

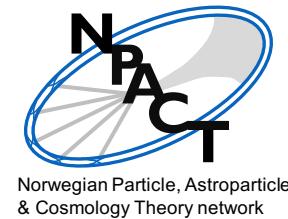
Towards symmetric discretization schemes via weak boundary conditions



Alexander Rothkopf

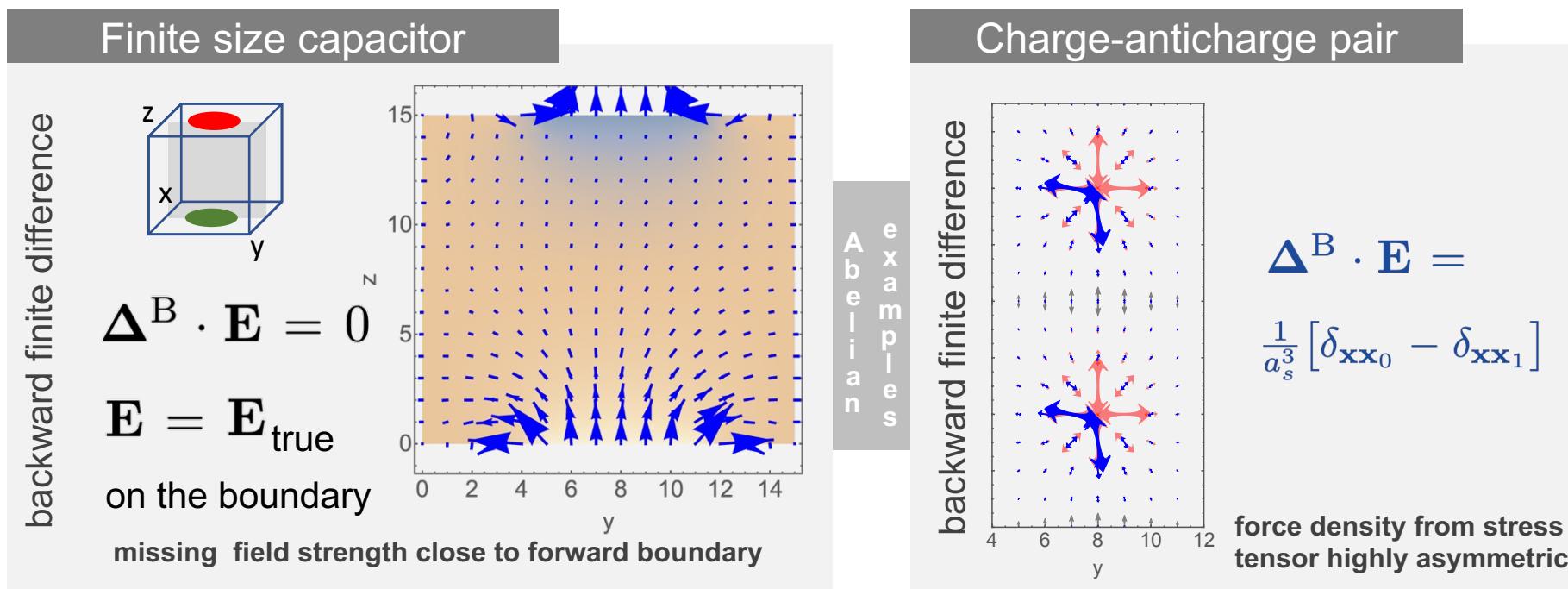
Faculty of Science and Technology
Department of Mathematics and Physics
University of Stavanger

based on: A.R. and J. Nordström [arXiv:2205.14028](https://arxiv.org/abs/2205.14028)
motivated by A.R. [arXiv:2102.08616](https://arxiv.org/abs/2102.08616)



Motivation

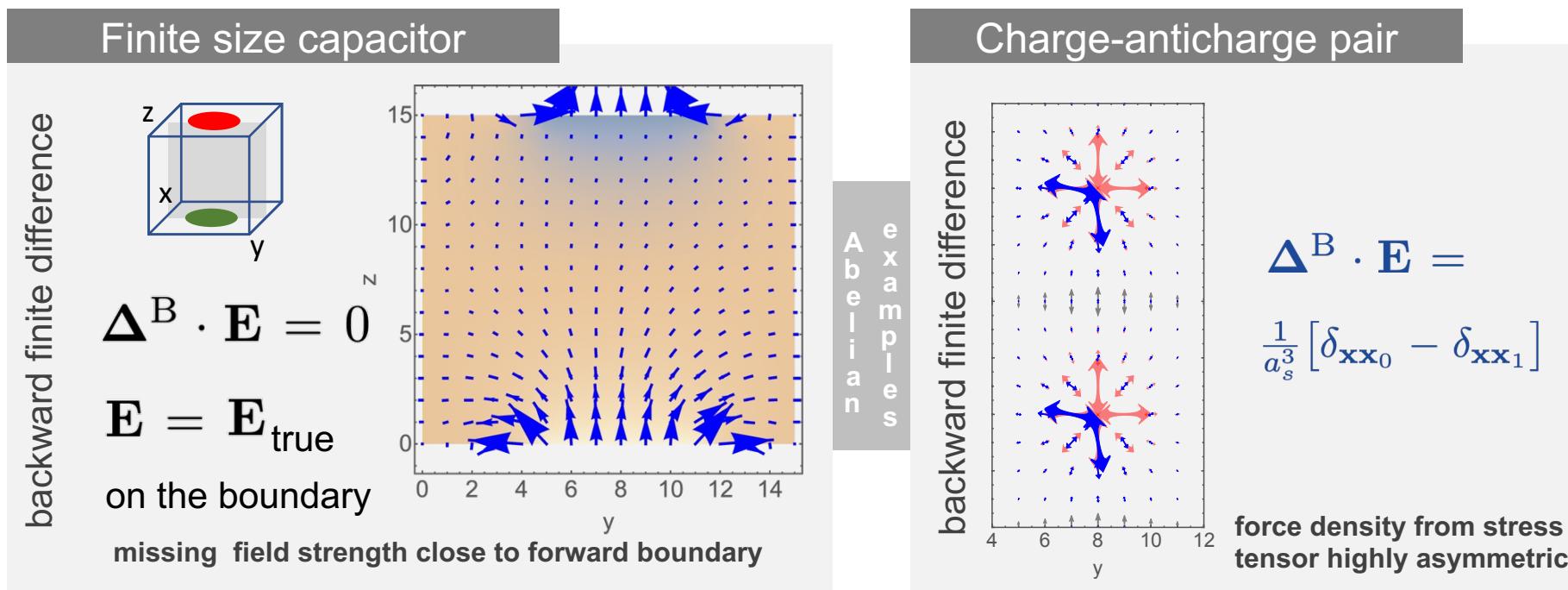
- Systems without translational invariance: **finite extent or presence of sources**
small system collisions at LHC, strong coupling cavity QED, quarkonium real-time dynamics ...
- Classical Wilson action corresponds to a **backward finite difference** Gauss-law



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

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

Symanzik's improvement program

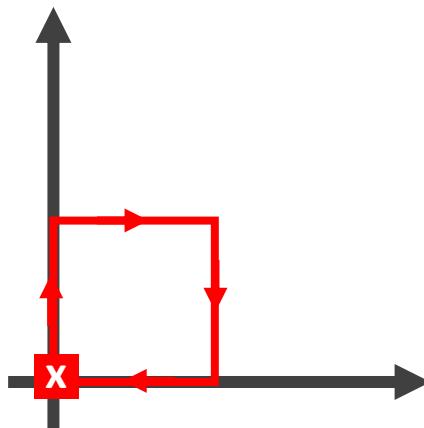
- Starting point is the Wilson plaquette action with forward finite differences

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

$$P_{\mu\nu,x}^{1\times 1} = U_{\mu,x} U_{\nu,x+a_\mu \hat{\mu}} U_{\mu,x+a_\nu \hat{\nu}}^\dagger U_{\nu,x}^\dagger = e^{ia_\mu a_\nu \tilde{F}_{\mu\nu,x}} + \mathcal{O}(a^2)$$

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

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



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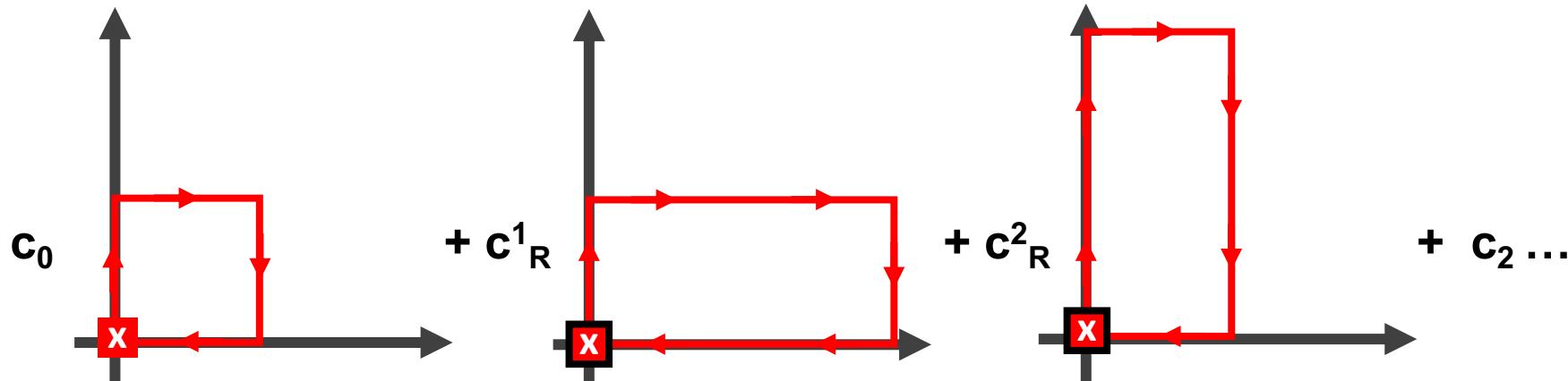
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- Improvement deployed in modern actions: higher order forward finite differences

