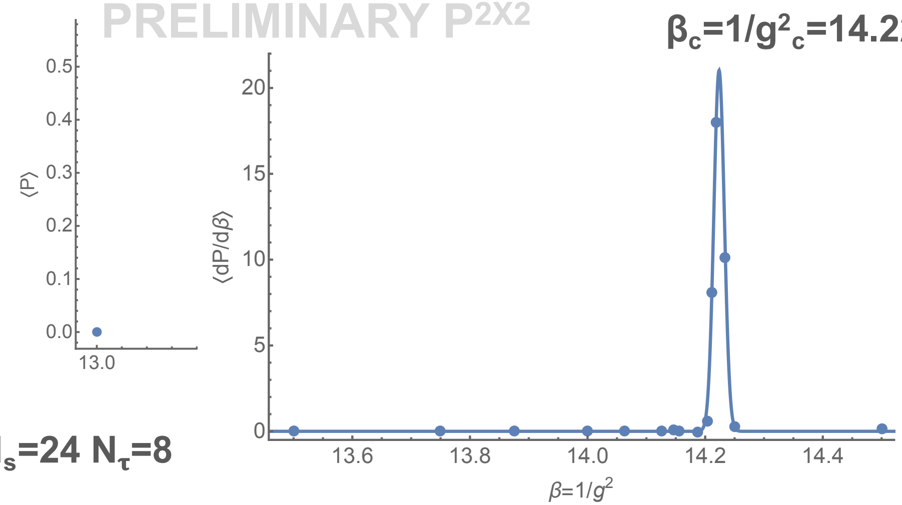


- Thermodynamics via plaquette sums: $$\frac{\varepsilon - 3p}{T^4} = \frac{N_\tau^3}{N_s^3}\left(a\frac{\partial\beta}{\partial a}\right)\left\langle \frac{\partial S}{\partial\beta}\right\rangle$$

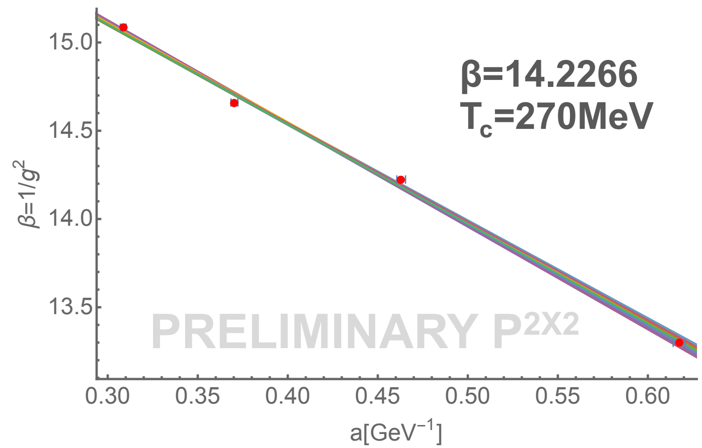
First steps towards quantization

University of Stavanger

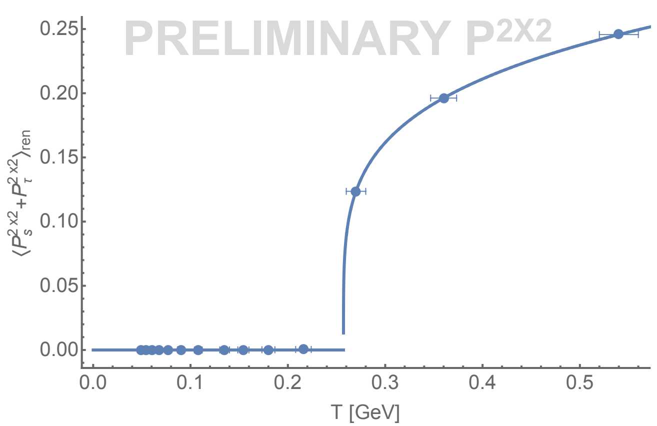
- P^{2x2} action in a standard PBC Langevin MC: rough scale setting & beta function



