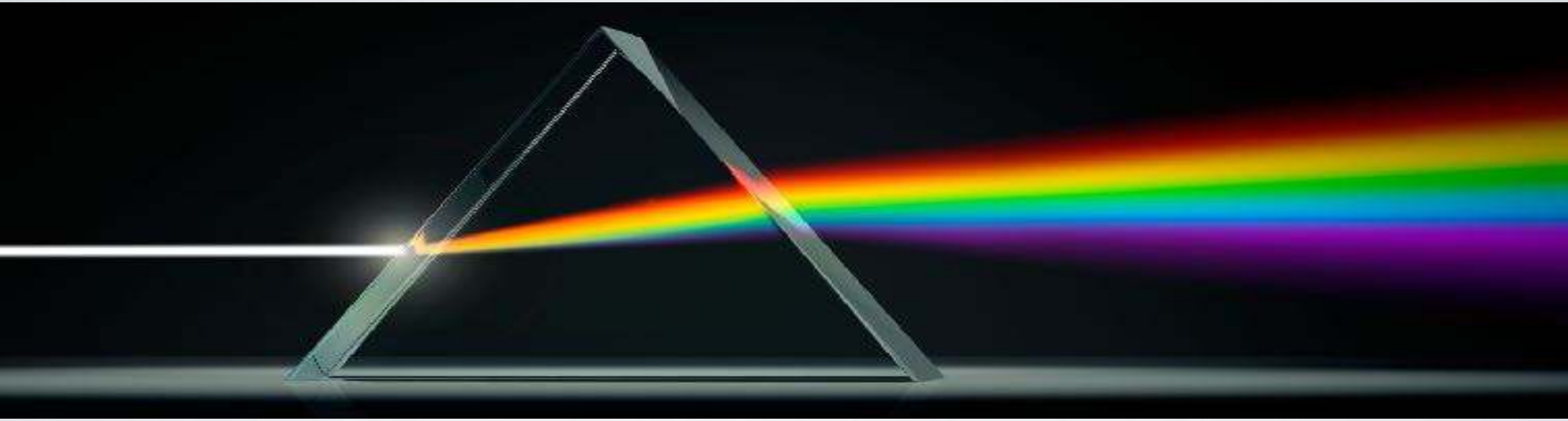
Simulations of QCD and QED with C* boundary conditions



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Marina Marinkovic (CERN, Trinity College Dublin)

Lattice2017

Overview

- **Simulation code**
  - Features
  - C* boundary conditions
  - Fermion representation
  - Lattice action
- **Exploratory studies**
  - Ensembles and parameters
  - QCD simulations
  - QCD+QED simulations

Simulation Code

Features

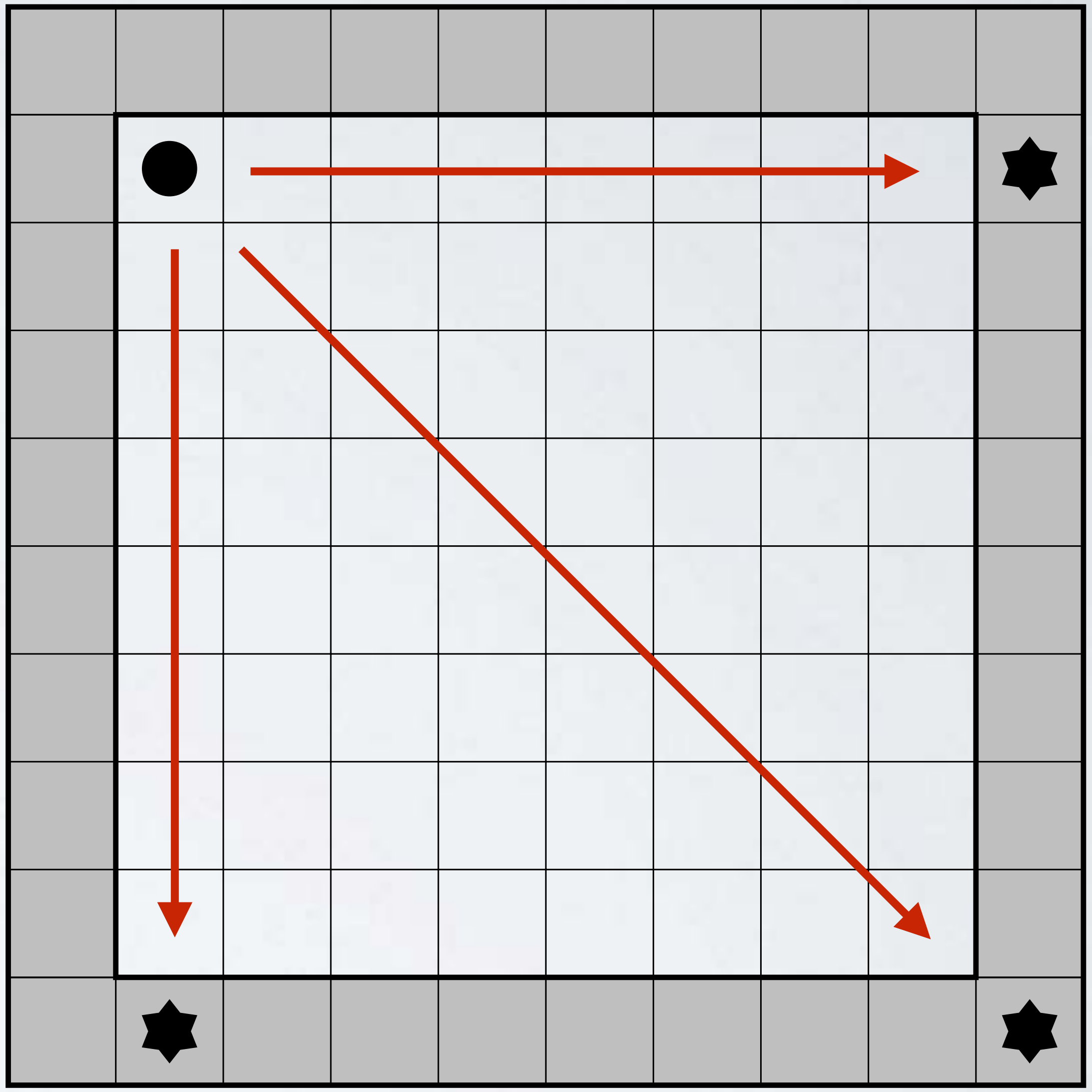
§ Del Debbio *et al* PRD (2008)

- **Modified version of the HiRep§ code**
  - Flexible code for BSM models
  - Can simulate QCD, QED and QCD+QED
  - Compact QED (with Fourier acceleration)
  - Rational approximations
  - Different boundary conditions
  - Wilson-Clover fermions
  - Lüscher-Weisz gauge action
  - OMF integrators
  - Charged and neutral meson correlators

Boundary Conditions

- C* boundary conditions

$$A_\mu(x+L) = -A_\mu(x)$$
$$\psi(x+L) = C^{-1}\bar{\psi}^T(x)$$
$$\bar{\psi}(x+L) = -\psi^T(x)C$$



- **Extended lattice**
  - Static boundary

$$U_\mu(x) \to U_\mu(x)^*$$

Lucini, Patella, Ramos, Tantalo

JHEP (2016)

FERMIONS

- **Fermion representation**
  - Consider fermions in the $3 \oplus \bar{3}$ representation

$$\chi = \begin{pmatrix} \psi \\ C^{-1}\bar{\psi}^T \end{pmatrix}, \qquad \chi(x+L) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \chi$$