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



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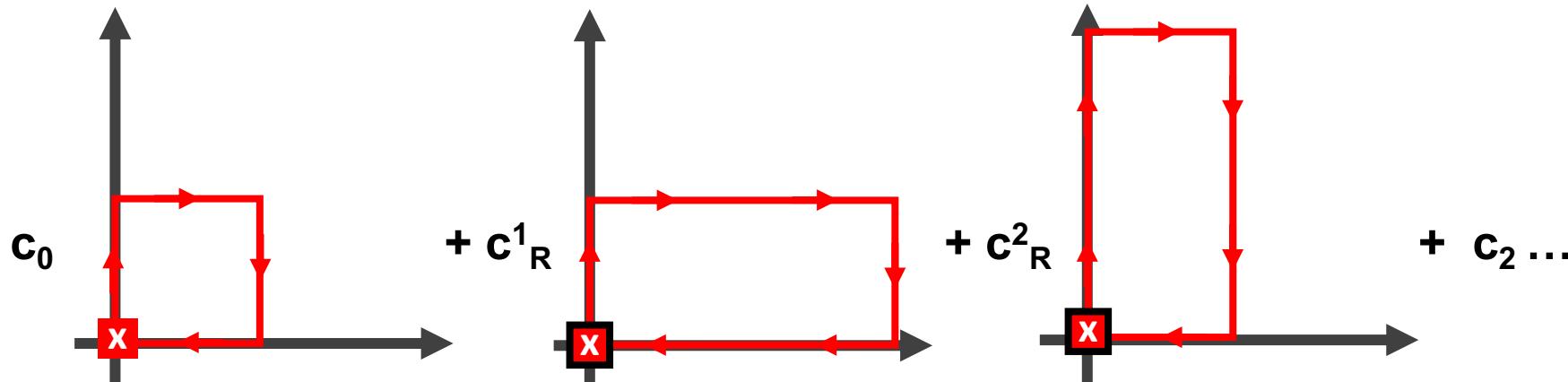
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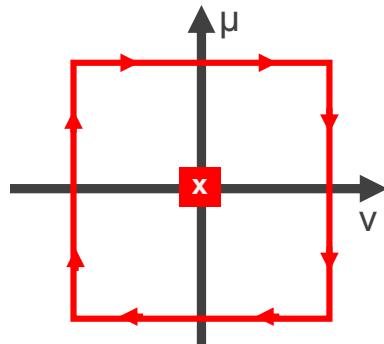
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- Does not realize a symmetric discretization of field strength around charges

A naïve symmetric discretization

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



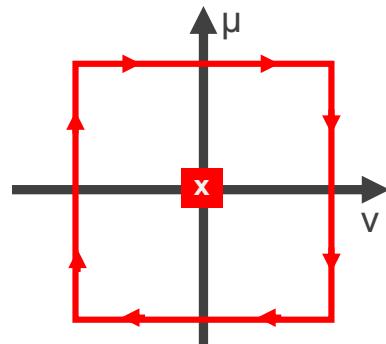
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$$\begin{aligned}
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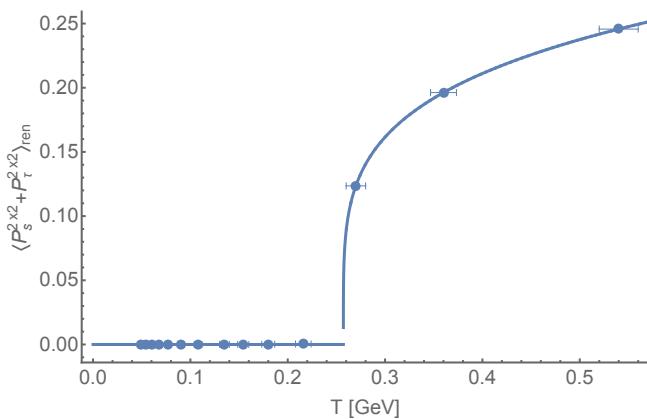


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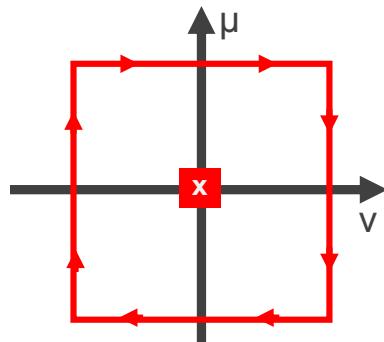
- Qualitatively consistent but trace anomaly too large



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

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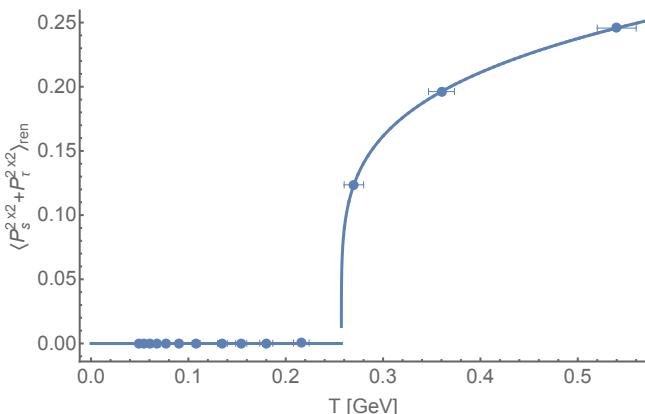


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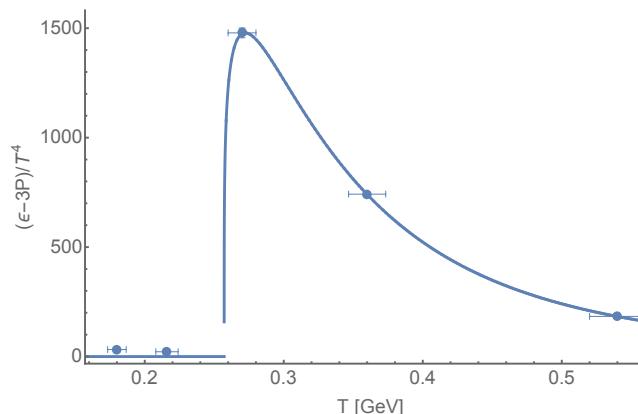
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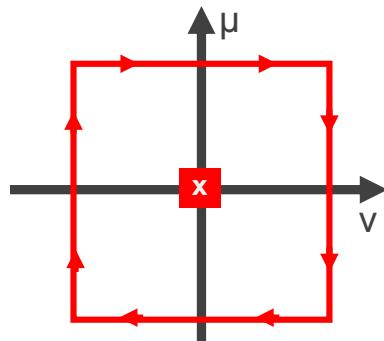


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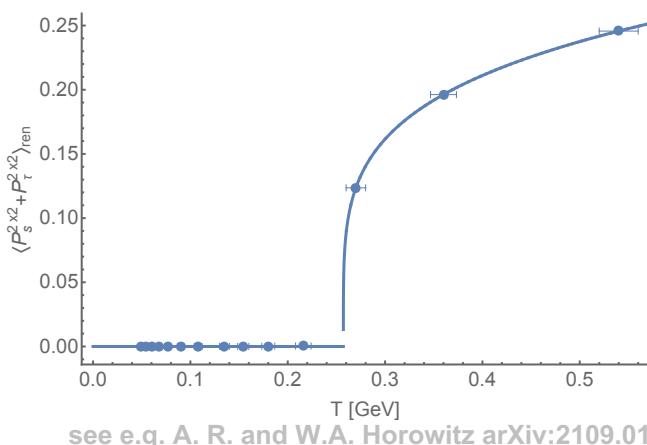


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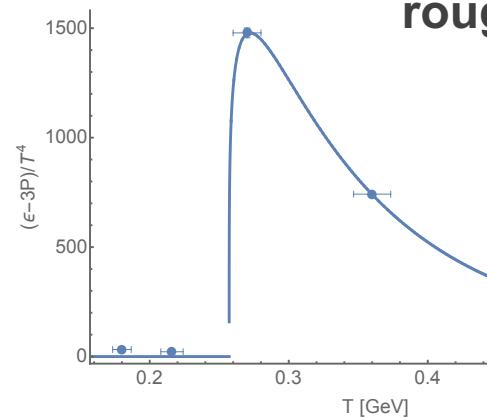
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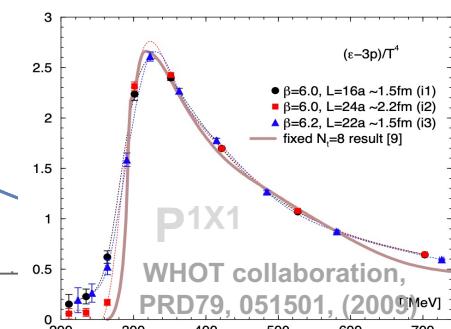
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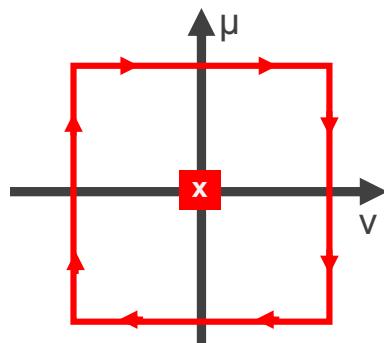


rougly factor 4x8x15



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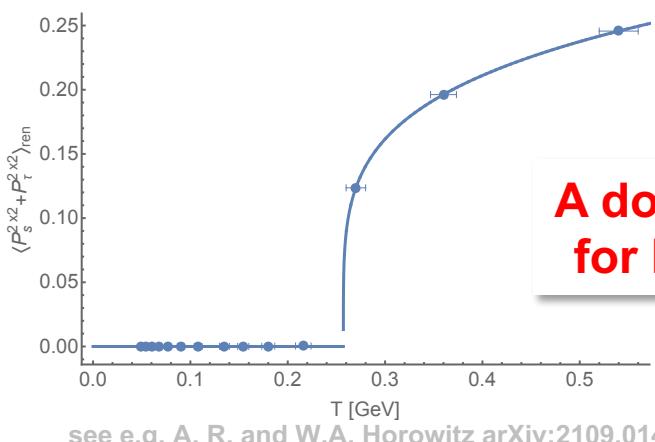


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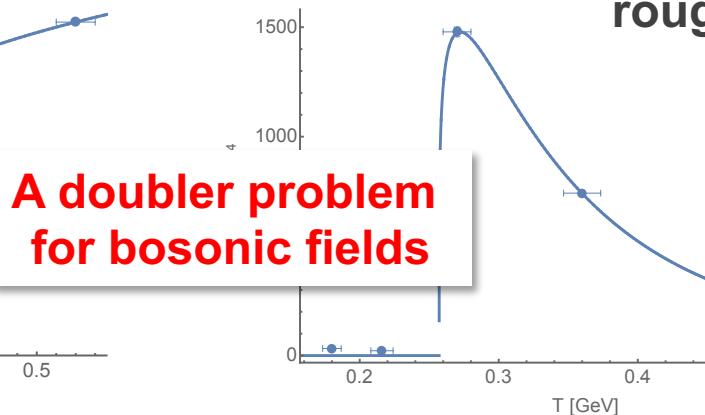
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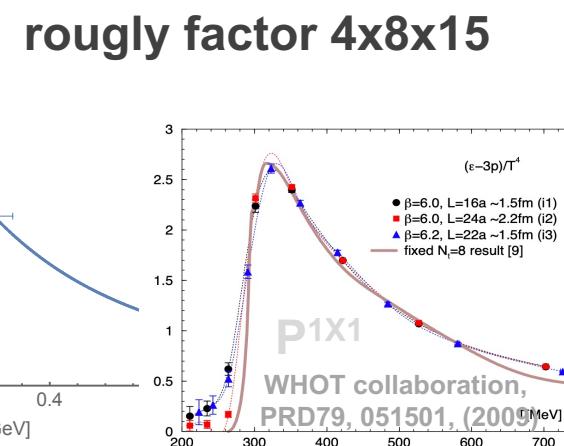
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A doubler problem for bosonic fields



