Fourier Acceleration of the Principal Chiral Model $SU(2) \otimes SU(2)$ in 2 Dimensions

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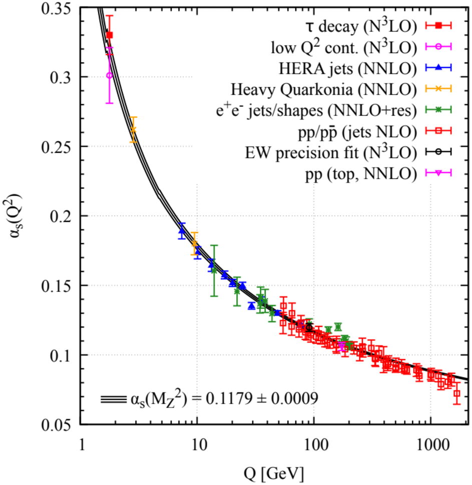
Set Up



R. L. Workman et al. (Particle Data Group), 'Review of Particle Physics', PTEP **2022**, 083C01 (2022)

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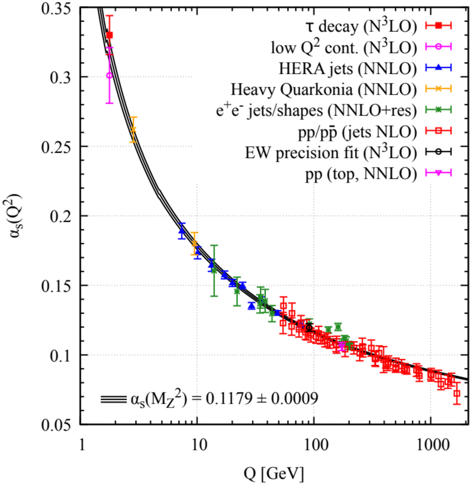
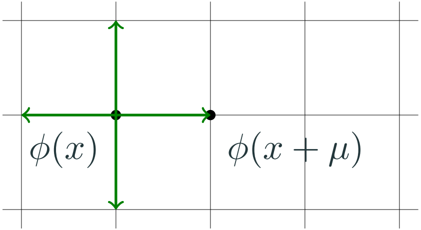


$SU(N) \otimes SU(N)$: gauge theory test bed

$$S = -2\beta \sum_{x,\mu} \mathrm{Re}\,\mathrm{tr}\left(\phi^\dagger(x)\phi(x+\mu)\right)$$

$\beta \sim 1/\text{coupling}$



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Objectives

1. Physics: QCD toy model with asymptotic freedom

2. Algorithm: simulation efficiency increase through Fourier Acceleration

Lattice Simulations
Discretizing space-time to simulate field theories fully non-perturbatively.

$$\langle O(\phi)\rangle = \int \mathcal{D}\phi\, O(\phi) \exp(iS_M[\phi]) \overset{t\to i\tau}{\to} \int \mathcal{D}\phi\, O(\phi) \exp(-S[\phi])$$

Fields follow probability density $\exp(-S[\phi])$.

Background

Lattice Simulations
Discretizing space-time to simulate field theories fully non-perturbatively.

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Monte Carlo
Independent, identically distributed samples $\{\phi_1, \ldots, \phi_N\}$, $\phi_i \sim \exp(-S[\phi])$.

$$\langle O(\phi)\rangle = \frac{1}{N}\sum_{i=1}^{N} O(\phi_i) + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

Hamiltonian Monte Carlo [1]

$$H[\phi, \pi] = \frac{1}{2}\pi \cdot \pi + S[\phi] \implies \dot{\phi} = \pi,\ \dot{\pi} = -\frac{dS}{d\phi} \tag{1}$$

[1] S. Duane et al., 'Hybrid Monte Carlo', Physics Letters B **195**, 216–222 (1987)

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Algorithm Steps

1. Start chain with arbitrary initial field configuration ϕ
2. Generate a momentum sample according to $\exp\left(-\frac{1}{2}\pi \cdot \pi\right)$
3. Candidate proposal: evolve $(\phi, \pi) \to (\phi', \pi')$ via Eq.1
4. Accept or reject: the candidate according to the Metropolis update

$$P(\phi \to \phi') = \min\left(1,\ \exp(-\Delta H)\right),\ \Delta H = H[\phi', \pi'] - H[\phi, \pi]$$