N_s=24 N_τ=8

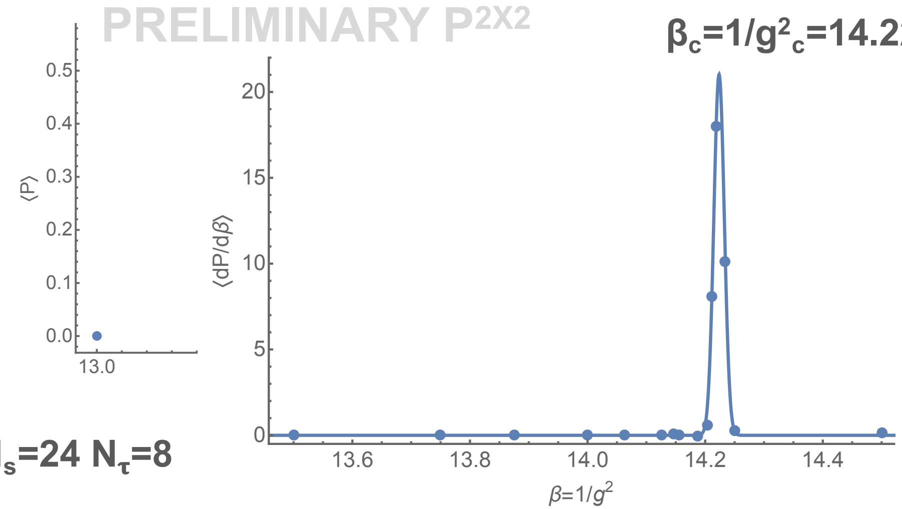


- Thermodynamics via plaquette sums: $$\frac{\varepsilon - 3p}{T^4} = \frac{N_\tau^3}{N_s^3}\left(a\frac{\partial\beta}{\partial a}\right)\left\langle\frac{\partial S}{\partial\beta}\right\rangle$$

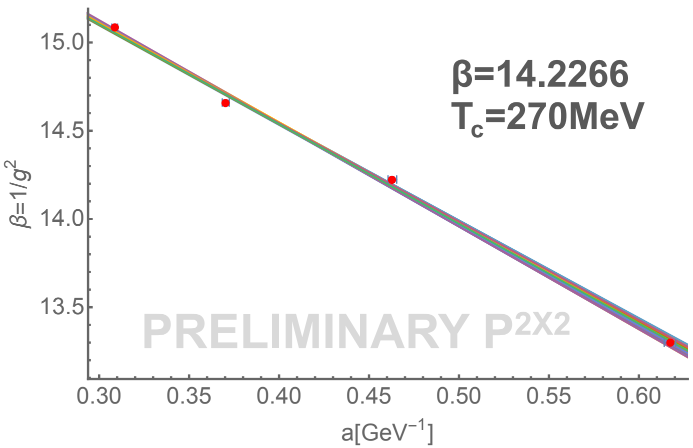


First steps towards quantization

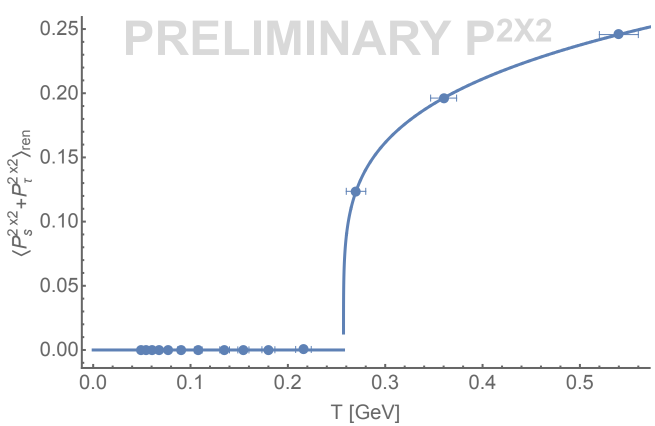
- P^{2x2} action in a standard PBC Langevin MC: rough scale setting & beta function

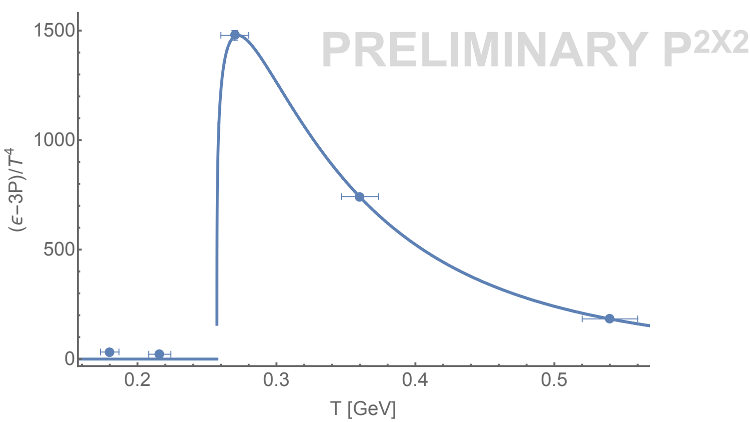


N_s=24 N_τ=8



- Thermodynamics via plaquette sums: $$\frac{\varepsilon - 3p}{T^4} = \frac{N_\tau^3}{N_s^3}\left(a\frac{\partial\beta}{\partial a}\right)\left\langle\frac{\partial S}{\partial\beta}\right\rangle$$