Doublers and the Wilson term

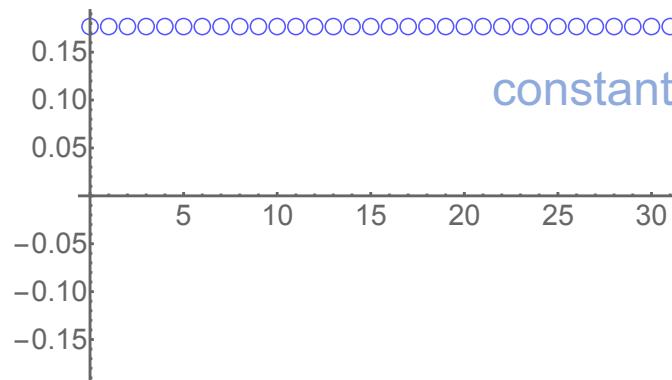
- Problem already apparent in finite difference schemes in one dimension

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

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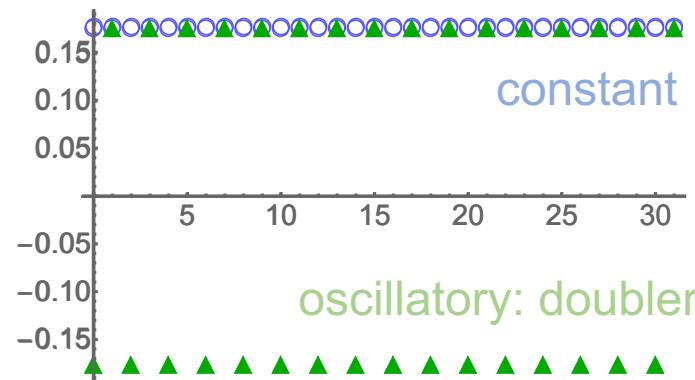


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zero eigenvalue eigenfunctions of D^C and $(D^C)^t$ distinct

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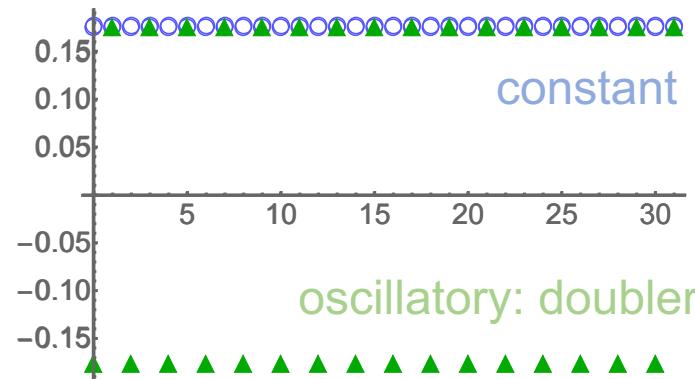


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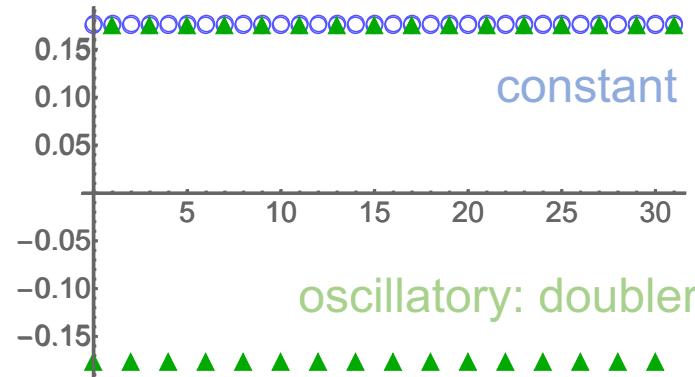
upwind modification

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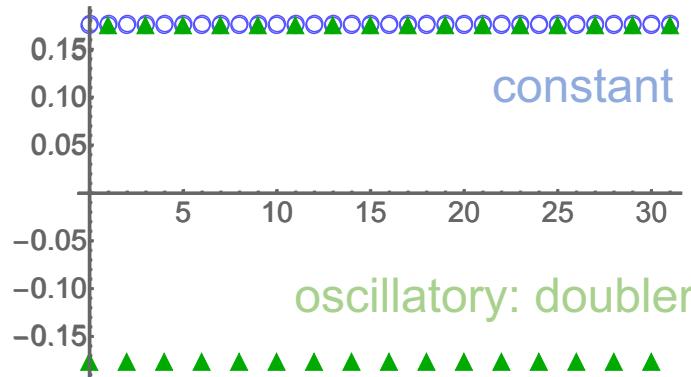
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Wilson term

- 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

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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)

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- For ODEs / PDEs well established (penalty term from boundary data):
see e.g. Lundquist, T., Nordström J., JCP 270, 86–104 (2014)

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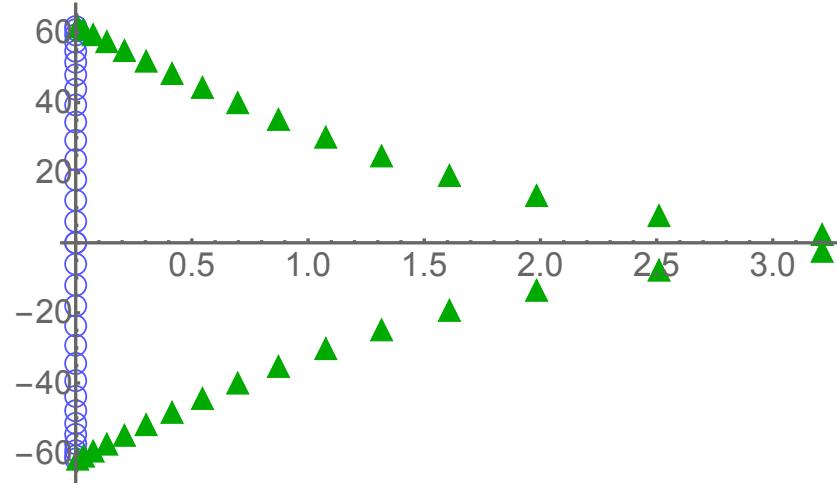
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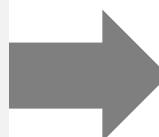
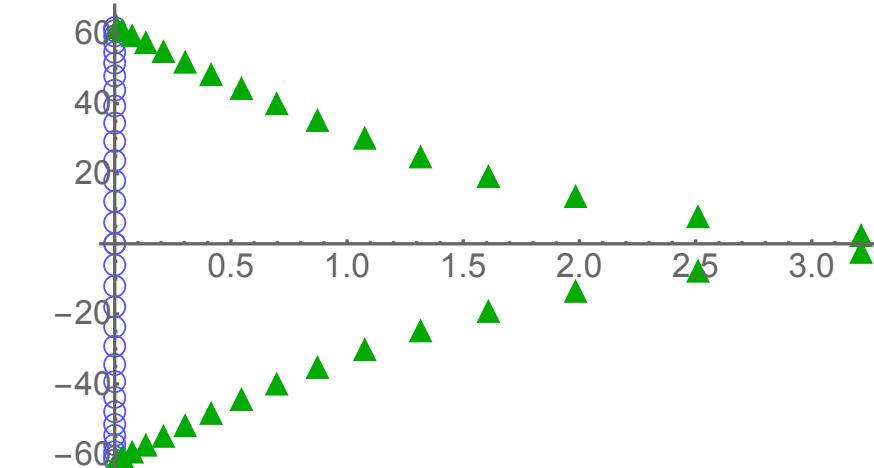
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$$\tilde{D}\mathbf{u} = \mathbf{g} - \frac{1}{a} E_0 \mathbf{u}_0$$

invertible \tilde{D} and modified inhomogeneous RHS

Introducing boundary data in the action

- In lattice applications (both classical statistical & path integral) action is central
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Introducing boundary data in the action

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- In an action we do not have an “=” sign to move boundary terms around

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A. Rothkopf, J. Nordström, arXiv:2205.14028

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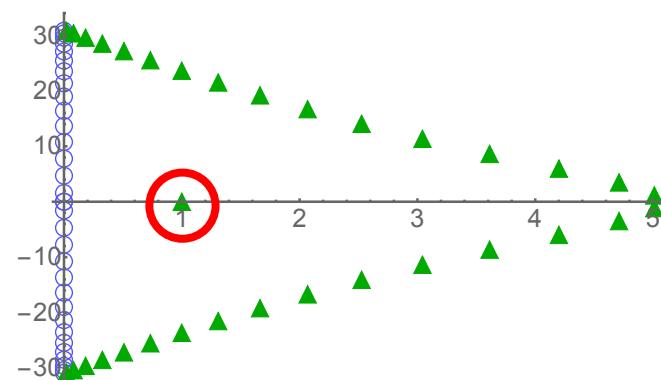
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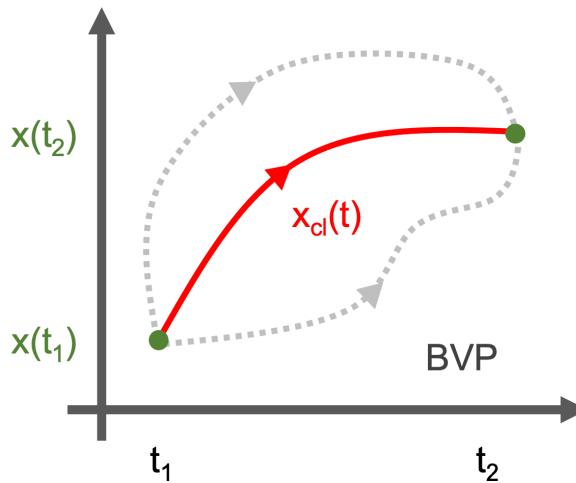
- + all zero modes are lifted
- + physical constant mode with correct boundary behavior now as unit EV