  - Rotated to basis where b.c.s. are diagonal

$$\eta = \begin{pmatrix} \psi_+ \\ -i\psi_- \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \psi + C^{-1}\bar{\psi}^T \\ -i(\psi - C^{-1}\bar{\psi}^T) \end{pmatrix}$$

$$\tilde{U} = \begin{pmatrix} \mathrm{Re}\, U & -\mathrm{Im}\, U \\ \mathrm{Im}\, U & \mathrm{Re}\, U \end{pmatrix} \longleftarrow$$ Easy in HiRep

FERMIONS

- **Path integral**
  - After change of basis the path integral can be evaluated

$$\int_{C^\star} [D\psi][D\bar{\psi}]\; e^{-\bar{\psi} D[U] \psi}$$

$$\downarrow$$

$$\int_K [D\eta]\; e^{+\frac{1}{2}\eta^T C D[\tilde{U}]\eta}$$

$$\downarrow$$

$$\mathrm{Pf}\; C D[\tilde{U}]$$

Fermions

- **Lattice fermions**
  - RHMC algorithm is needed

$$|\mathrm{Pf}\ CD[\tilde{U}]| = \sqrt{\det D[\tilde{U}]}$$

$$\mathrm{Pf}\ CD[\tilde{U}] = \int [D\phi][D\phi^*]\ e^{-\phi^\dagger \{D[\tilde{U}]^\dagger D[\tilde{U}]\}^{-1/4} \phi}$$

ACTION

- **Lattice action**
  - Wilson-Clover fermions
  - Plaquette action for QED field
  - Lüscher-Weisz action for QCD field

$$
\begin{aligned}
D\phi(x) &= (4+m)\phi(x) \\
&\quad - \frac{1}{2}\sum_{\mu}(1-\gamma_\mu)V_\mu(x)^n U_\mu(x)\phi(x+\hat{\mu}) + (1+\gamma_\mu)V_\mu^\dagger(x-\hat{\mu})^n U_\mu^\dagger(x-\hat{\mu})\phi(x-\hat{\mu}) \\
&\quad + \frac{i}{4}\sum_{\mu,\nu}\sigma_{\mu\nu}\left\{\mathrm{c}_{\mathrm{sw}}^{\mathrm{QCD}} F_{\mu\nu}^{\mathrm{QCD}}(x) + \mathrm{c}_{\mathrm{sw}}^{\mathrm{QED}} F_{\mu\nu}^{\mathrm{QED}}(x)\right\}\phi(x)
\end{aligned}
$$

- At tree-level $\mathrm{c}_{\mathrm{sw}}^{\mathrm{QED}} = n$ where *n* is a function of the fermion charge

Exploratory studies

Exploratory Studies

PRELIMINARY

Ensembles

- QCD simulations with $N_f = 3$ at the symmetric point

Ensemble	$L^3 \times T$	β	κ	c_{sw}	b.c.s.	MDU
A1	$16^3 \times 32$	3.40	0.13675962	1.986246	PPPP	1000
A2	$16^3 \times 32$	3.40	0.13675962	1.986246	CCCP	1500
A3	$24^3 \times 48$	3.40	0.13675962	1.986246	CCCP	693
B1	$16^3 \times 32$	3.55	0.13700000	1.824865	CCCP	1000
B2	$24^3 \times 48$	3.55	0.13700000	1.824865	CCCP	1000

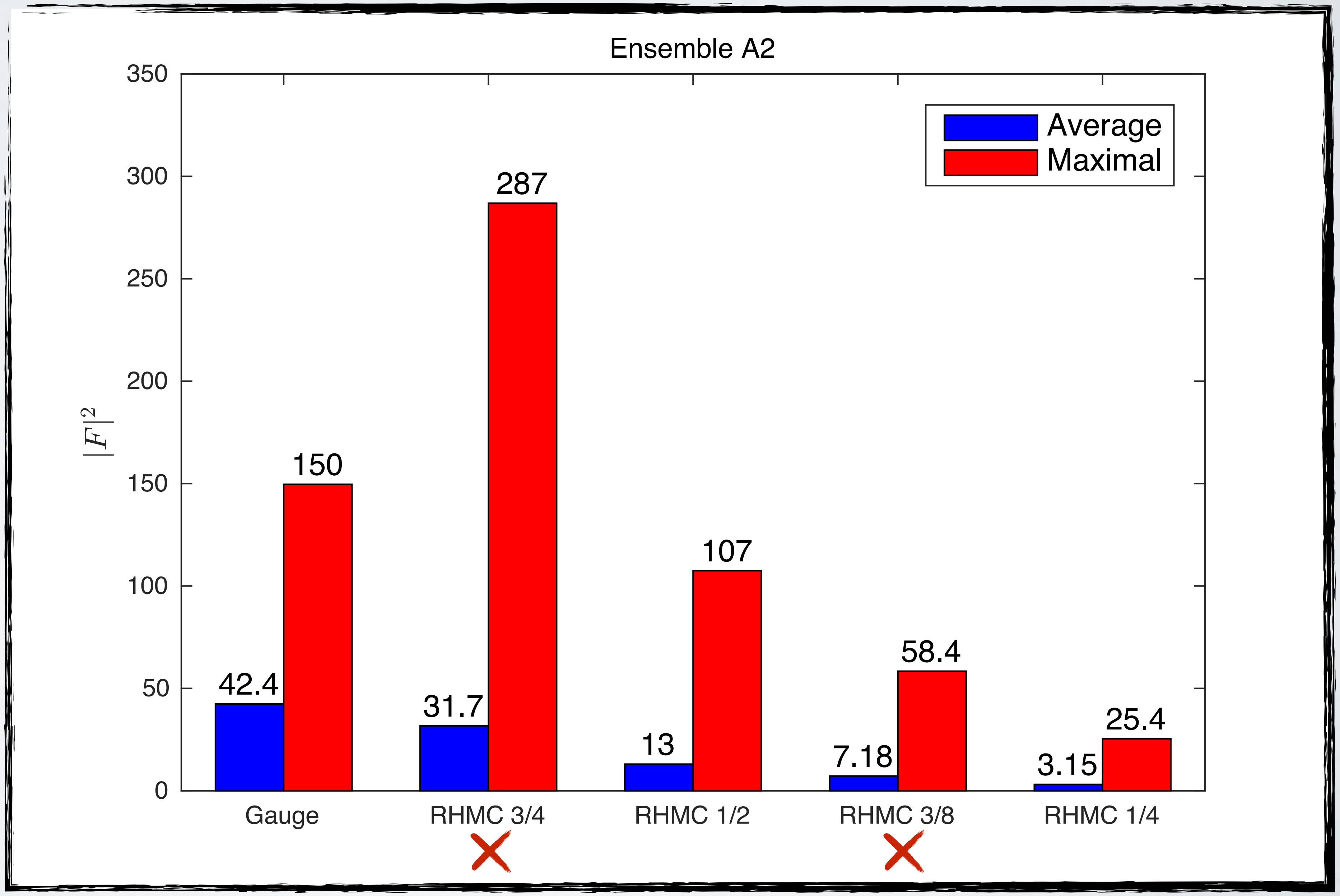
- QCD+QED simulations with $N_f = 2 + 1$

Ensemble	$L^3 \times T$	β	α	q_f	κ	c_{sw}^{QCD}	b.c.s.	MDU
Q1	$16^3 \times 32$	3.55	0.05	$\{+2/3, -1/3, -1/3\}$	0.13700000	1.824865	CCCP	1000
Q2	$16^3 \times 32$	3.55	1/137	$\{+2/3, -1/3, -1/3\}$	0.13700000	1.824865	CCCP	500