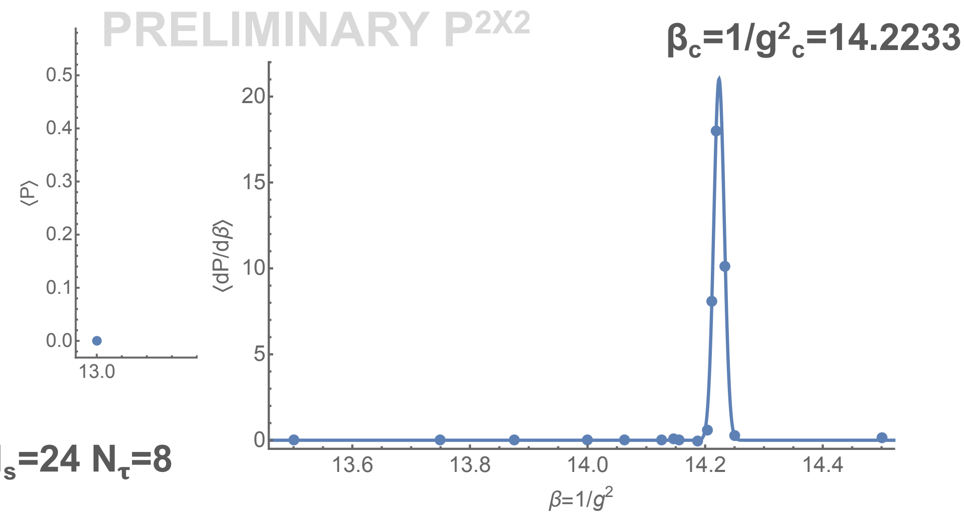




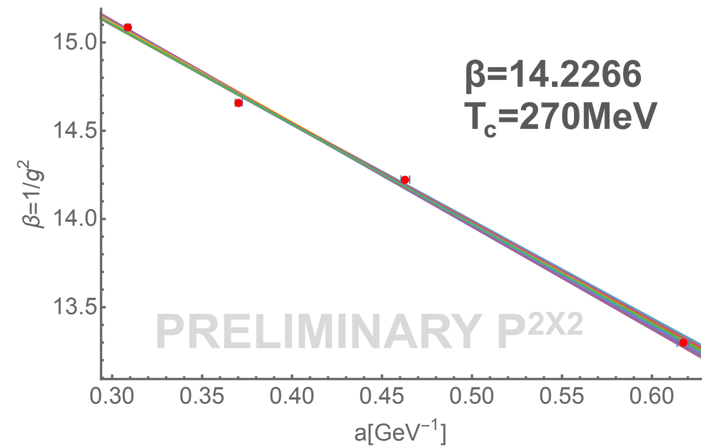
First steps towards quantization

University of Stavanger

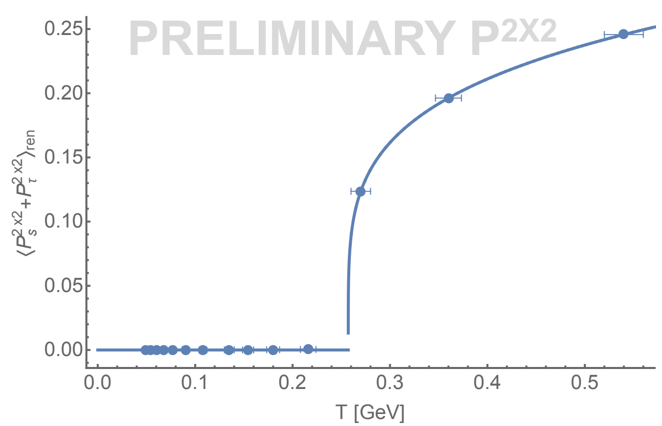
- P^{2x2} action in a standard PBC Langevin MC: rough scale setting & beta function

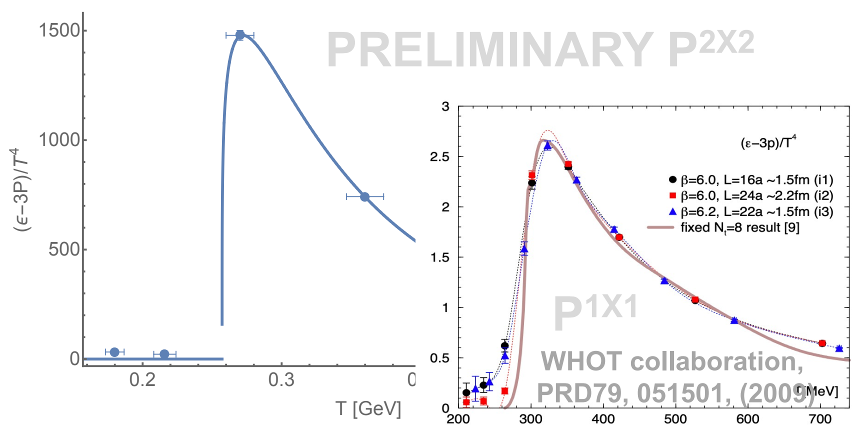


$N_s=24$ $N_\tau=8$



- Thermodynamics via plaquette sums: $$\frac{\varepsilon-3p}{T^4}=\frac{N_\tau^3}{N_s^3}\left(a\frac{\partial\beta}{\partial a}\right)\left\langle\frac{\partial S}{\partial\beta}\right\rangle$$



