Pion-Pion Scattering in the Non-Linear Sigma Model

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Outline

1. Introduction & Background
2. Klein-Gordon Simulation
3. Non-Linear Sigma Model Simulation
4. Conclusion

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   - Lattice Field Theory
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   - Gibbs Sampler
   - Observable Calculation
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Klein-Gordon Theory

- Klein-Gordon theory[1,2] describes a non-interacting scalar boson
- Lattice action[3]

$$S(\phi) = \sum_{\mathbf{x}} \phi(\mathbf{x}) \left(\frac{2d + (am)^2}{2} \phi(\mathbf{x}) - \sum_{i=1}^{d} \phi(\mathbf{x} + \mathbf{e}_i) \right).$$

  - d: lattice dimension
  - a: lattice spacing
  - m: boson mass

[1] Klein, *Z. Phys.* **37**, 895-906 (1926).
[2] Gordon, *Z. Phys.* **40**, 117-133 (1926).
[3] Rothe, *Lattice Gauge Theories: An Introduction*, 3rd ed., ch. 3 (2005).

Non-Linear Sigma Model

- Non-linear sigma model[4] describes a scalar field $\boldsymbol{\phi} = (\sigma, \boldsymbol{\pi})$ taking values in a target manifold $\mathcal{M} = S^{N-1}$
- $N = 4$: $SU(2)$ NLSM/chiral model[5]
- Lattice action

$$S(\boldsymbol{\phi}) = -\frac{\beta}{2} \sum_{\mathbf{x}} \mathrm{Tr} \left[\boldsymbol{\phi}(\mathbf{x}) \left(\lambda_0 \mathbb{I} + \sum_{i=1}^{d} \boldsymbol{\phi}^\dagger(\mathbf{x} + \mathbf{e}_i) \right) \right]$$

- $$\boldsymbol{\phi} = \sigma \mathbb{I} + i \sum_{k=1}^{3} \pi_k \tau_k \in SU(2)$$

$$\det \boldsymbol{\phi} = \sigma^2 + \boldsymbol{\pi}^2 = 1 \implies (\sigma, \boldsymbol{\pi}) \in S^4$$

[4] Gellmann et al., *Nuovo Cim.* **16**, 705-726 (1960).
[5] Gürsey, *Nuovo Cim.* **16**, 230-240 (1960).

Two-Point Correlation

- Define

$$\Phi(t) \equiv \sum_{i=1}^{d-1} \sum_{x_i=1}^{L_i} \phi((x_1, \ldots, \ldots, x_{d-1}, t))$$

$$c(\delta) \equiv \sum_{t=1}^{T} \Phi(t)\, \Phi(t+\delta)$$

- $c(\delta)$: two-point correlation function[6,7]
- General form[8]

$$c(\delta) \propto e^{-am\,\delta} + e^{-am(T-\delta)} + k$$

[6] Peskin et al., *An Introduction to Quantum Field Theory*, ch. 4.2 (1995).
[7] Rothe, *Lattice Gauge Theories: An Introduction*, 3rd ed., ch. 2 (2005).
[8] Rothe, *Lattice Gauge Theories: An Introduction*, 3rd ed., ch. 10.1 (2005).

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Markov Chain Monte Carlo Methods

- Randomly generate a sequence of states independent of previous states to calculate expected values for some distribution $\lambda(\phi)$
- Metropolis-Hastings algorithm[9,10,11]
  - Current state ν
  - Propose state ξ according to some $q(\xi, \nu)$
  - Accept ξ as next state with probability

$$\alpha(\xi, \nu) = \min\left(\frac{q(\nu, \xi)\lambda(\xi)}{q(\xi, \nu)\lambda(\nu)}, 1\right)$$

- Gibbs sampler:[12,11] $q(\xi, \nu) \propto \lambda(\xi) \implies \alpha = 100\%$

[9] Metropolis et al., *J. Chem. Phys.* **21**, 1087-1092 (1953).
[10] Hastings, *Biometrika* **57**, 97-109 (1970).
[11] Ross, *Simulation*, 5th ed., ch. 12 (2005).
[12] Geman et al., *IEEE Trans. Pattern Anal. Mach. Intell.* **6**, 721-741 (1984).