Application to initial value problems (IVP)

- Long term goal: gauge invariant real-time quantum dynamics of QCD
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IVP challenge: standard $\delta S[x,v]/\delta x(t)=0$ only as boundary value problem

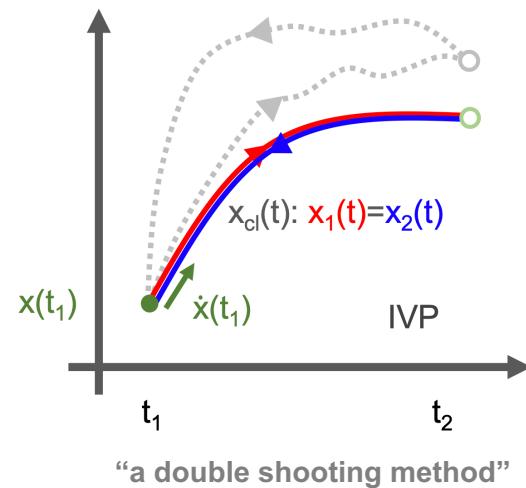
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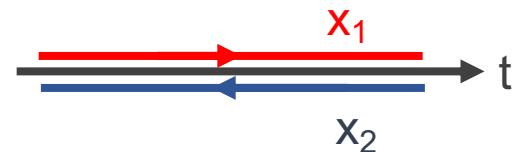
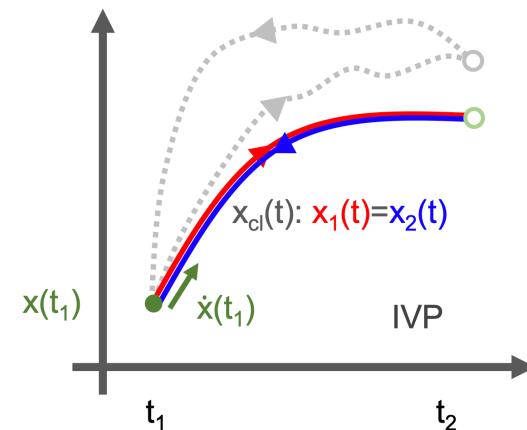


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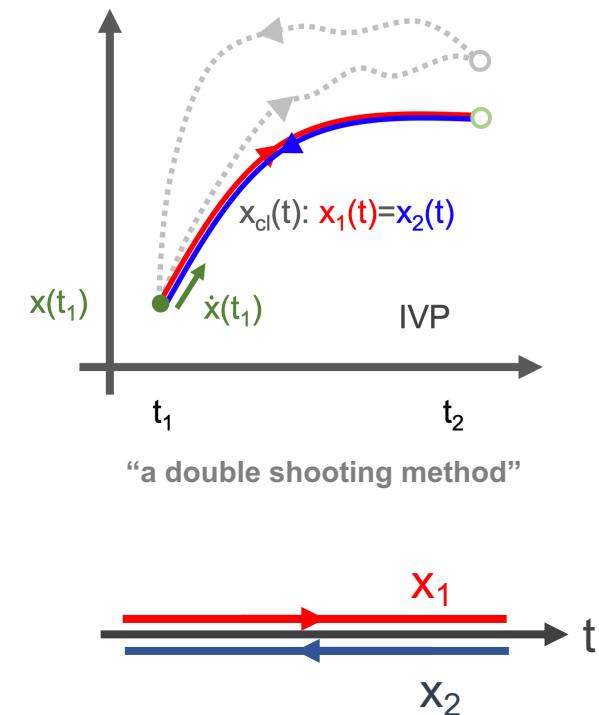
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$$x_- = x_1 - x_2$$

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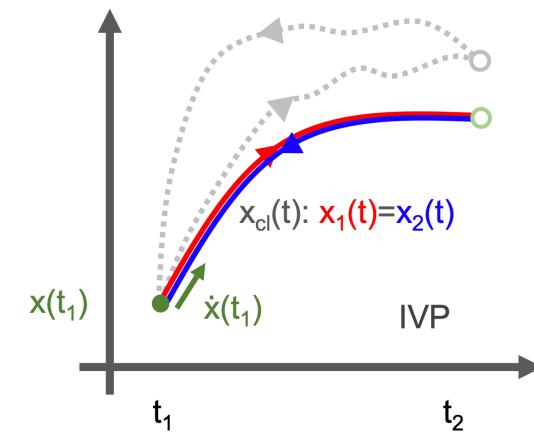


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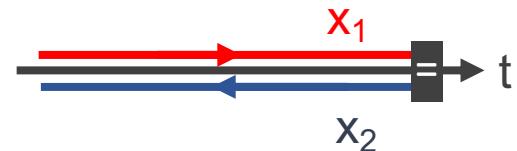
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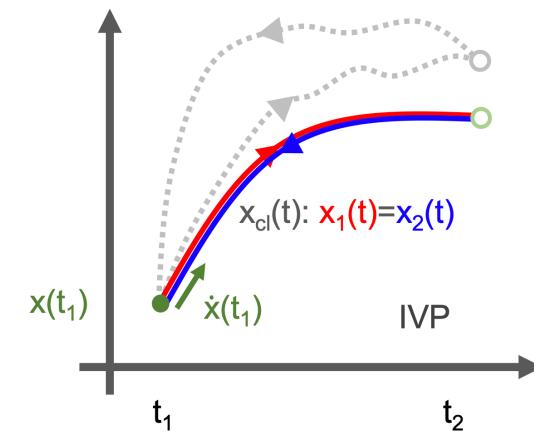
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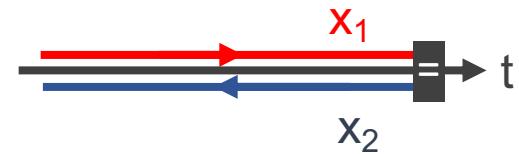
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$$\frac{\delta S_{\text{IVP}}[x_\pm]}{\delta x_-} \Big|_{x_-=0, x_+=x_{\text{class}}} = 0$$



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Implementation with Lagrange multipliers

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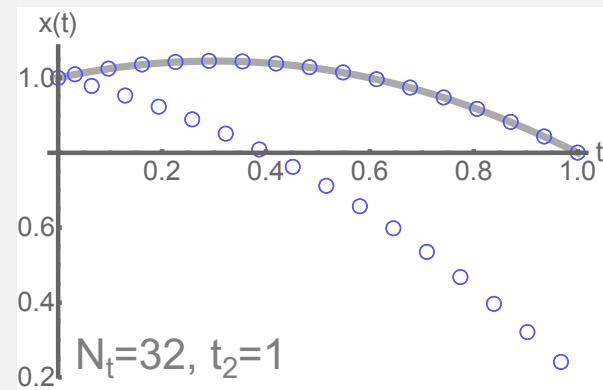
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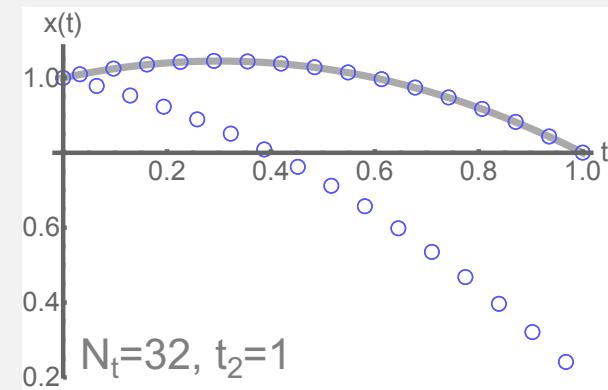
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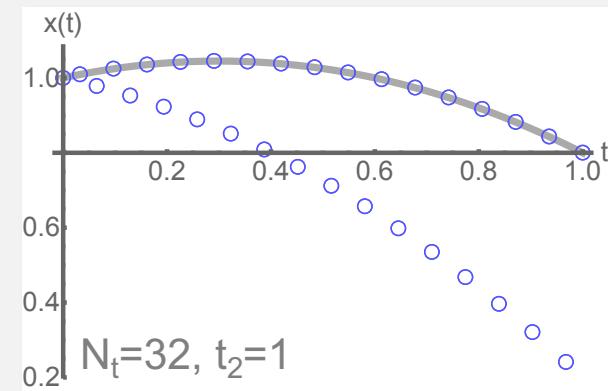
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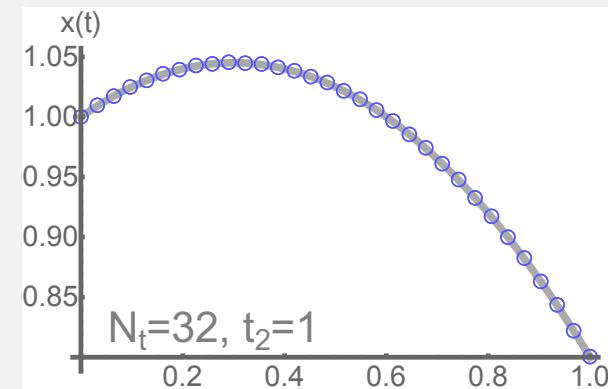
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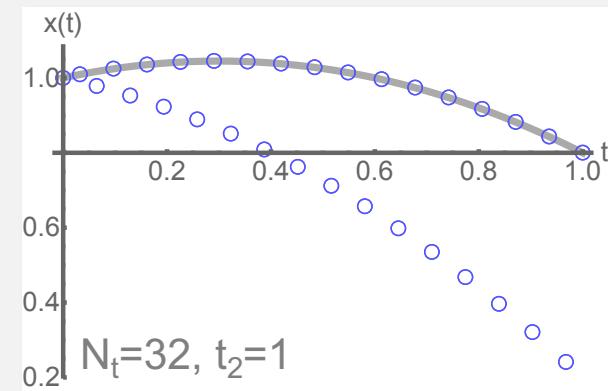
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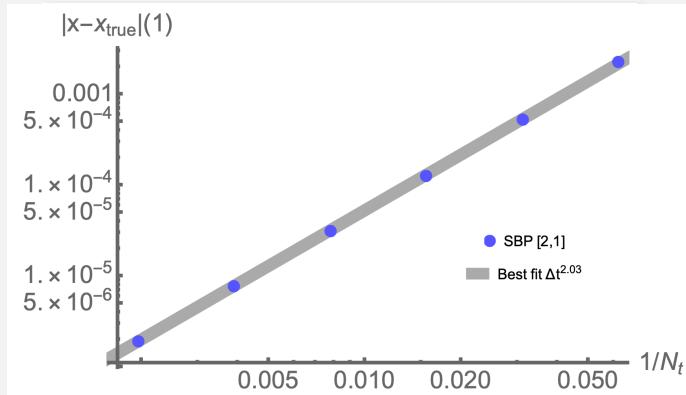