5. Repeat steps 2 - 4 until the chain has the desired length

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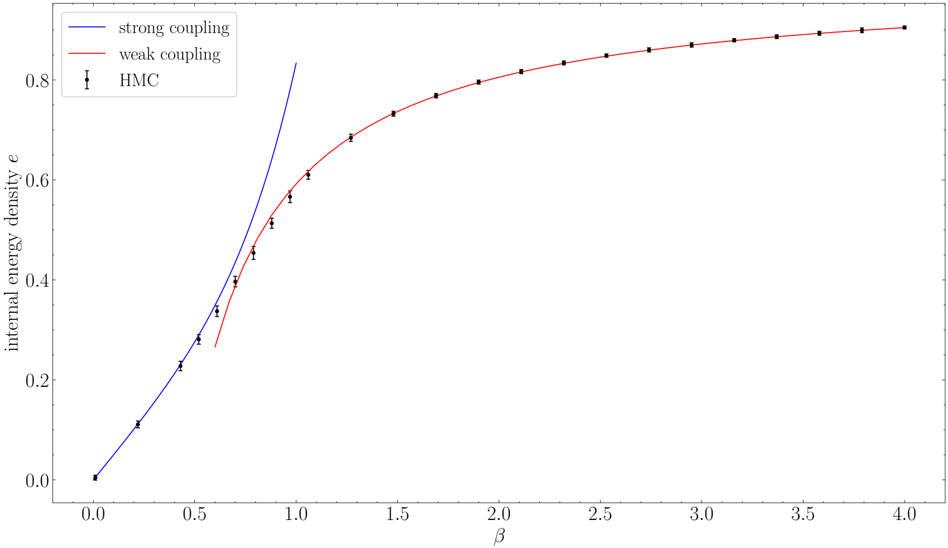
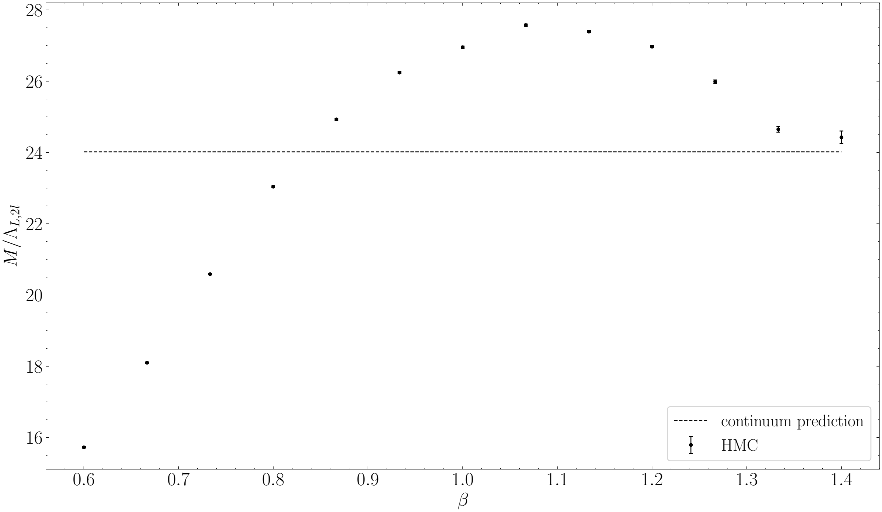
Simulation Test



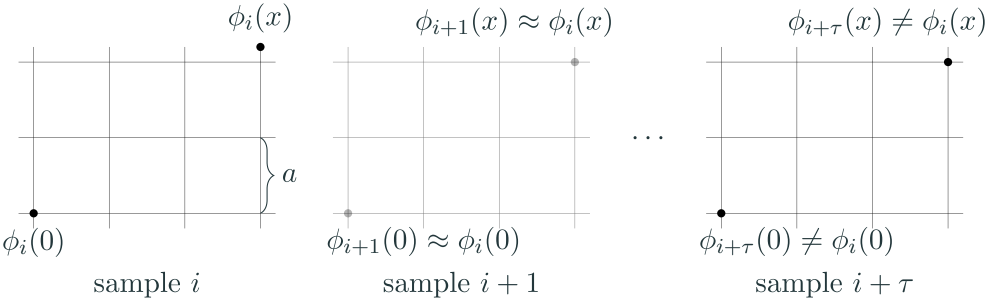
Results: Physics



P. Rossi and E. Vicari, 'Two-dimensional SU(N) × SU(N) chiral models on the lattice', Phys. Rev. D **49**, 1621–1628 (1994)