Autocorrelation

- Initial state far from equilibrium: discard first D states
- Naïve MSE $= \frac{\text{variance}}{\text{no. of samples}} \neq$ true MSE
  - Binning method:[13] average samples into bins, binned MSE $= \frac{\text{variance of binned samples}}{\text{no. of binned samples}} \to$ true MSE as bin size $\to \infty$
  - Integrated autocorrelation time[14] for estimator $\hat{\mu}$

$$\tau_{\hat{\mu}} = \frac{\text{true MSE}}{\text{naïve MSE}} = \frac{\text{total no. of samples}}{\text{effective no. of ind. samples}}$$

[13] Knechtli et al., *Lattice Quantum Chromodynamics...*, ch. 2 (2017).
[14] Sokal, Cargése Summer School (1996).

Error Calculation

Random variables $A_1, \ldots, A_N$ with mean μ

- Sample mean $\hat{\mu}$: binning method
- Estimating $f(\mu)$
  - Average of $f(A_i)$ does not converge to $f(\mu)$[15]
  - Jackknife method[16,17] for independent samples

$$\hat{f}_i = f\left(\frac{1}{N-1}\sum_{k\neq i} A_k\right),$$

$$\hat{f}_{\text{jack}} = \frac{1}{N}\sum_{i=1}^{N}\hat{f}_i, \quad \widehat{\text{MSE}}(\hat{f}) = \frac{N-1}{N}\sum_{i=1}^{N}\left(\hat{f}_i - \hat{f}_{\text{jack}}\right)^2$$

  - Dependent samples: combine jackknife & binning

[15] Berg, *Markov Chain Monte Carlo Simulations...*, ch. 2.7 (2004).
[16] Quenouille, *Biometrika* **43**, 353-360 (1956).
[17] Tukey, *Ann. Math. Stat.* **29**, 614 (1958).

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Motivation

- Debug & verify calculations by analytic comparison
- Optimising approaches to writing programmes
- Compare efficiency of different MCMC algorithms
- Determine relationships between $\tau_{\hat{c}(\delta)}$ and system parameters (lattice size, dimensionless mass am)

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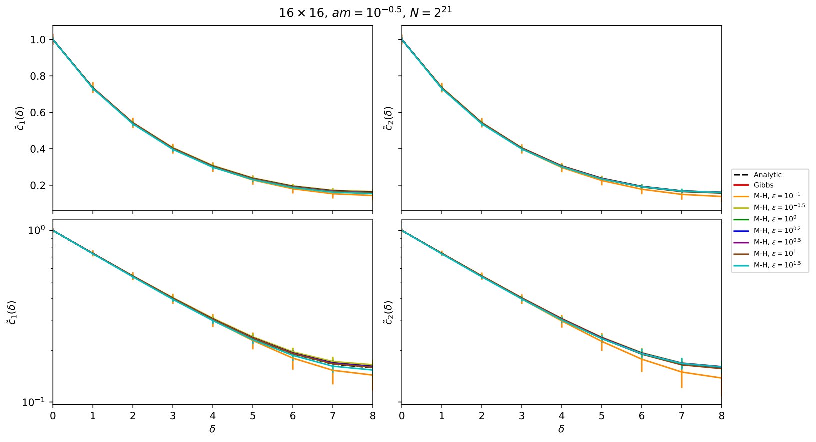
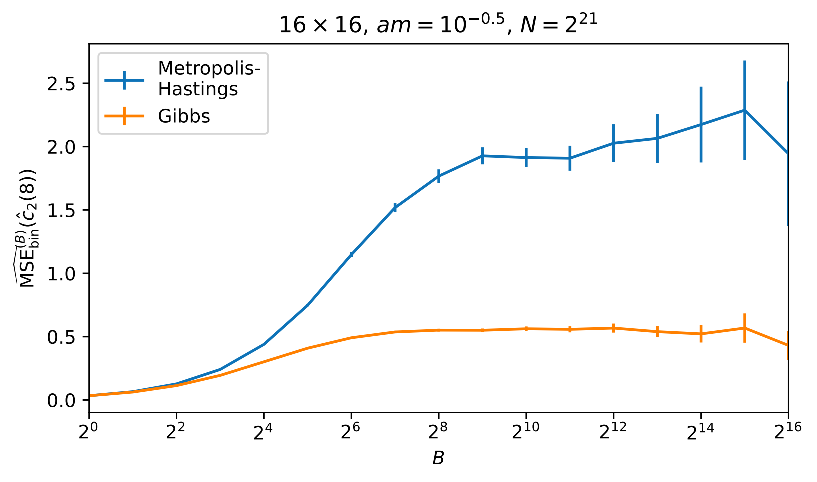
Analytic Comparison