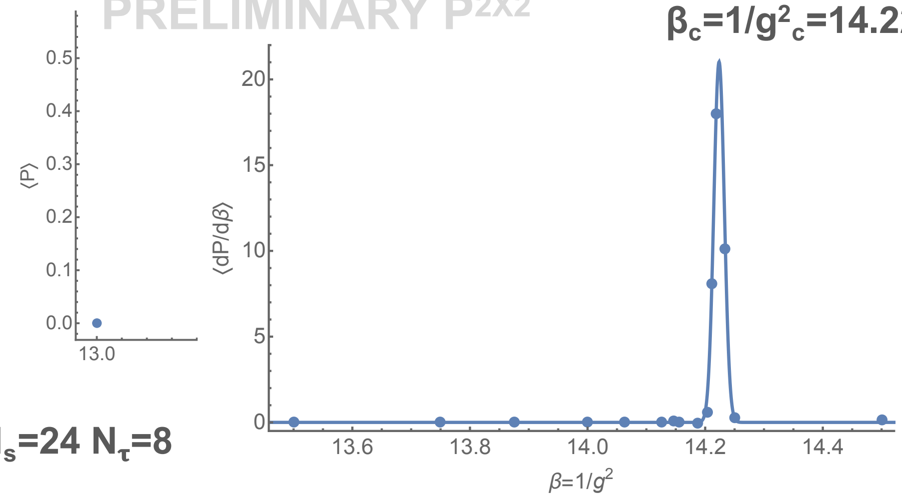


First steps towards quantization

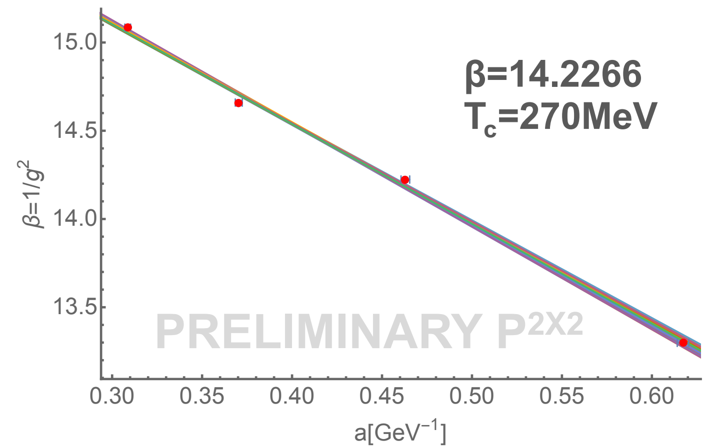
University of Stavanger

- P^{2x2} action in a standard PBC Langevin MC: rough scale setting & beta function

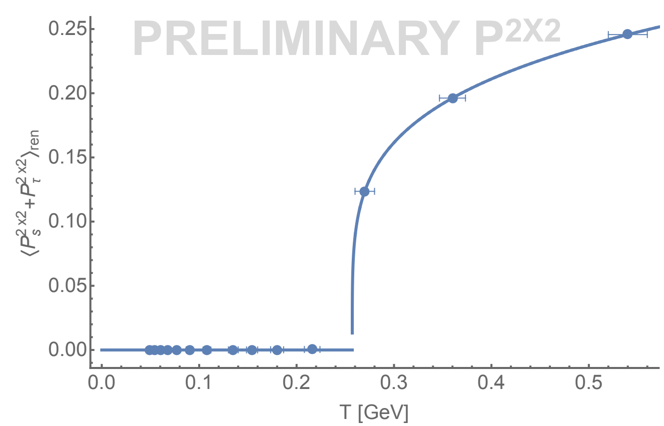
$\beta_c=1/g^2_c=14.2233$



N_s=24 N_τ=8



- Thermodynamics via plaquette sums: $$\frac{\varepsilon-3p}{T^4}=\frac{N_\tau^3}{N_s^3}\left(a\frac{\partial\beta}{\partial a}\right)\left\langle\frac{\partial S}{\partial\beta}\right\rangle$$



What about normalization?