Regularization with initial value data

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

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

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



Conclusion & Outlook

- 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**
- 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)

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

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

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

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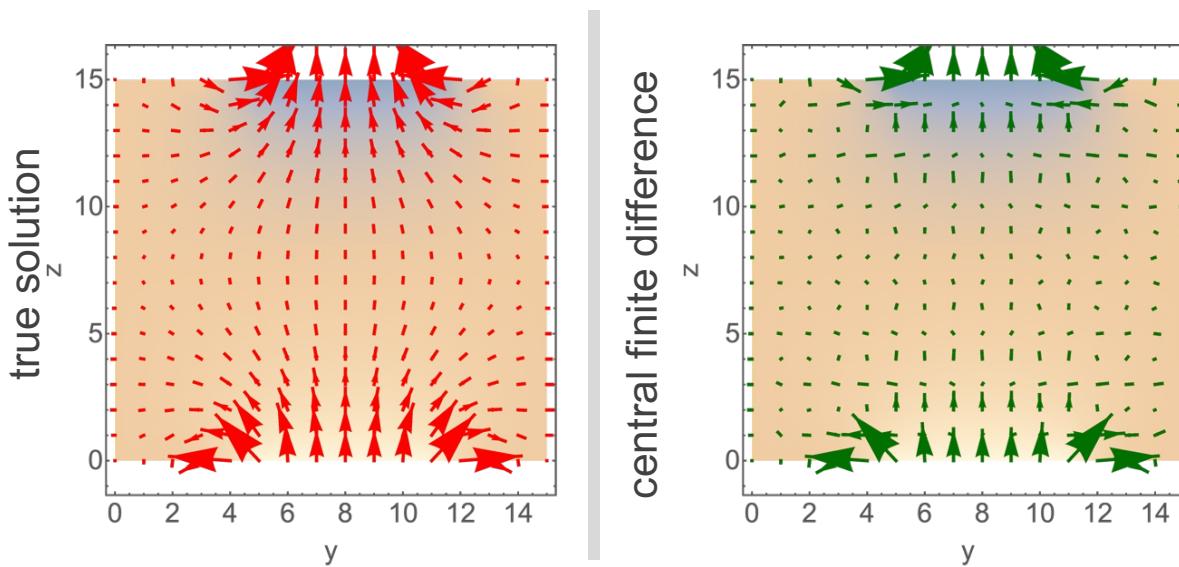
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- Central finite difference on interior not enough, need genuine SBP form of FD



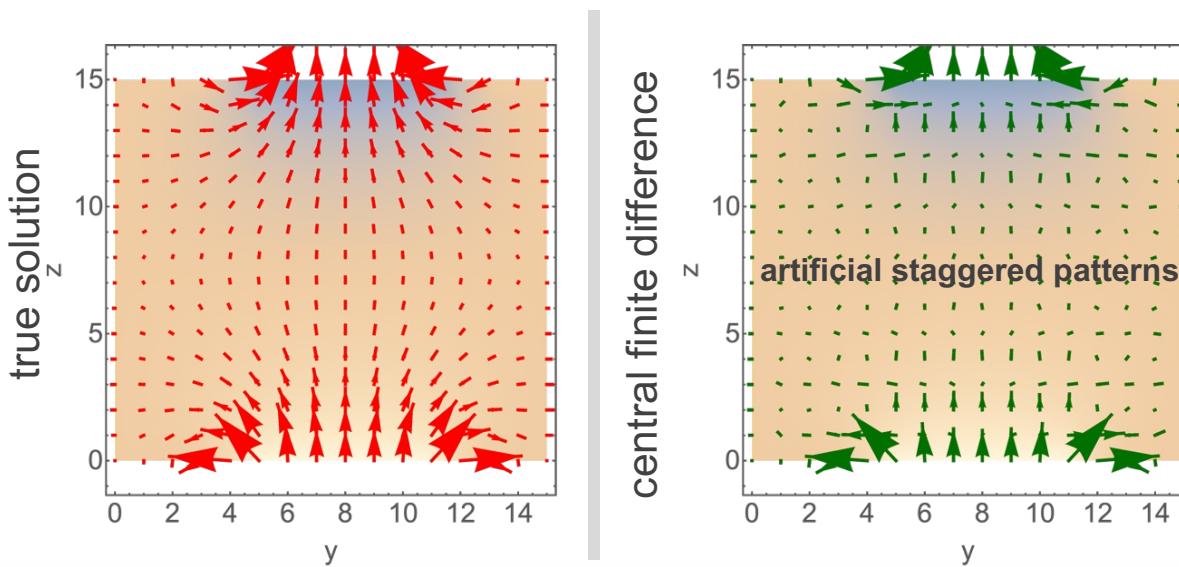
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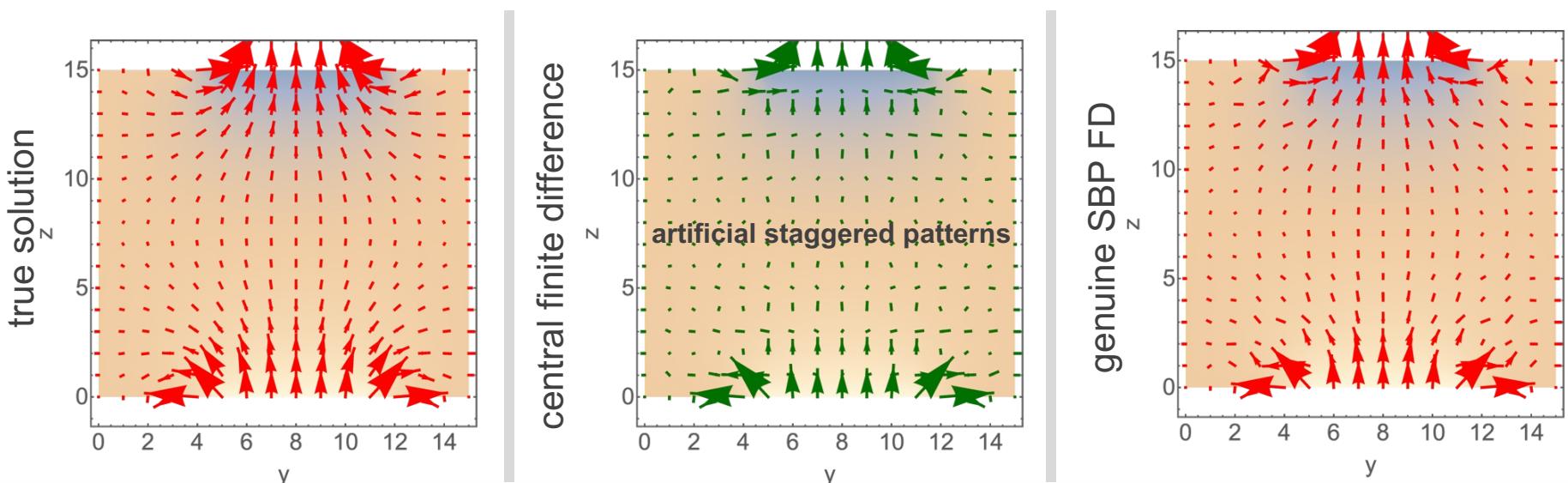
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Challenge II

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

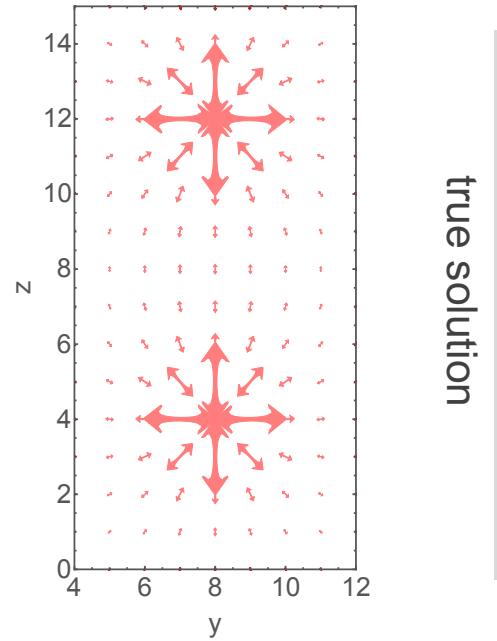
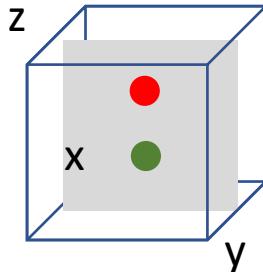
$$\Theta^{ij} = \frac{1}{4\pi} (g^{i\mu} F_{\mu\lambda} F^{\lambda j} + \frac{1}{4} g^{ij} F_{\mu\lambda} F^{\mu\lambda}) \quad \mathbf{f} = \nabla \cdot \boldsymbol{\Theta} + \partial \mathbf{S} / \partial t$$

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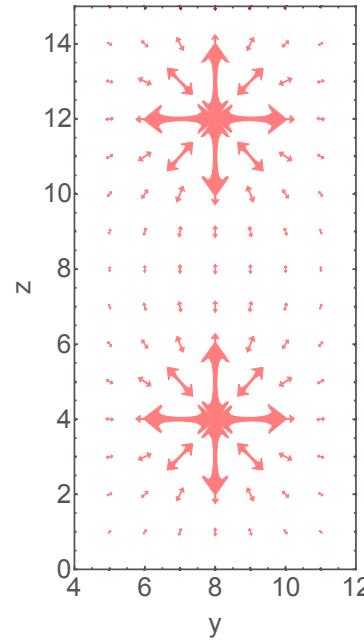
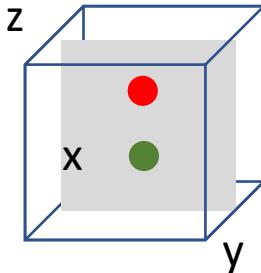
true solution

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true solution backward finite difference