QCD

Tuning the RHMC

- Reduce number of integrations steps by a factor of **five** by using two pseudofermions in N_f = 3 simulations



Clark, Kennedy
PRL (2007)

- **Comparison with CLS**
  - We have smaller volumes and less statistics
  - Agreement within 5% on our largest volumes

Ensemble	m_q	$m_{\pi,K}$	$f_{\pi,K}$	m_{ρ,K^*}	t_0	$m_\pi L$
A1	0.00868(35)	0.2006(82)	0.0486(21)	0.425(35)	2.960(48)	3.2
A2	0.00877(24)	0.1820(47)	0.0562(12)	0.396(28)	2.879(34)	2.9
A3	0.00901(12)	0.1819(16)	0.06022(96)	0.371(18)	2.901(10)	4.3
H101§	0.009202(45)	0.18302(57)	0.06351(34)	–	2.8469(59)	5.8
B1	0.00665(23)	0.1866(65)	0.0305(24)	0.397(21)	5.01(10)	3.0
B2	0.006805(93)	0.1324(28)	0.04597(51)	0.295(27)	5.259(41)	3.2
H200§	0.006856(30)	0.13717(76)	0.04704(43)	–	5.150(25)	4.4

§ Bruno, Korzec, Schaefer
PRD (2017)

QCD+QED

Operators

- **Coulomb operator**
  - Unique gauge-invariant extension of operator in Coulomb gauge

$$\Psi_c(x) = e^{-iq\int d^3y\, \partial_k A_k(x_0,\mathbf{y})\Phi(\mathbf{y}-\mathbf{x})}\, \psi(x)$$

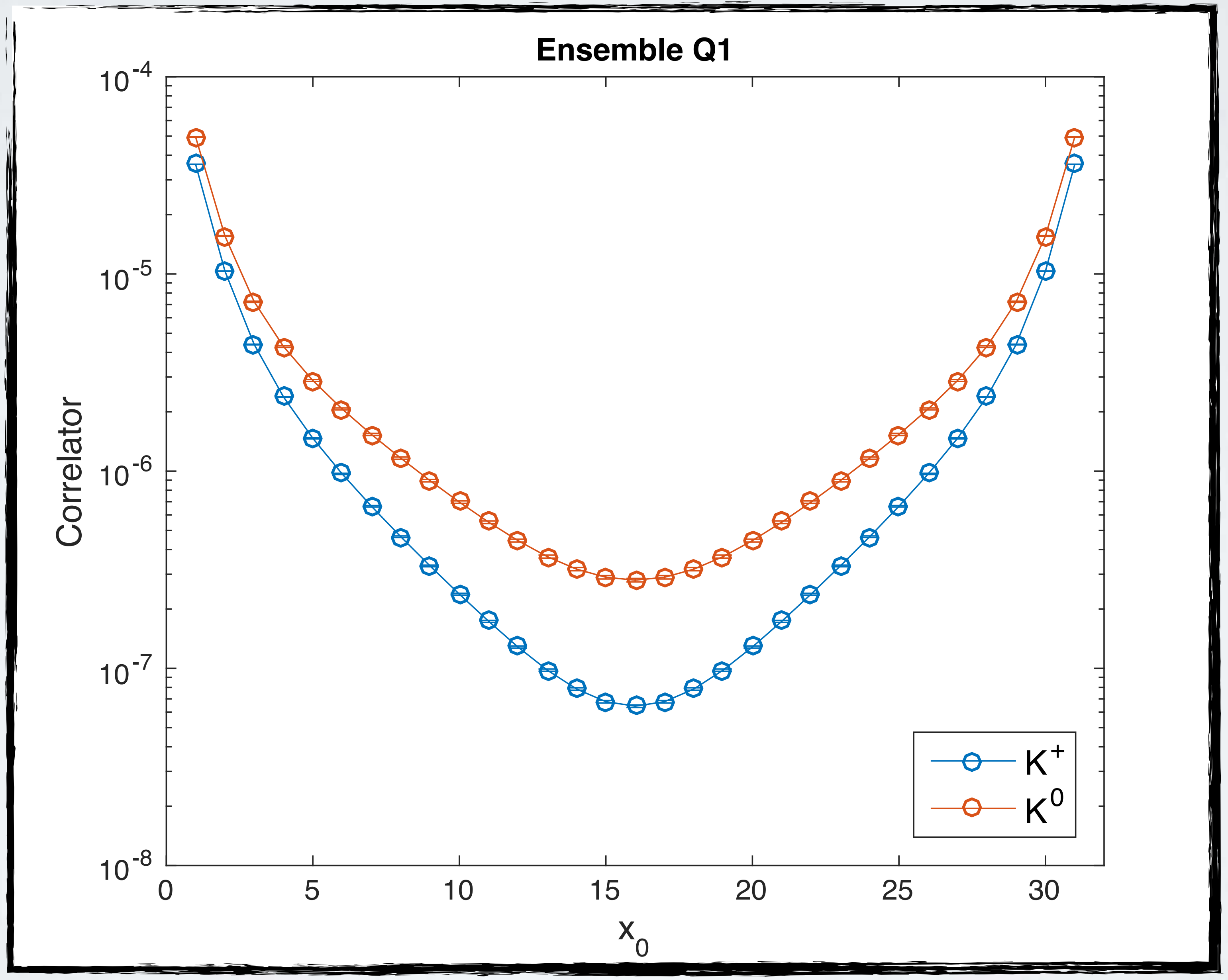
$$\partial_k\partial_k\Phi(\mathbf{x}) = \delta^3(\mathbf{x})$$
$$\Phi(\mathbf{x}+L) = -\Phi(\mathbf{x})$$

- **String operator**
  - Simple discretisation

$$\Psi_s(x) = e^{-\frac{iq}{2}\int_{-x_k}^{0} ds\, A_k(x+s\hat{k})}\, \psi(x)\, e^{+\frac{iq}{2}\int_{0}^{L-x_k} ds\, A_k(x+s\hat{k})}$$