Critical Slowing Down

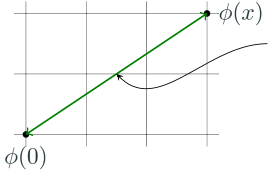
$$\omega^2(p) = m^2 + p^2 \quad \Longrightarrow \quad \text{unequal evolution rates}$$



Integrated Autocorrelation Time τ
Average number of steps in the chain separating uncorrelated configurations.

$\Longrightarrow$ effective number of samples: $N' = N/\tau$

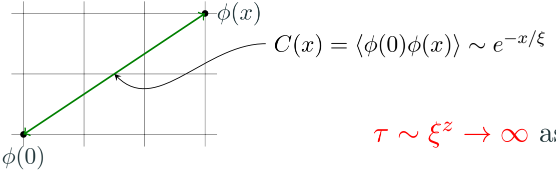
Phase Transition



$$C(x) = \langle \phi(0)\phi(x) \rangle \sim e^{-x/\xi}$$

$$\tau \sim \xi^z \to \infty \text{ as } L \to \infty,\ a \to 0$$

Phase Transition



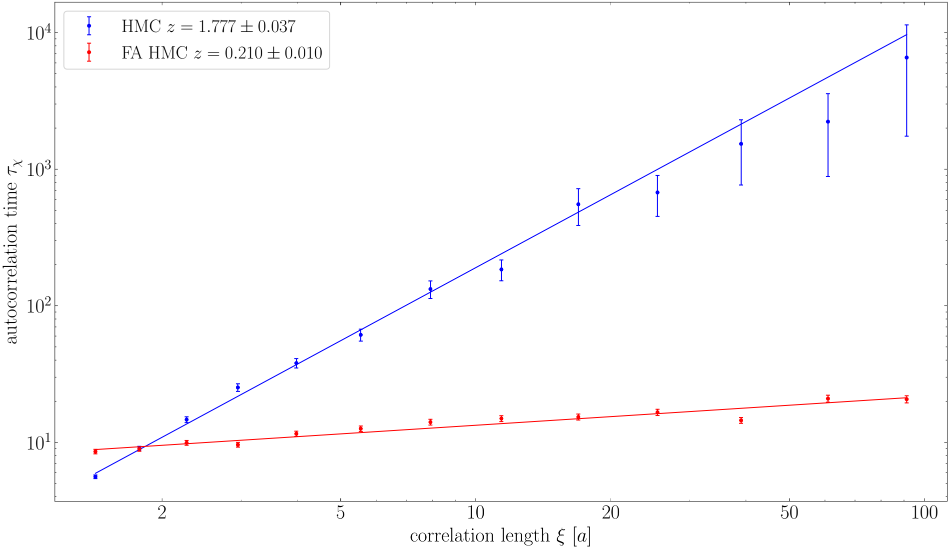
$\tau \sim \xi^z \to \infty$ as $L \to \infty$, $a \to 0$

Fourier Acceleration

$$H[\phi, \pi] = \frac{1}{2}\pi \cdot K^{-1} \cdot \pi + \frac{1}{2}\phi \cdot K \cdot \phi, \quad K^{-1} = (\partial^2 + M^2)^{-1} \text{ with acceleration mass M}$$

- Fast modes are slowed, slow modes are accelerated
- $\dot{\phi} = K^{-1} \cdot \pi, \quad \dot{\pi} = -\frac{dS}{d\phi}$
  K difficult to invert in real space but diagonal in Fourier space
  $\implies$ update ϕ and sample $\pi \sim \exp\left(-\frac{1}{2}\pi \cdot K^{-1} \cdot \pi\right)$ in Fourier space