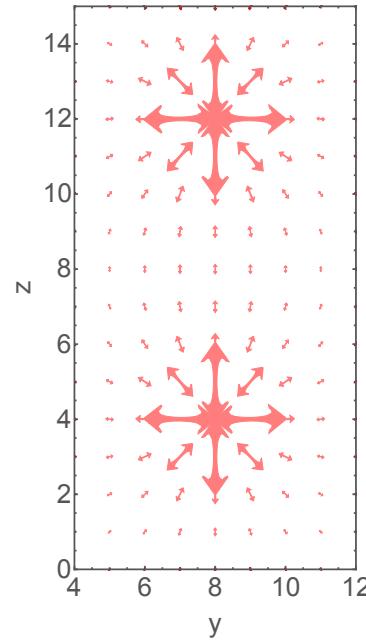
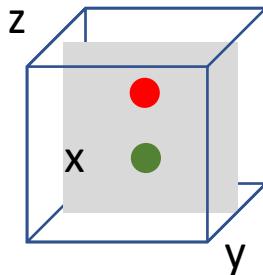
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Challenge II

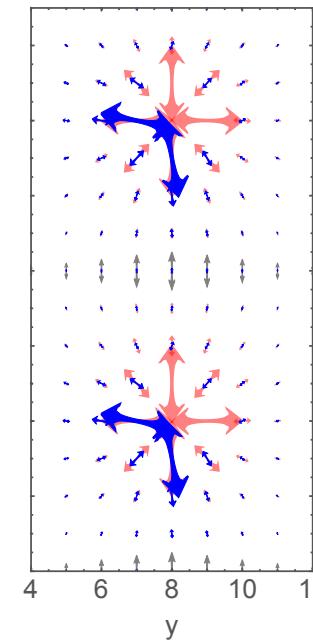
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true solution
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- Need a symmetric discretization, but naïve central finite differences do not respect the integral form of the Gauss law

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

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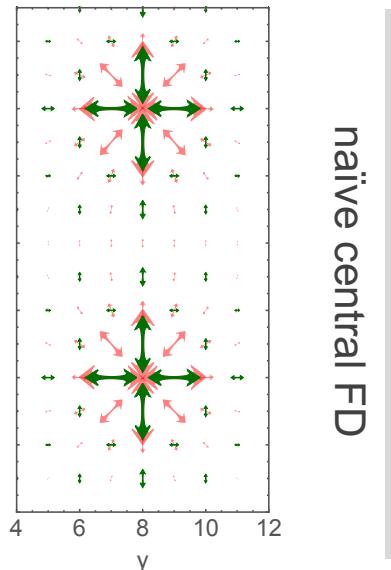
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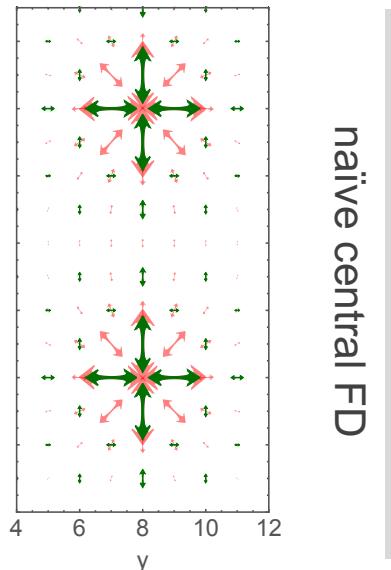
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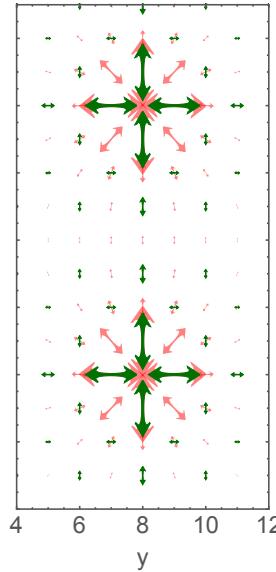
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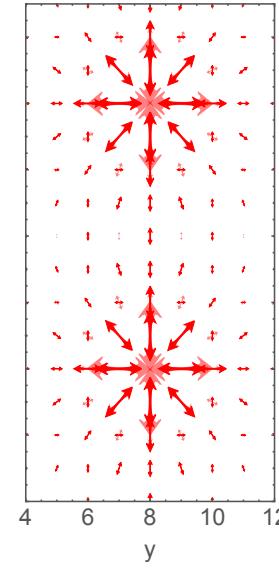
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naïve central FD



finite volume central FD

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

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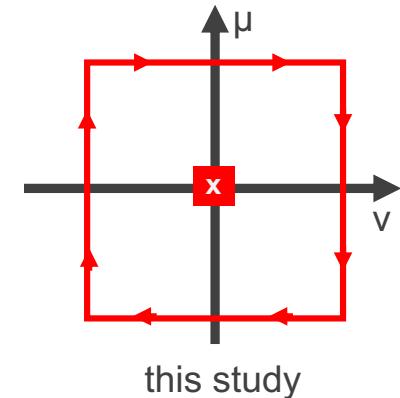
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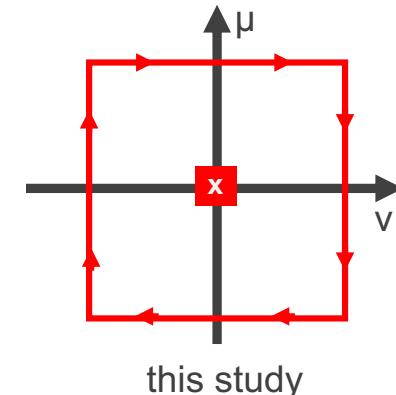
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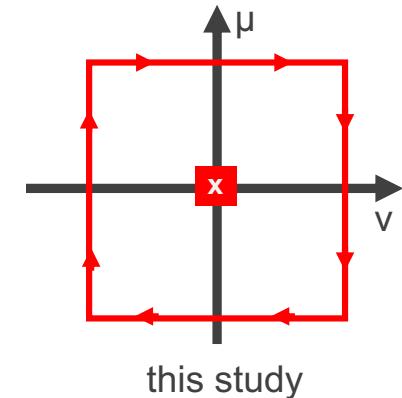
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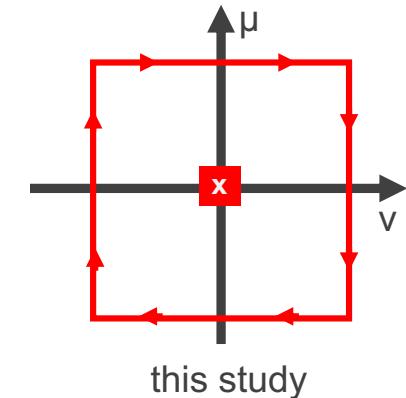
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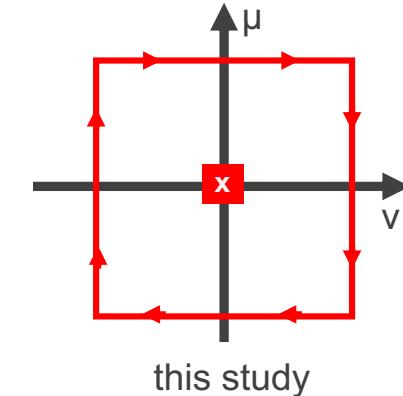
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Szymanzik program:
 $P^{1\times 1} + P^{1\times 2} + P^{2\times 2} + \dots$ (not SBP)

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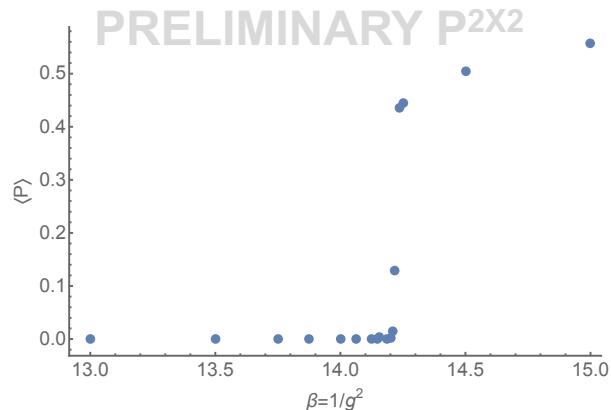
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$$\tilde{F}_{\mu\nu,x} = \Delta_\mu^{\text{SBP}} A_{\nu,x} - \Delta_\nu^{\text{SBP}} A_{\mu,x} + i[A_{\mu,x}, A_{\nu,x}]$$

First steps towards quantization

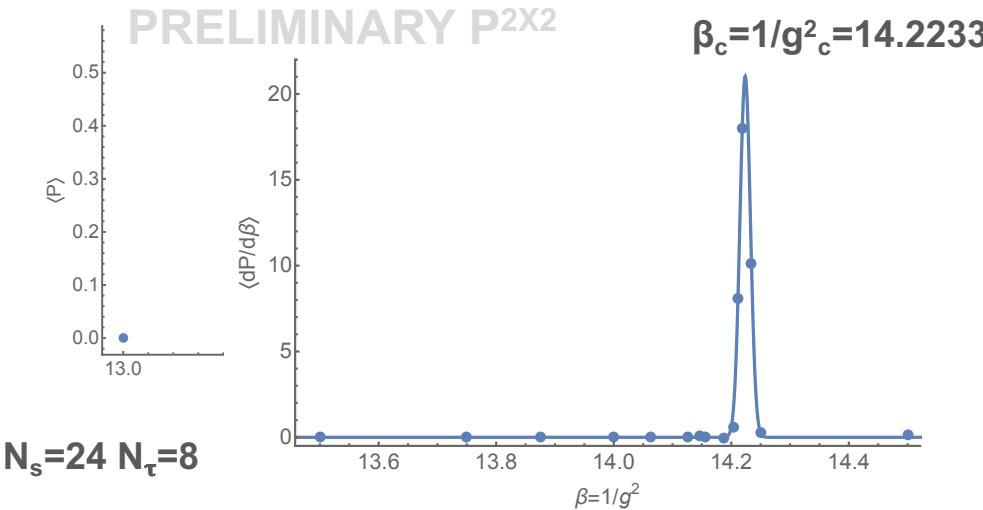
- P^{2x2} action in a standard PBC Langevin MC: rough scale setting & beta function