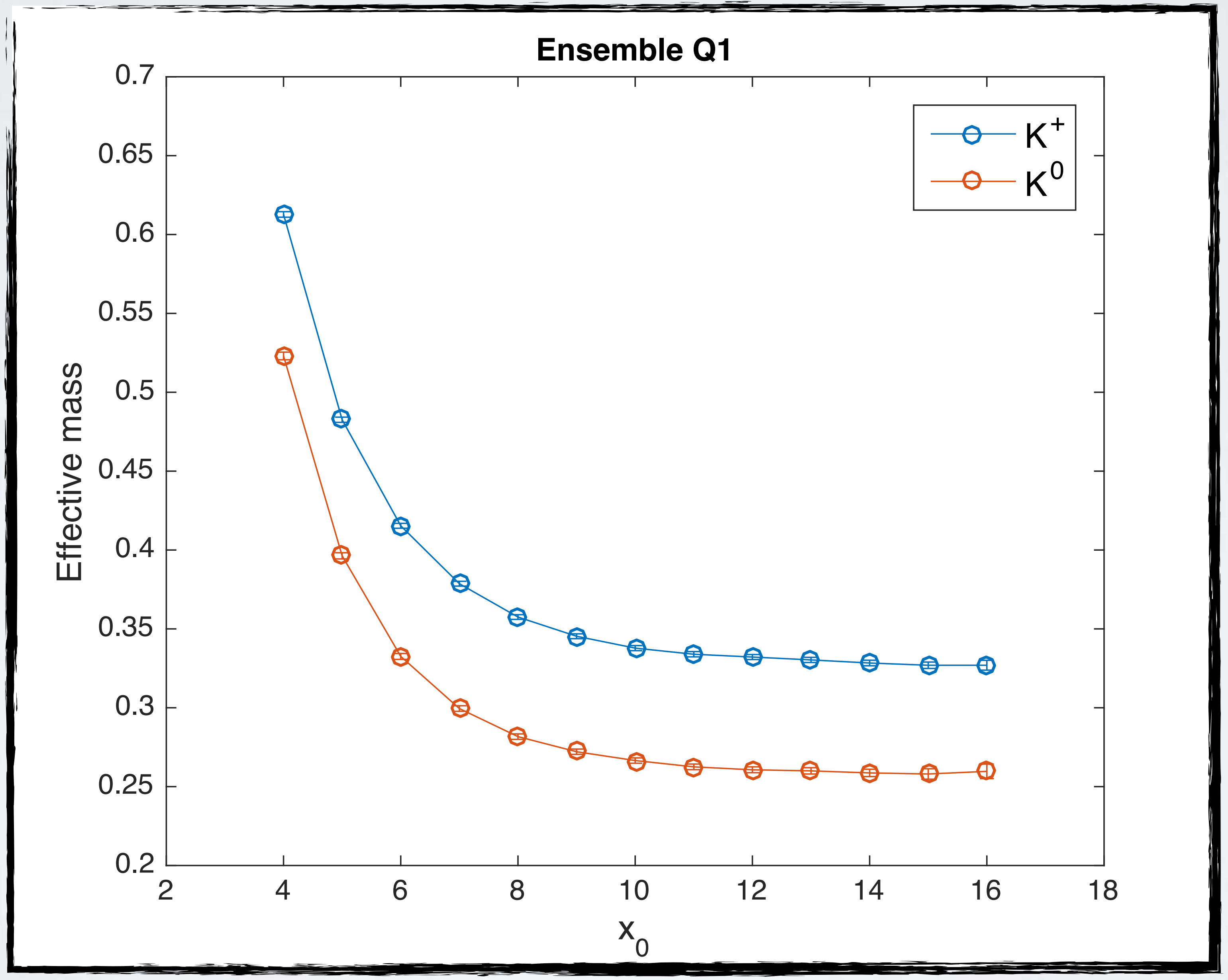
QCD+QED

- **Ensemble Q1 with α = 0.05**
  - Charged and neutral Kaon correlator



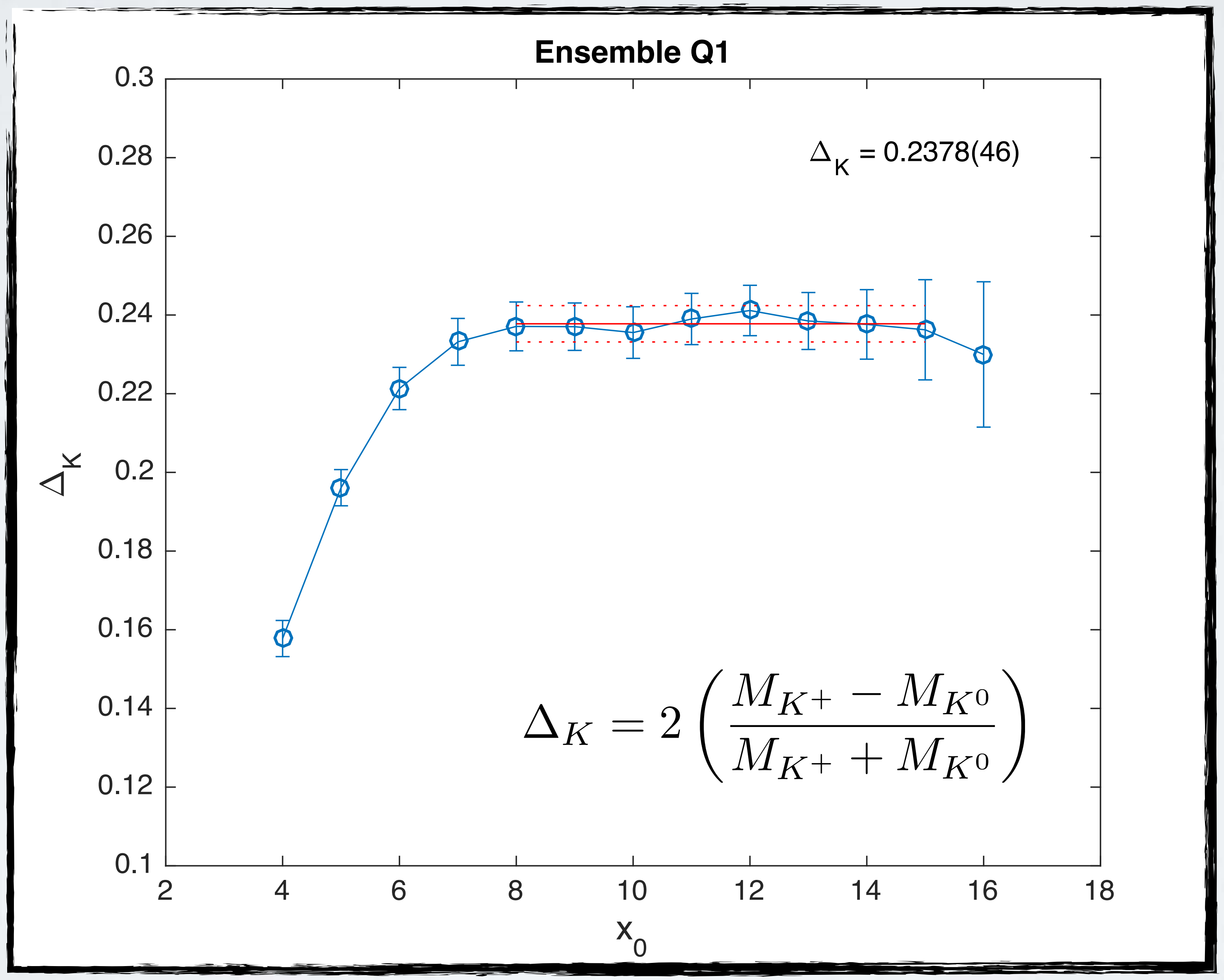
QCD+QED

- Ensemble Q1 with α = 0.05
  - Charged and neutral Kaon effective masses



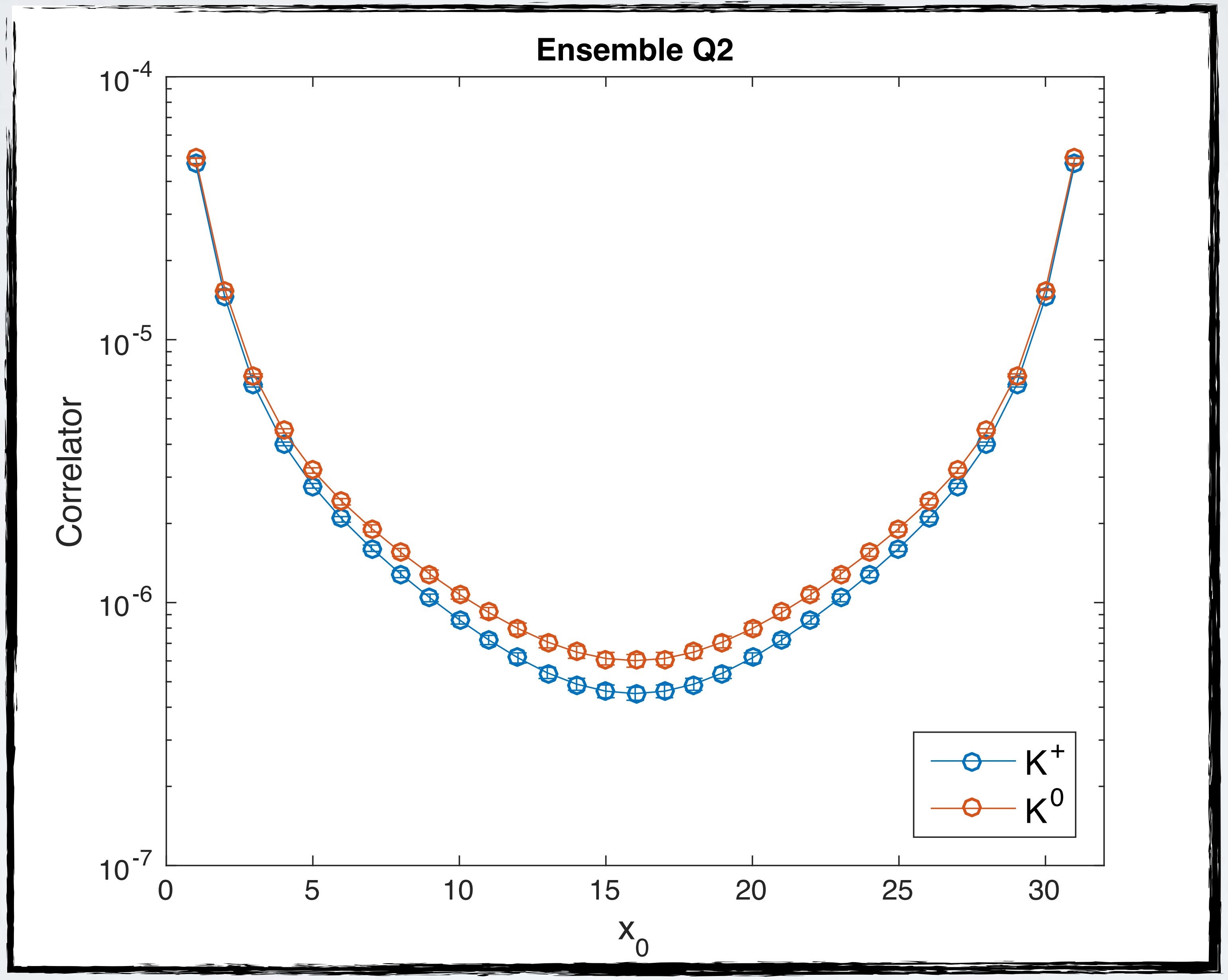
QCD+QED

- **Ensemble Q1 with α = 0.05**
  - Charged and neutral Kaon mass splitting



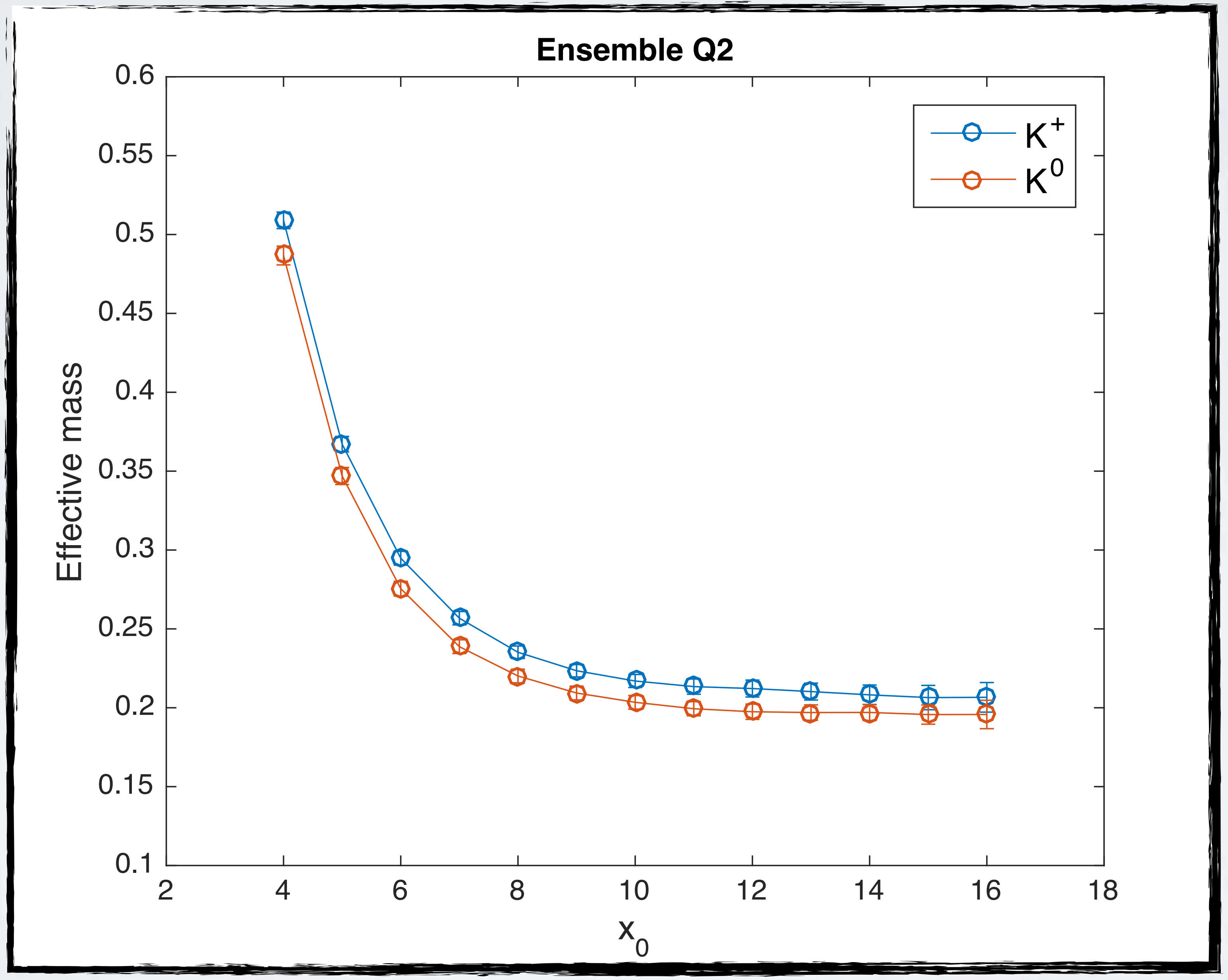