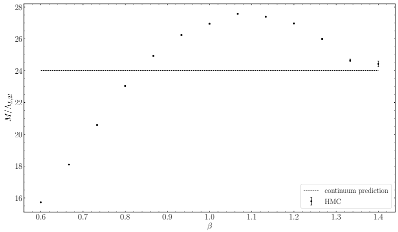
Results: Algorithm



Conclusion

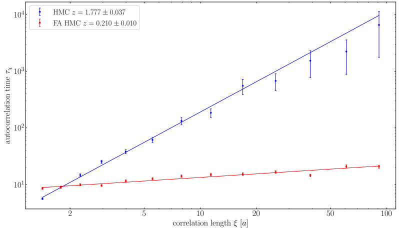
Summary

1. Onset of asymptotic freedom
2. Successful Fourier Acceleration



Future Work

1. Improved coupling
2. Acceleration mass
3. $SU(N) \otimes SU(N)$



References

[1] R. L. Workman et al. (Particle Data Group), 'Review of Particle Physics', PTEP **2022**, 083C01 (2022).

[2] S. Duane, A. D. Kennedy, B. J. Pendleton and D. Roweth, 'Hybrid Monte Carlo', Physics Letters B **195**, 216–222 (1987).

[3] P. Rossi and E. Vicari, 'Two-dimensional $\mathrm{SU}(N) \times \mathrm{SU}(N)$ chiral models on the lattice', Phys. Rev. D **49**, 1621–1628 (1994).

Backup

Dynamics on S^3

$$SU(2) \ni \phi = e^{i\alpha_i \sigma_i} = \cos\alpha\, \mathbb{1}_2 + i \sin\alpha\, (\hat{\boldsymbol{\alpha}} \cdot \boldsymbol{\sigma}) = a_0 \mathbb{1}_2 + i a_i \sigma_i$$

$$a_0 = \cos\alpha,\ a_i = \hat{\boldsymbol{\alpha}}_i \sin\alpha,\ \alpha = |\boldsymbol{\alpha}|,\ \hat{\boldsymbol{\alpha}} = \boldsymbol{\alpha}/\alpha.$$

Degrees of freedom: scalar fields α_μ.

Unitarity and $\det\phi = 1$ require

$$|a|^2 = a_0^2 + a_1^2 + a_2^2 + a_3^2 = 1 \implies a_0 = \sqrt{1 - a_i^2} = 1 - \frac{1}{2} a_i^2 + \dots$$

$$\therefore \phi = a_0 \mathbb{1}_2 + i a_i \sigma_i = \mathbb{1}_2 + i a_i \sigma_i - \frac{1}{2} a_i^2 \dots$$

HMC for $SU(2) \otimes SU(2)$

Equations of Motion

$$\pi_i(x,t) \equiv \frac{d}{dt}\alpha_i(x,t) = \dot{\alpha}_i(x,t) \implies \dot{\phi}(x,t) = i\pi_i(x,t)\sigma_i\phi(x,t) = i\pi_x\phi_x$$

$$H(\phi,\pi) = \frac{1}{4}\sum_x \operatorname{tr}\pi_x\pi_x + S(\phi) = \frac{1}{2}\sum_x \pi_i(x,t)\pi_i(x,t) + S(\phi)$$

$$\dot{H} = 0 \implies \dot{\pi}_x = -i\beta\sum_\mu \left(\phi_{x+\mu} + \phi_{x-\mu}\right)\phi_x^\dagger - \text{h.c.}$$