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

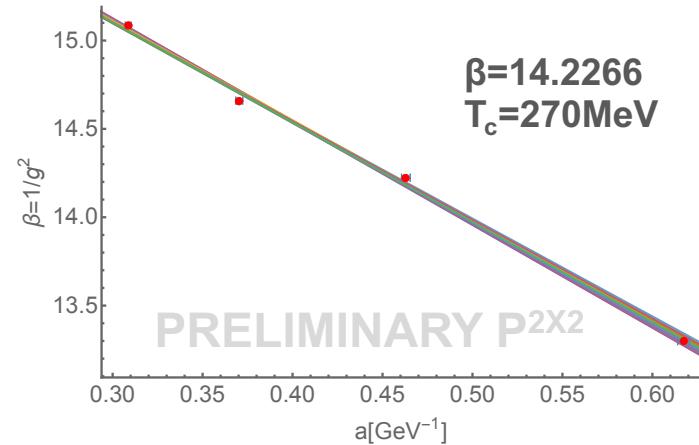
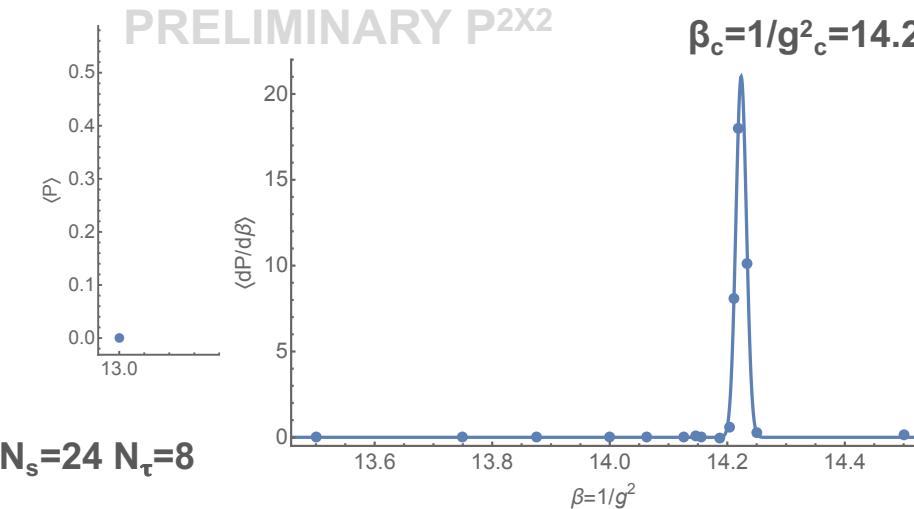
First steps towards quantization

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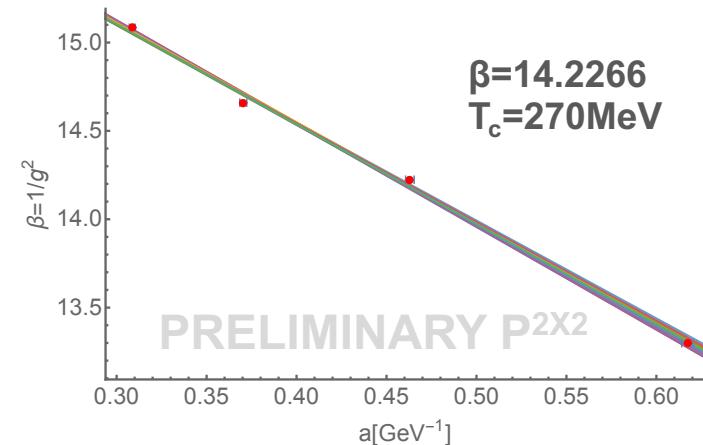
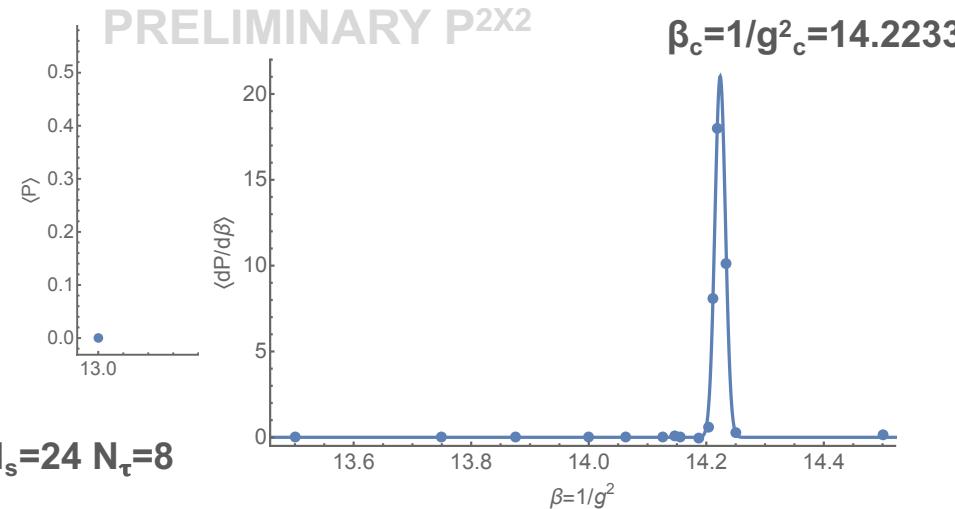
First steps towards quantization

- P²x2 action in a standard PBC Langevin MC: rough scale setting & beta function



First steps towards quantization

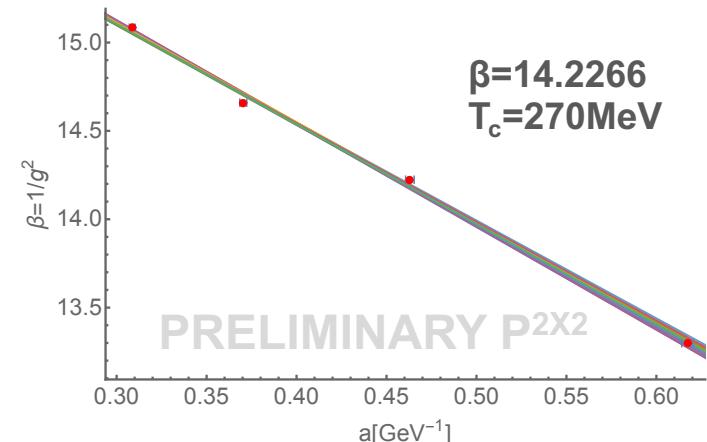
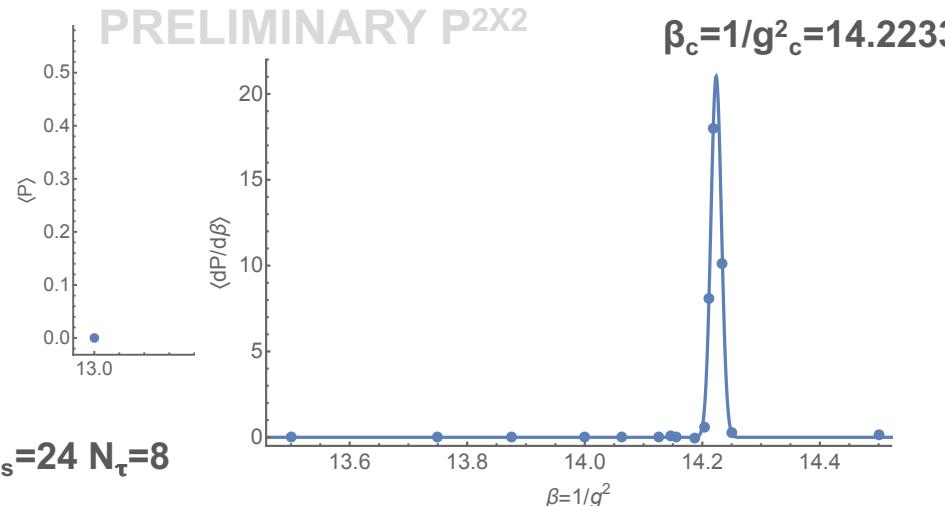
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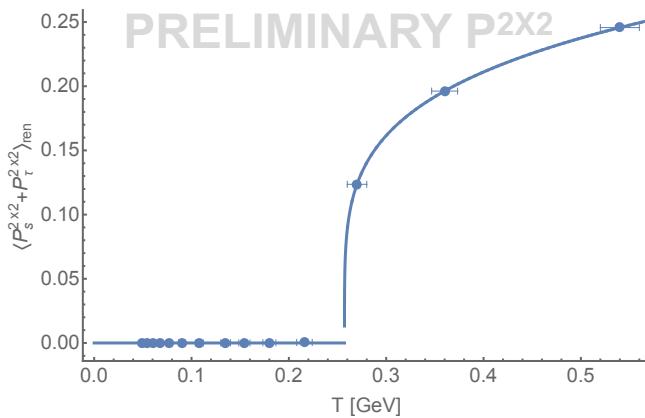
- Thermodynamics via plaquette sums:
$$\frac{\varepsilon - 3p}{T^4} = \frac{N_\tau^3}{N_s^3} \left(a \frac{\partial \beta}{\partial a} \right) \left\langle \frac{\partial S}{\partial \beta} \right\rangle$$

First steps towards quantization

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

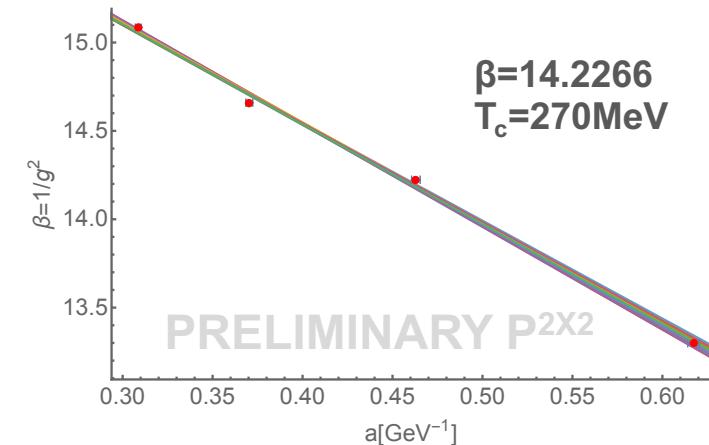
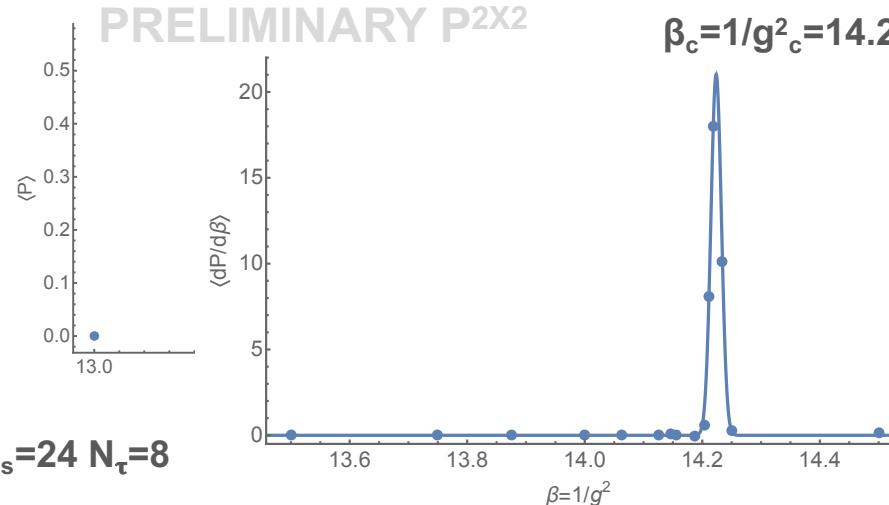