Binning Method



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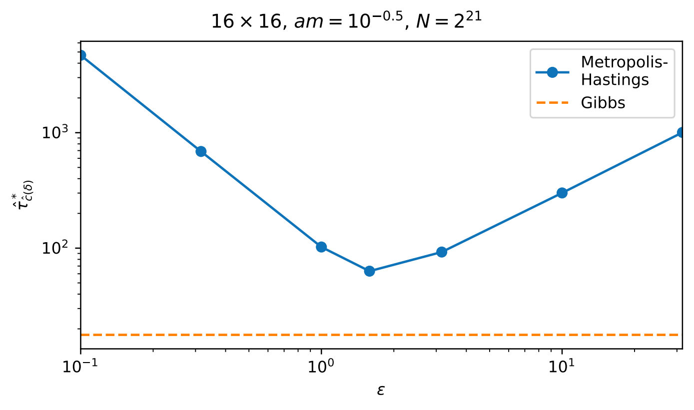
Metropolis-Hastings Algorithm Procedure

1. Calculate $\kappa^2 = \frac{1}{2d+(am)^2}$.
2. Choose a lattice site $\mathbf{x}$ and calculate $\gamma(\mathbf{x}) = \sum_{i=1}^{d} \left(\phi(\mathbf{x}-\mathbf{e}_i) + \phi(\mathbf{x}+\mathbf{e}_i)\right)$.
3. Generate a proposed value $\phi'(\mathbf{x}) \sim \phi(\mathbf{x}) + \mathcal{U}(-\varepsilon, \varepsilon)$.
4. Calculate $\psi(\mathbf{x}) = \phi(\mathbf{x}) - \kappa^2\gamma(\mathbf{x})$ and $\psi'(\mathbf{x}) = \phi'(\mathbf{x}) - \kappa^2\gamma(\mathbf{x})$.
5. If $|\psi'(\mathbf{x})| \leqslant |\psi(\mathbf{x})|$, then set $\phi(\mathbf{x}) = \phi'(\mathbf{x})$. Otherwise, generate $U \sim \mathcal{U}(0,1)$ and set $\phi(\mathbf{x}) = \phi'(\mathbf{x})$ if $U < \exp\left[-\frac{(\psi'(\mathbf{x}))^2 - (\psi(\mathbf{x}))^2}{2\kappa^2}\right]$.
6. Repeat steps 2-5 for each lattice site.

Gibbs Sampler Procedure

1. Calculate $\kappa^2 = \frac{1}{2d+(am)^2}$.
2. Choose a lattice site $\mathbf{x}$ and calculate $\gamma(\mathbf{x})$.
3. Generate a proposed value $\phi'(\mathbf{x}) \sim \mathcal{N}\left(\kappa^2\gamma(\mathbf{x}), \kappa^2\right)$.
4. Set $\phi(\mathbf{x}) = \phi'(\mathbf{x})$.
5. Repeat steps 2-4 for each lattice site.