QCD+QED

- **Ensemble Q2 with α = 1/137**
  - Charged and neutral Kaon correlator



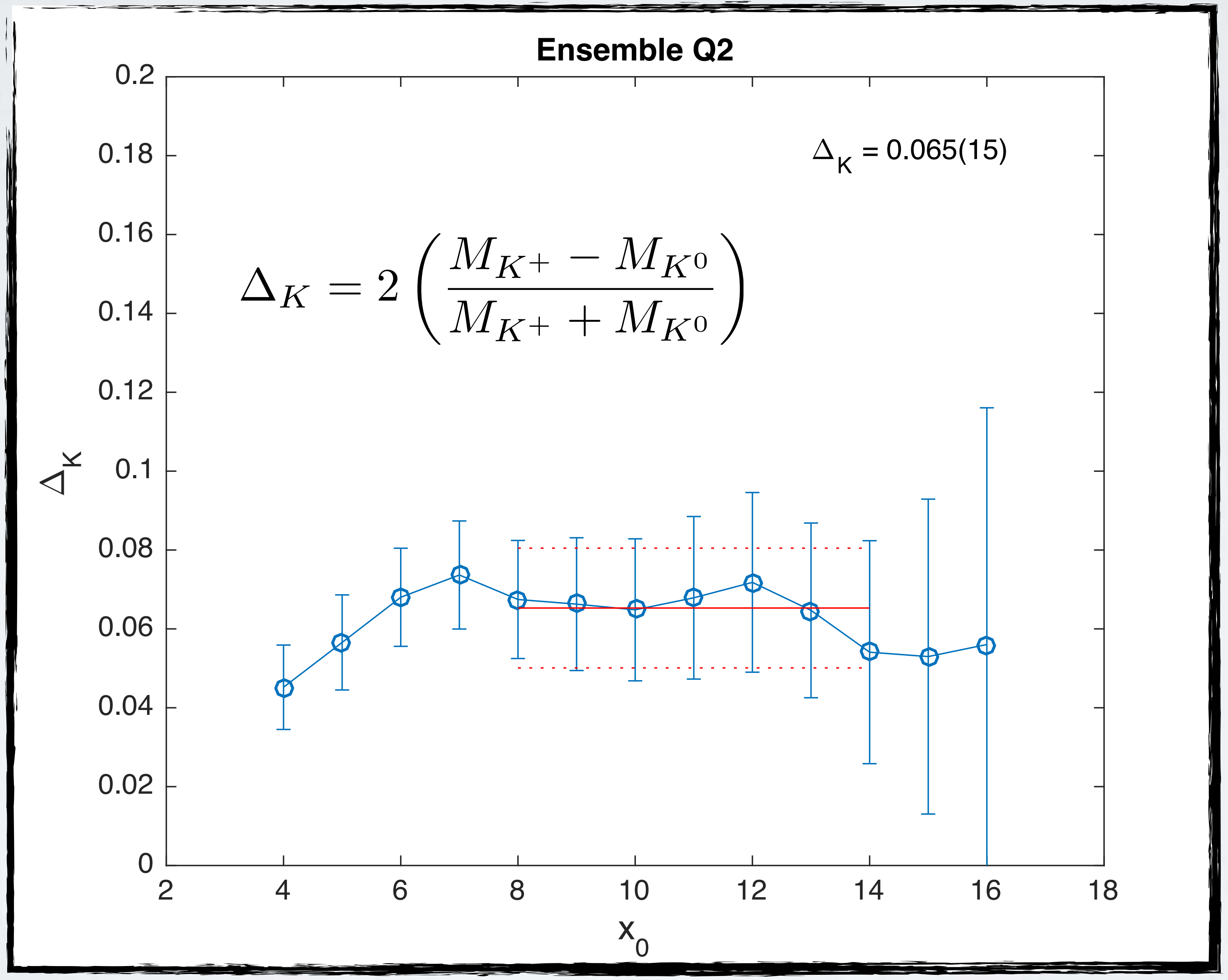
QCD+QED

- Ensemble Q2 with α = 1/137
  - Charged and neutral Kaon effective masses



QCD+QED

- Ensemble Q2 with α = 1/137
  - Charged and neutral Kaon mass splitting



Conclusions

- Simulation code is working
- Simulations with C* boundary conditions works both for QCD and QCD+QED
- Masses of charged hadrons can be extracted in a gauge invariant way with a good signal
- More results are on the way!

Conclusions

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- More results are on the way!

Thank you!

Backup Slides

Fourier Acceleration

- **Evolution of U(1) field is controlled by the eigenvalues of the Laplacian — not all modes evolve equally fast**
  - Change momenta in HMC algorithm