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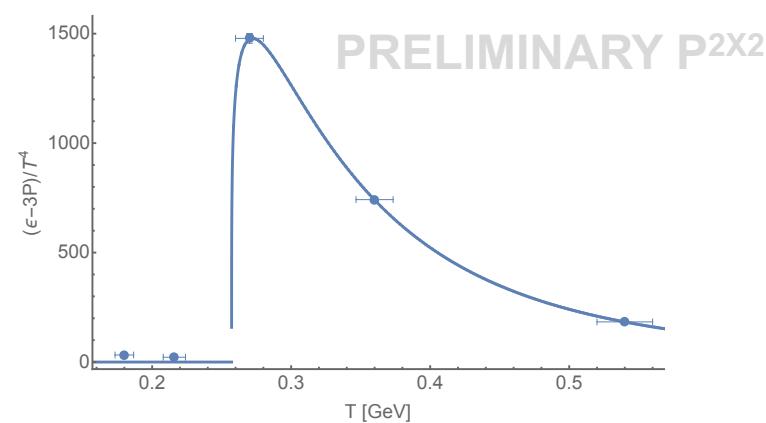
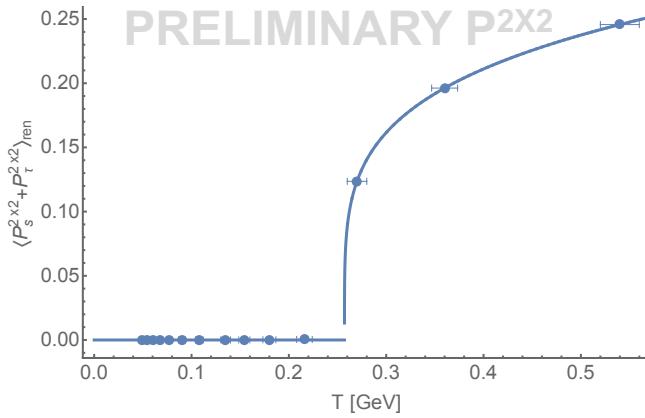


First steps towards quantization

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

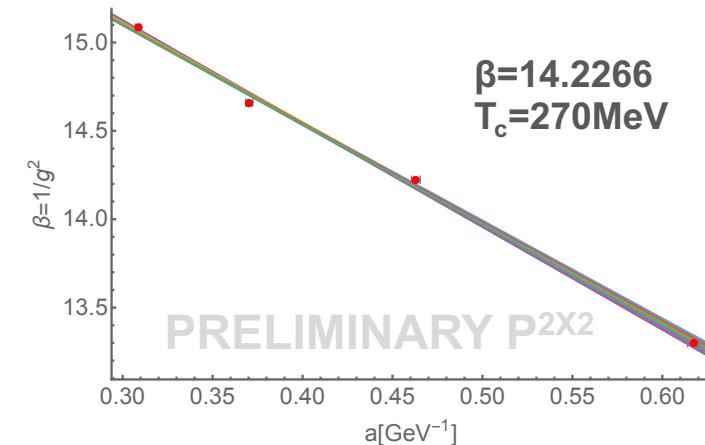
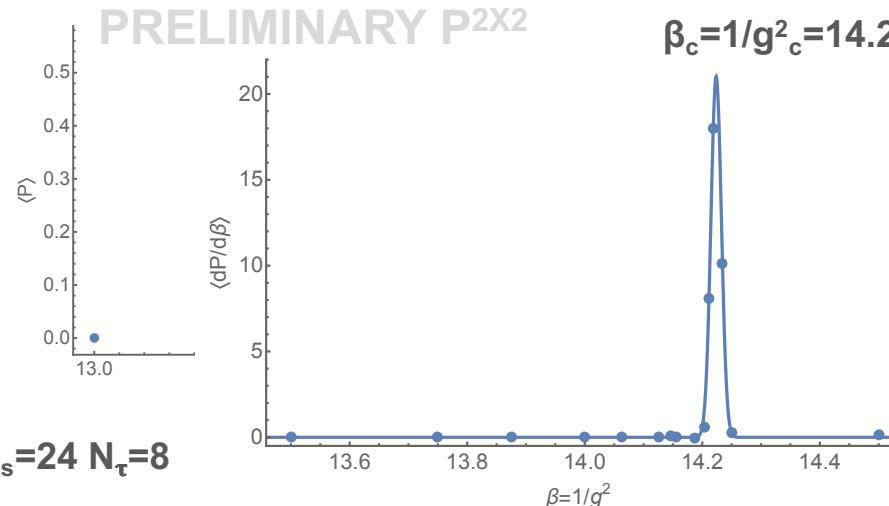


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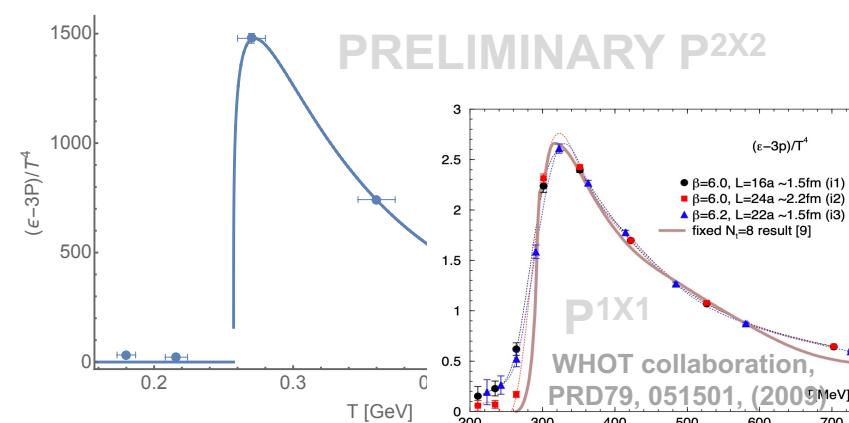
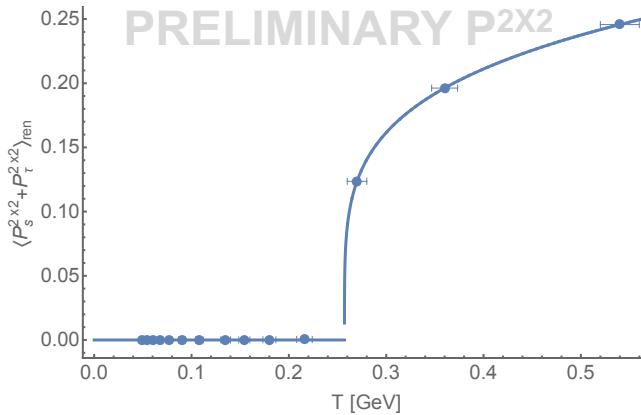


First steps towards quantization

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

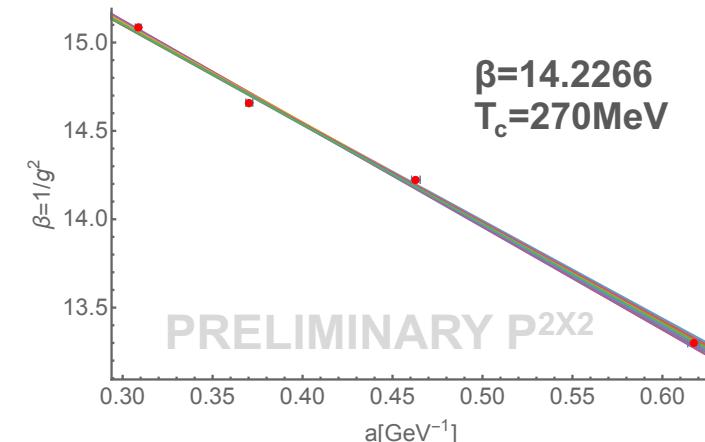
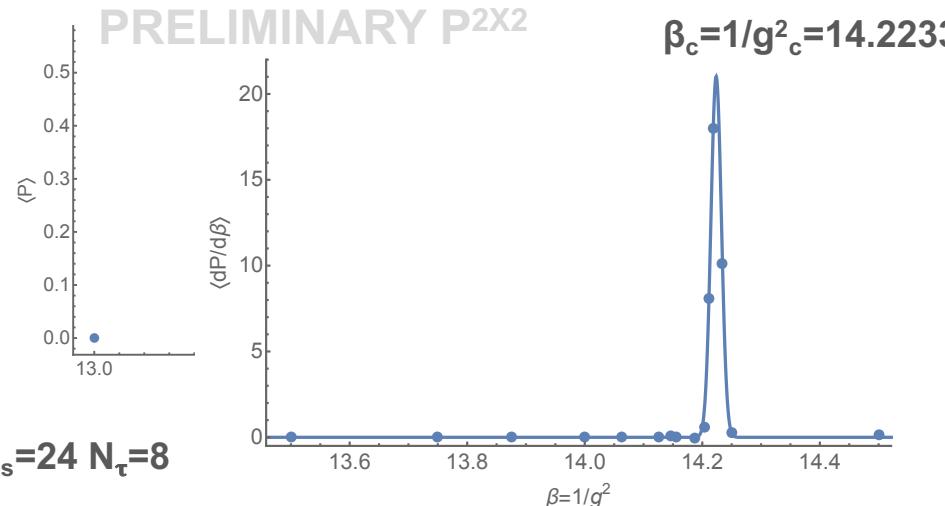


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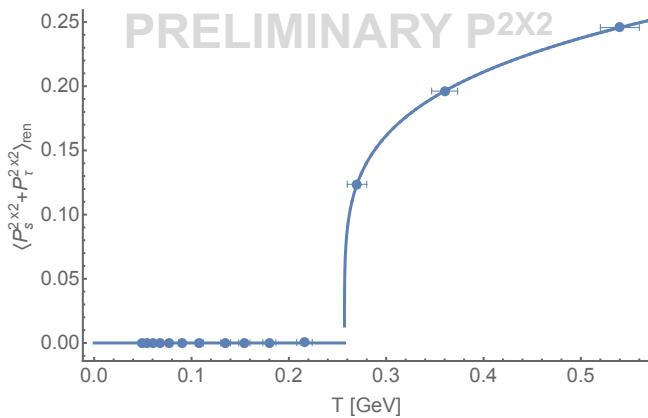


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What about
normalization?