Autocorrelation



- Metropolis-Hastings: optimal $\hat{\tau}_{\hat{c}(\delta)} = 63.21$ for $\varepsilon = 1.58$
- Gibbs: $\hat{\tau}_{\hat{c}(\delta)} = 17.75$

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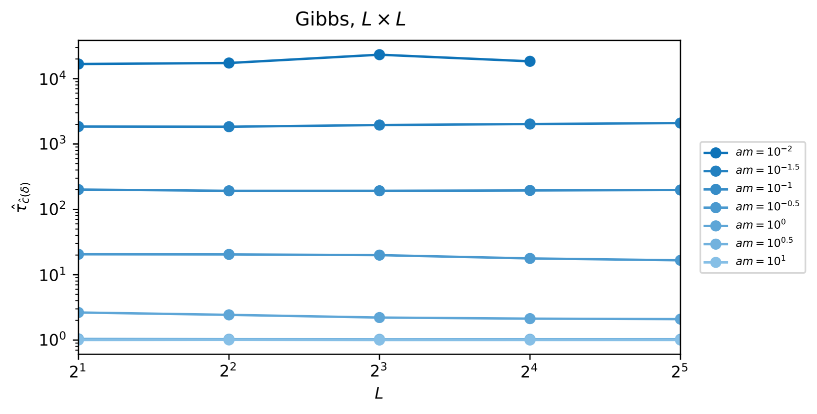
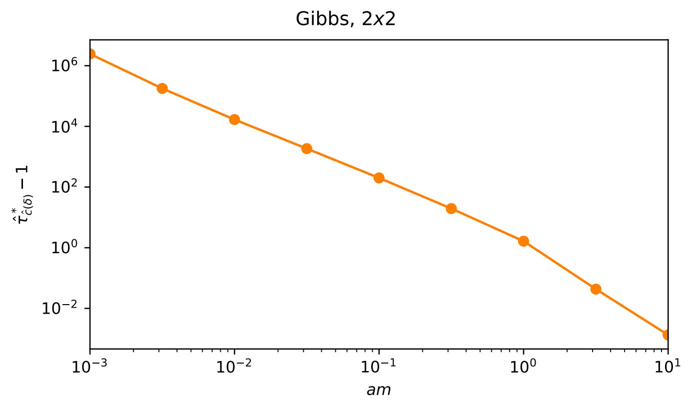
Lattice Size



Mass



- $\tau_{\hat{c}(\delta)} - 1 \propto am^{-2}$ for $am < 1$

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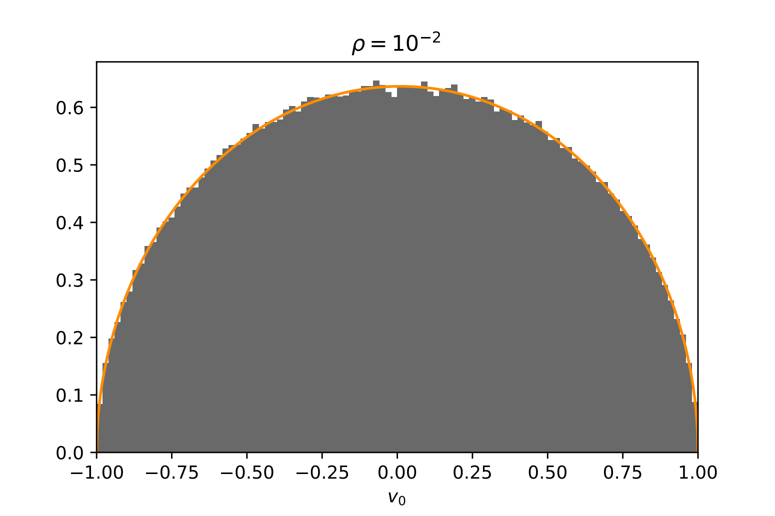
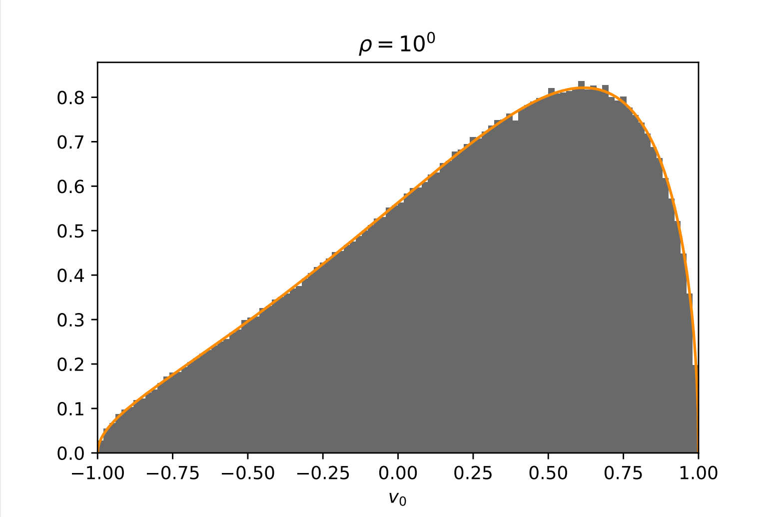
Procedure

