HIC for FAIR
Helmholtz International Center

*PhD defence*

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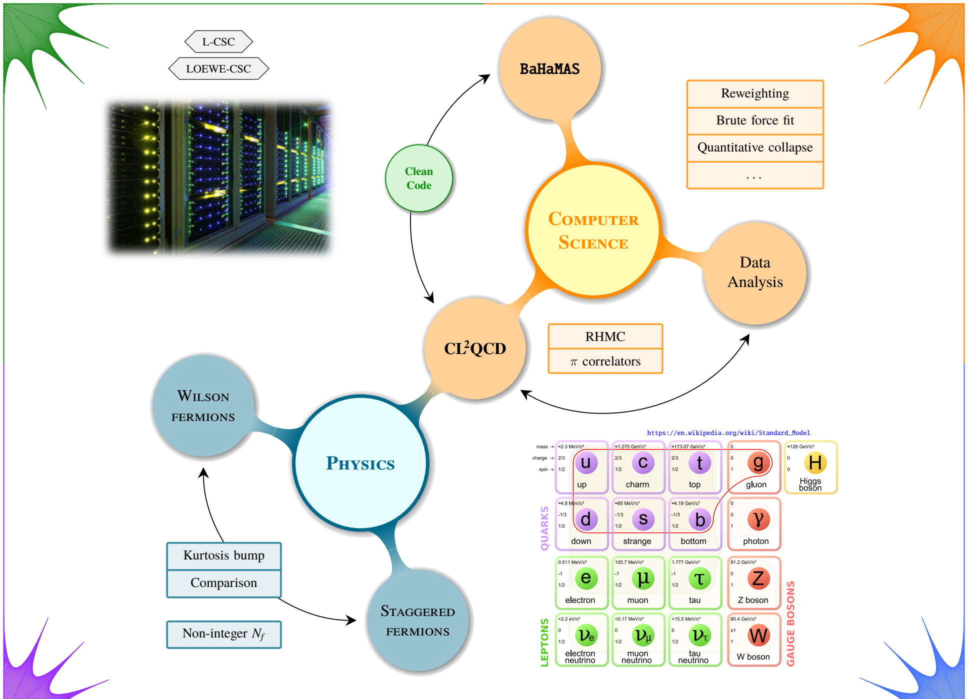
# The QCD phase diagram at purely imaginary chemical potential from the lattice

**Alessandro Sciarra**

**Supervisors:** Prof. Dr. Owe Philipsen
Prof. Dr. Stefan Schramm

GOETHE UNIVERSITÄT FRANKFURT AM MAIN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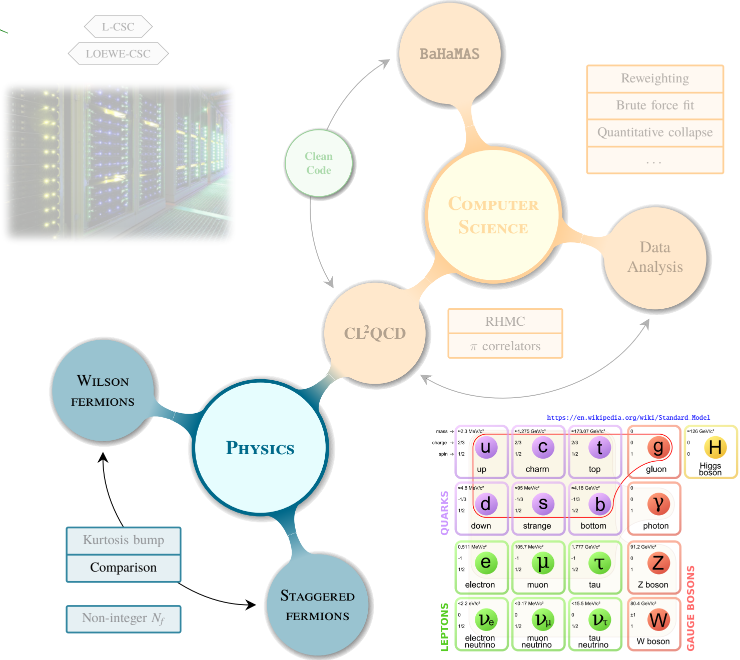
QUARKS
LEPTONS
GAUGE BOSONS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# Outline of the talk

1. Physics background
2. LQCD: why and how?
3. Finite Temperature LQCD at $\mu^2 \leqslant 0$
4. Two flavour QCD at $\mu = \imath\,\mu_I^{\mathrm{RW}}$