$$\mathcal{H} = \sum_x \pi(x) O(x,y) \pi(y)$$

  - Where

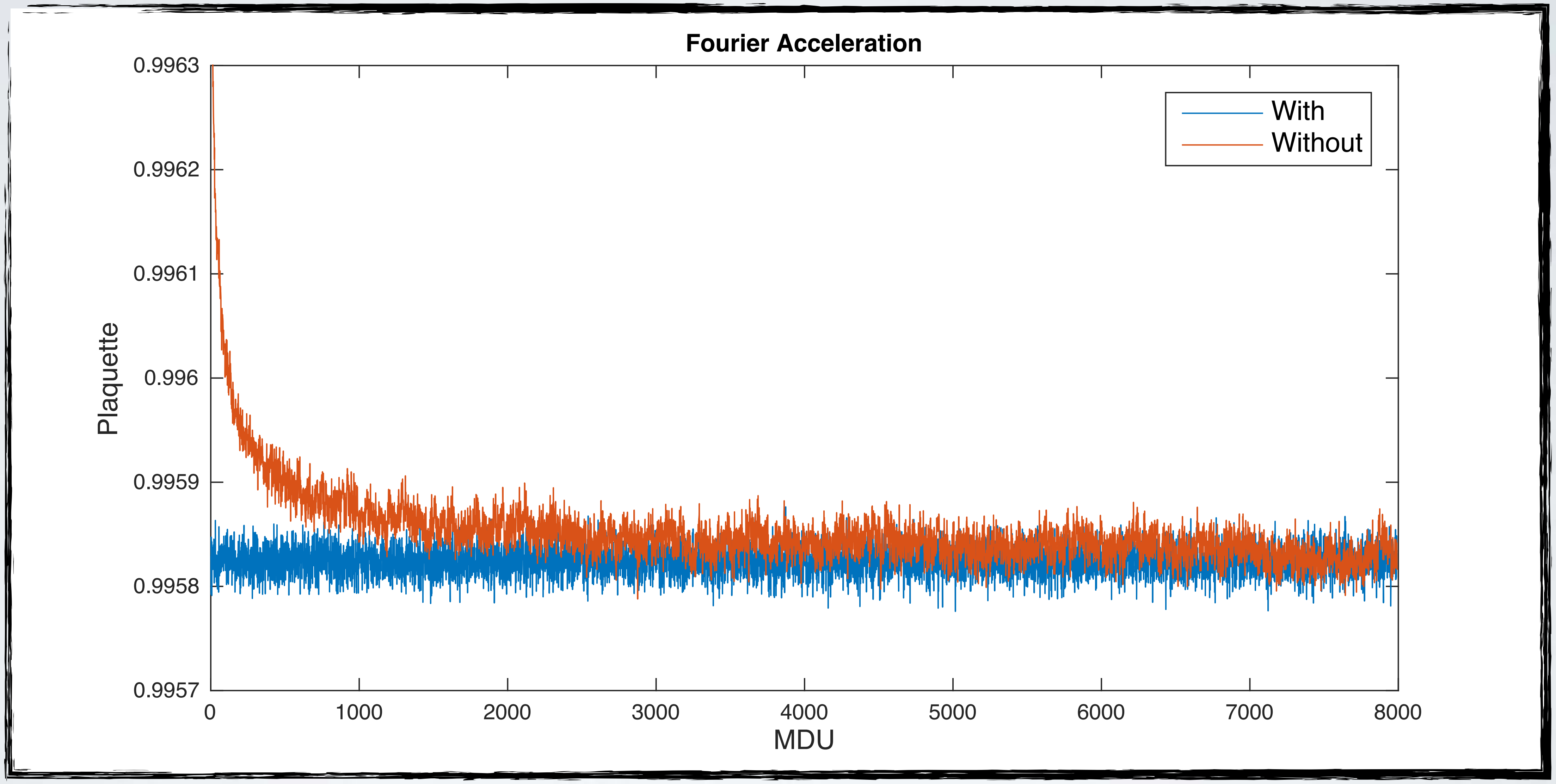
$$O = \frac{1}{-\partial^* \partial}$$

  - Field update

$$\phi(x, t + \delta t) = \phi(x,t) + \delta t O(x,y) \pi(y, t + \delta t/2)$$

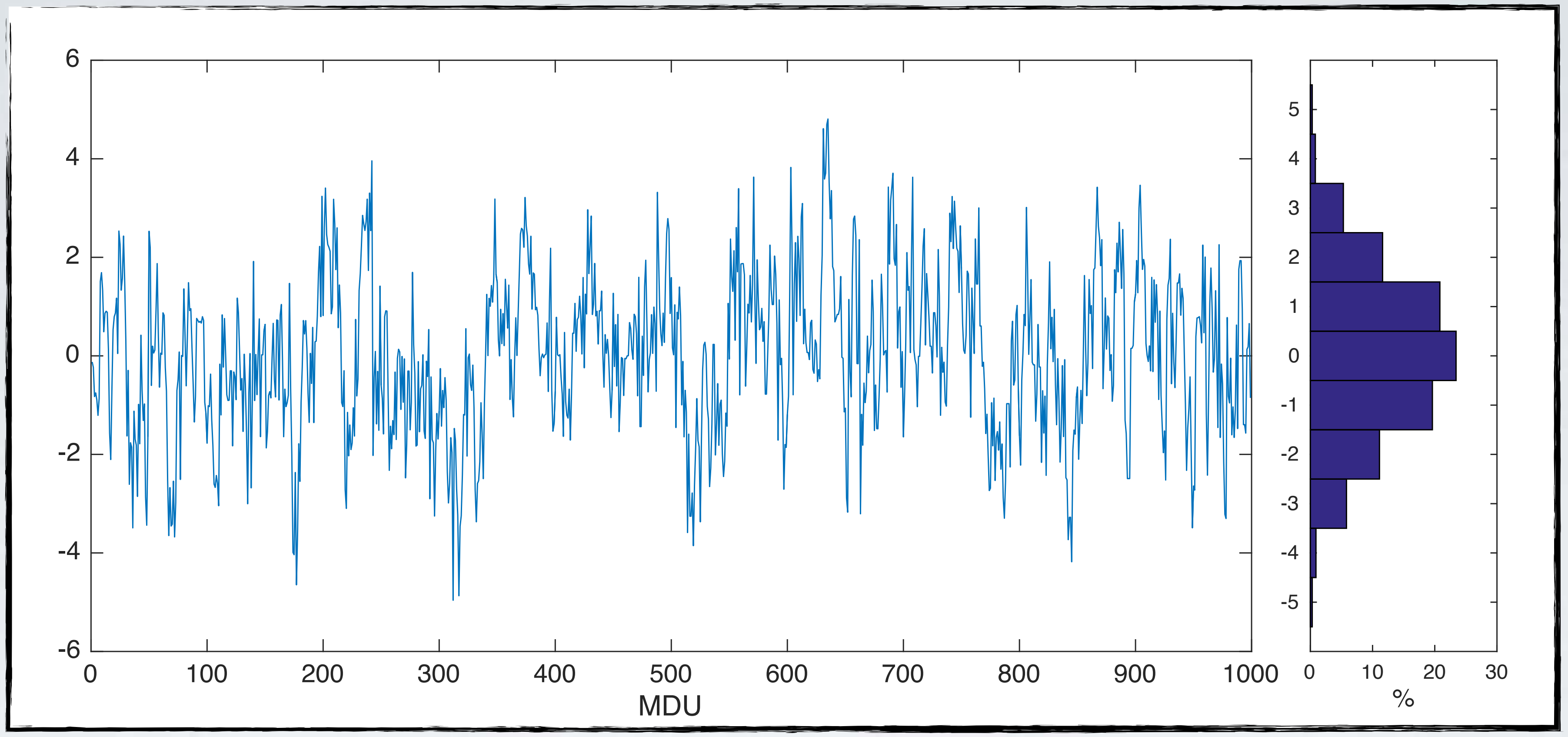
Fourier Acceleration

- Thermalisation of pure gauge at $\beta = 60$

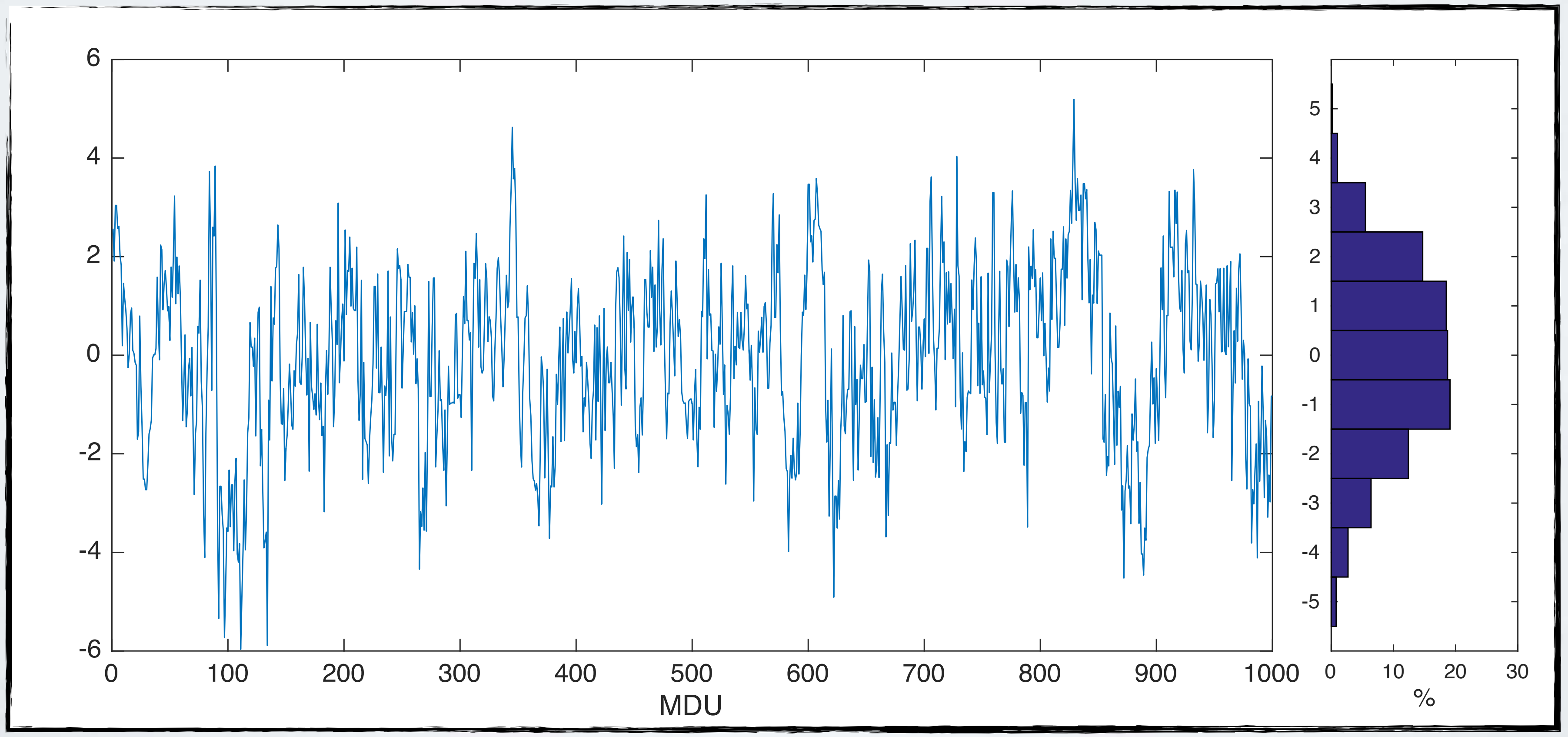


TOPOLOGY

A1

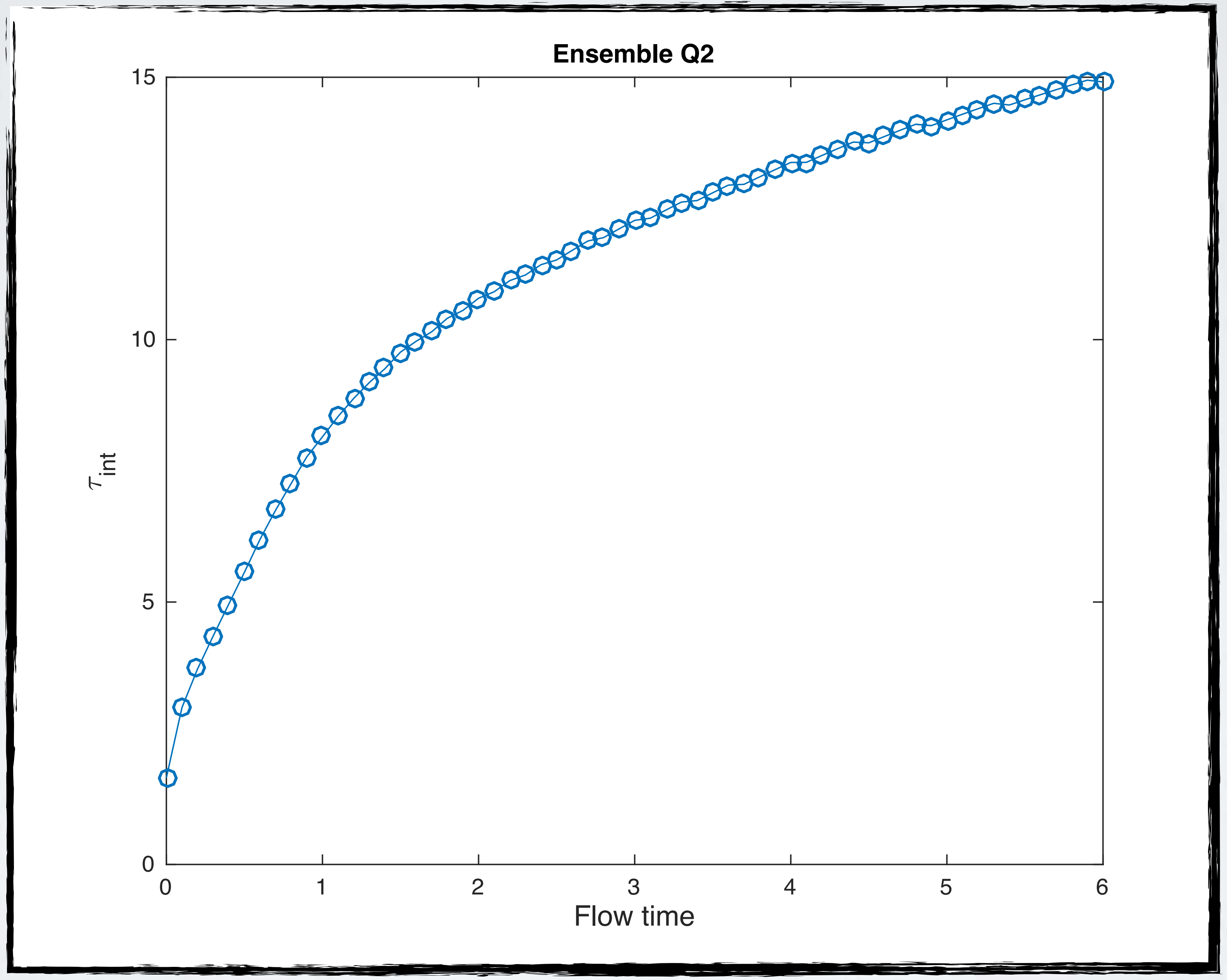


A2



Autocorrelation

- Autocorrelation of E(t) with clover discretisation



OPERATORS

- **Interpolating operators**
  - Gauge invariant and electrically charged

$$\Psi_J(x) = e^{iq\int d^4y\, A_\mu(y) J_\mu(y-x)}\,\psi(x)$$

$$\partial_\mu J_\mu(x) = \delta^4(x)$$
$$J_\mu(x+L) = -J_\mu(x)$$

$$J_\mu(x) \sim \delta(x_0)$$

OPERATORS

- **Coulomb operator**
  - Unique gauge-invariant extension of operator in Coulomb gauge

$$\Psi_c(x) = e^{-iq\int d^3y\, \partial_k A_k(x_0,\mathbf{y})\Phi(\mathbf{y}-\mathbf{x})}\,\psi(x)$$

$$\partial_k \partial_k \Phi(\mathbf{x}) = \delta^3(\mathbf{x})$$
$$\Phi(\mathbf{x}+L) = -\Phi(\mathbf{x})$$

- **String operator**
  - Discretisation is non-trivial