1. Choose a lattice site $\mathbf{x}$ and calculate $\mathbf{\Sigma}(\mathbf{x}) = \lambda_0 \mathbb{I} + \sum_{i=1}^{d} (\phi(\mathbf{x} - \mathbf{e}_i) + \phi(\mathbf{x} + \mathbf{e}_i))$.
2. Generate $A \sim \mathcal{N}\left(0, \frac{1}{2}\right)$, $B \sim \mathrm{Exp}(1)$, and $U \sim \mathcal{U}(0,1)$, and set $v_0 = 1 - \frac{A^2+B}{\beta\sqrt{\det \mathbf{\Sigma}(\mathbf{x})}}$.
3. If $2U^2 > v_0 + 1$, return to step 2.
4. Generate $n_1 \sim \mathcal{U}(-1,1)$ and $\theta \sim \mathcal{U}(0,2\pi)$, set $n_2 = \sqrt{1-n_1^2}\cos\theta$ and $n_3 = \sqrt{1-n_1^2}\sin\theta$, and set $v_i = n_i\sqrt{1-v_0^2}$ for $i = 1,2,3$.
5. Calculate $v = v_0 + i\sum_{k=1}^{3} v_k \tau_k$ and set $\phi(\mathbf{x}) = v \cdot \frac{\mathbf{\Sigma}(\mathbf{x})}{\sqrt{\det \mathbf{\Sigma}(\mathbf{x})}}$.
6. Repeat steps 1-5 for each lattice site.