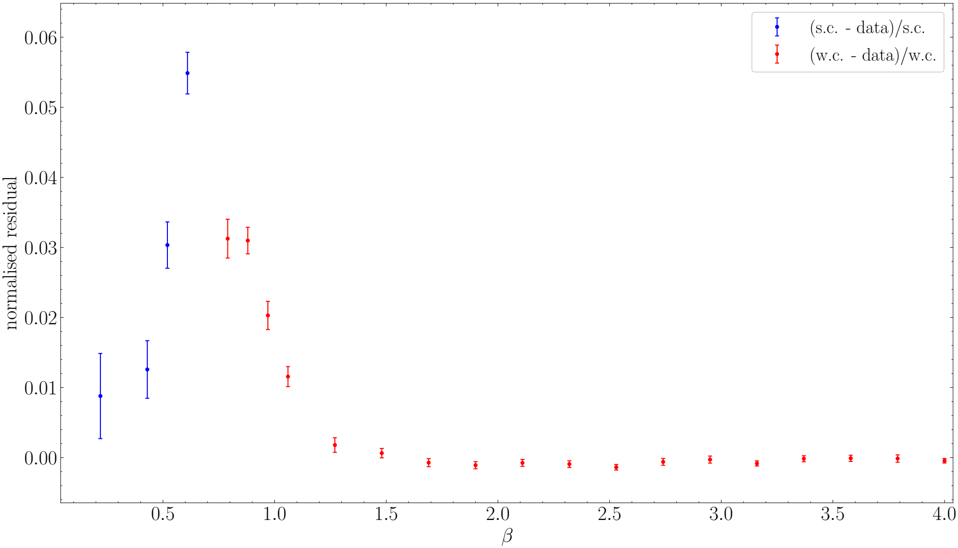
Fourier Acceleration

$$\tilde{K} = \sum_\mu 4\sin^2\pi\frac{k_\mu}{L}, \quad \tilde{K}^{-1}(M) = \left(\sum_\mu 4\sin^2\pi\frac{k_\mu}{L} + M^2\right)^{-1}$$

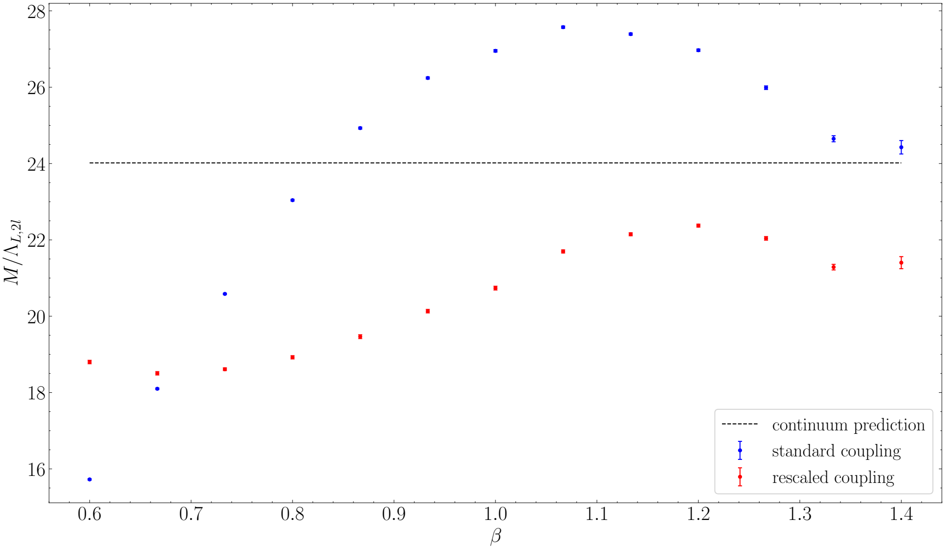
$$H(\phi,\pi) = \frac{1}{4}\sum_{x,y}\operatorname{tr}\pi_x K^{-1}_{x,y}(M)\pi_y + S(\phi)$$

$$\implies \dot{\alpha}_i(x,t) = K^{-1}(M)\pi_i(x,t), \ \dot{\phi}_x = iK^{-1}(M)\pi_x\phi_x$$

Coupling Expansion Residuals



Improved Coupling Prescription



Critical Slowing Down

Scalar Field Theory

$$H(\phi,\pi) = \frac{1}{2}\pi \cdot \pi + S(\phi), \quad S(\phi) = \frac{1}{2}\phi \cdot \left(m^2 - \partial^2\right) \cdot \phi = \frac{1}{2}\phi \cdot K(m) \cdot \phi$$

$$\implies \dot{\phi} = \pi, \quad \dot{\pi} = -\frac{\partial S}{\partial \phi} \qquad \implies \qquad \omega^2(p) = m^2 + p^2$$

Degree of Critical Slowing Down

$$\frac{\omega^2_{max}}{\omega^2_{min}} = \frac{m^2 + p^2_{max}}{m^2 + p^2_{min}} \to \infty$$

as $L \to \infty$ (i.e. $p_{min} \to 0$) and $a \to 0$ (i.e. $p_{max} \to \infty$).

Acceleration Mass Parameter