$$\Psi_s(x) = e^{-\frac{iq}{2}\int_{-x_k}^{0} ds\, A_k(x+s\hat{k})}\,\psi(x)\, e^{+\frac{iq}{2}\int_0^{L-x_k} ds\, A_k(x+s\hat{k})}$$

OPERATORS

- **Redefine perturbative expansion for U(1) field**
  - Introduce tunable parameter

$$U_\mu(x) = e^{i\omega A_\mu(x)}$$

  - Gauge action is unchanged when

$$\beta_{\mathrm{QED}} = \frac{1}{\omega^2 e^2}$$

  - Modify fermion coupling

$$n = \frac{q_f}{\omega}, \qquad \bar{\psi} U^n \psi \to q_f A_\mu \bar{\psi}\psi$$

OPERATORS

- **Choice of tunable parameter**
  - For QED we can use $\omega = 1/2$ such that

$$n = \begin{cases} +2 & \text{positron} \\ -2 & \text{electron} \end{cases}$$

  - For QCD+QED we can use $\omega = 1/6$ such that

$$n = \begin{cases} +4 & \text{up quark} \\ -2 & \text{down quark} \end{cases}$$

OPERATORS

- Discretised string operator

$$\Psi_s(x) = \left(\prod_{s=-x_k}^{-1} U_k(x + s\hat{k}) \right)^{\frac{n}{2}} \psi(x) \left(\prod_{s=0}^{L-x_k-1} U_k^\dagger(x + s\hat{k}) \right)^{\frac{n}{2}}$$

- Discretised Coulomb operator

$$\Psi_c(x) = \Psi_s(x) e^{+\frac{in}{2} \sum_{s=0}^{L} A_k^c(x+s\hat{k})}$$

$$A_\mu^c(x) = \Delta^{-1} \partial_k^* F_{k\mu}(x)$$

- In Coulomb gauge $A_\mu^c(x) = A_\mu(x)$ and $\Psi_c(x) = \psi(x)$