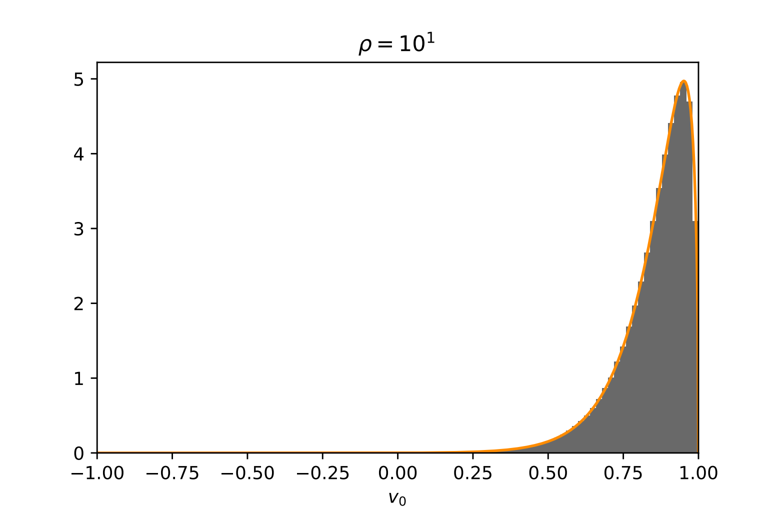
Debugging & Verification



Debugging & Verification



Debugging & Verification



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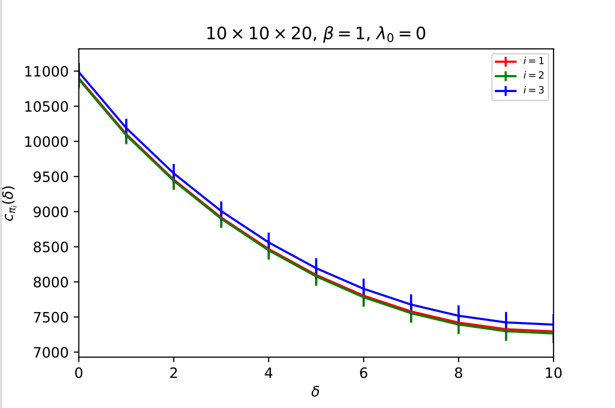
Two-Point Correlations

- $(\sigma, \boldsymbol{\pi}) \implies c_\sigma(\delta),\ c_{\pi_1}(\delta),\ c_{\pi_2}(\delta),\ c_{\pi_3}(\delta)$



- $c_\pi(\delta) = \sum_{i=1}^{3} c_{\pi_i}(\delta)$

Mass

- $c(\delta) = e^{-am\,\delta} + e^{-am(T-\delta)} + k$
- Small $\delta \implies c(\delta) \approx k_1 e^{-am\,\delta} + k_2$
- $\ldots$
- $am \approx \ln\left\{ \frac{c(0)-c(2)+\sqrt{[c(0)-c(2)]^2-4[c(1)-c(2)][c(0)-c(1)]}}{2[c(1)-c(2)]} \right\}$
- $am(c(\delta)) \implies \widehat{am}$ using jackknife

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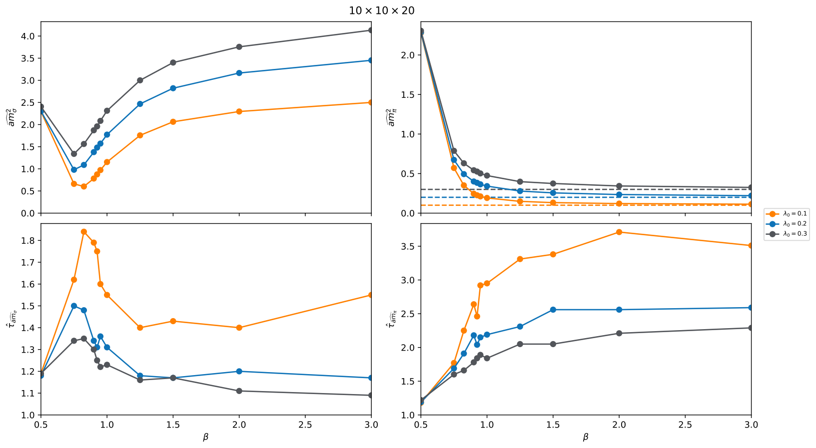
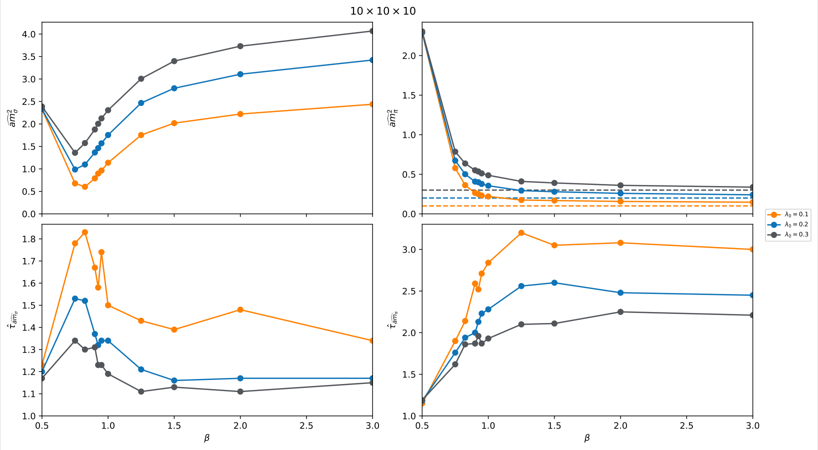
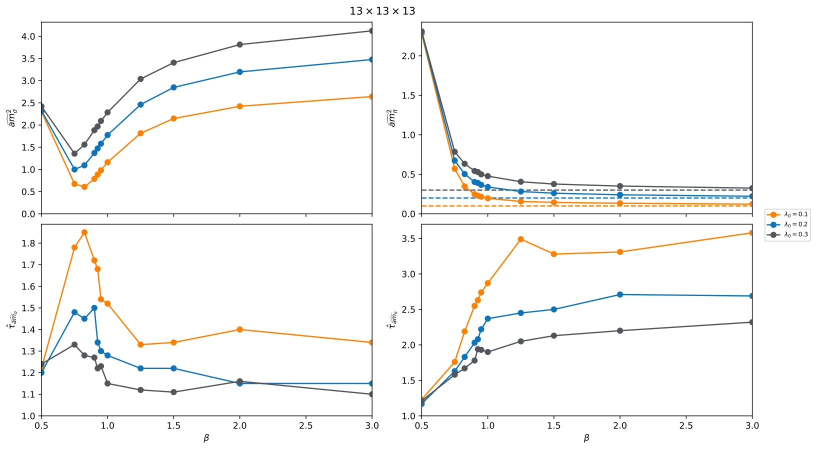
am_σ and am_π



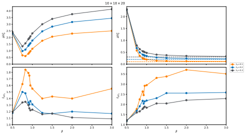
am_σ and am_π

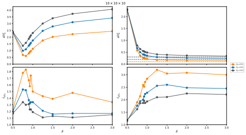


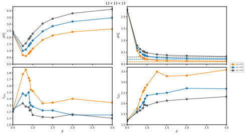
am_σ and am_π



am_σ and am_π







- Masses independent of lattice size
- Autocorrelation times maximised when mass minimised
- am_σ has a λ_0-dependent minimum
- $(am_\pi)^2 \to \lambda_0$ as $\beta \to \infty$

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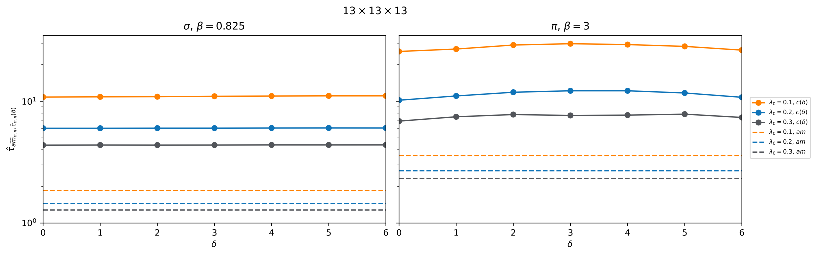
$\tau_{\widehat{am}}$ and $\tau_{\hat{c}(\delta)}$



- $\tau_{\widehat{am}} < \tau_{\hat{c}(\delta)}$
- $\tau_{\sigma} < \tau_{\pi}$

$\therefore$ Algorithm efficiency depends on observable

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Project Summary

- Klein-Gordon theory
  - Verified results via analytic comparison & statistical theory
  - Found Gibbs $>$ Metropolis-Hastings
  - Autocorrelation depends on am, independent of lattice size
- Non-linear sigma model
  - Used code and results from Klein-Gordon study
  - Investigated particle mass behaviour on system parameters
  - Observable determines algorithm efficiency

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