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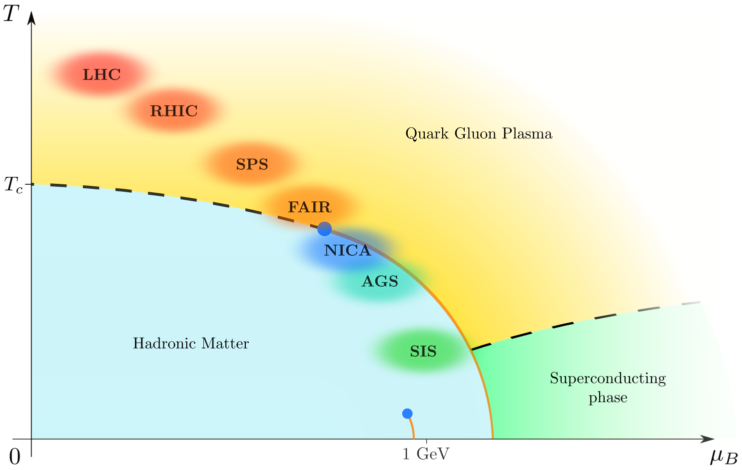

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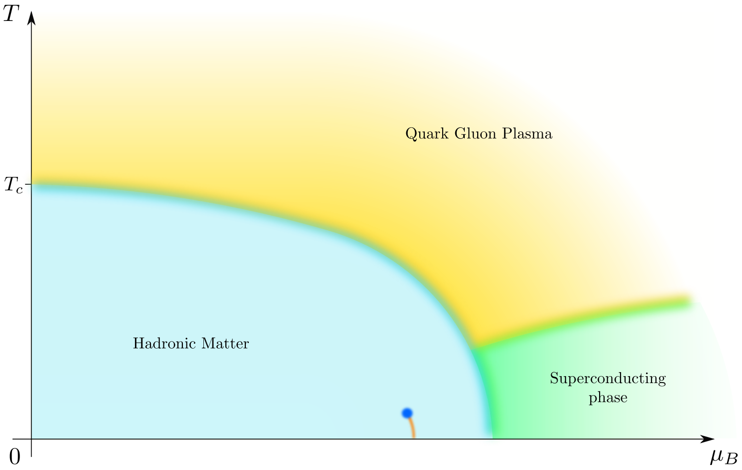

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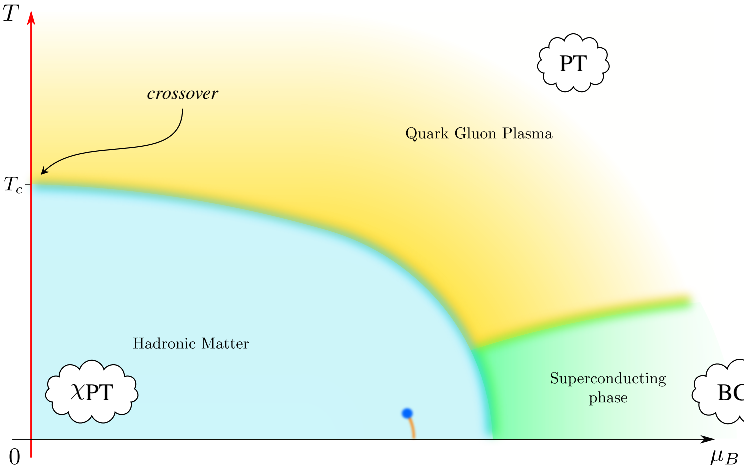
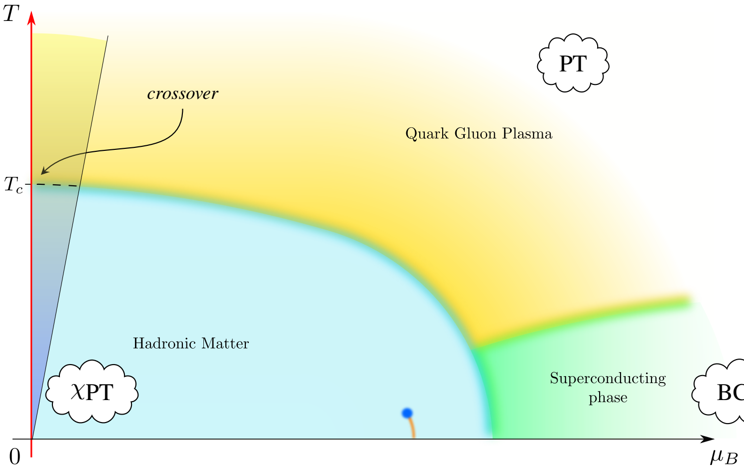



*Pure* LQCD available only at $\mu_B = 0$

# The conjectured QCD phase diagram




LQCD + reweighting to access $\mu_B/T \lesssim 1$ region

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# QCD on the lattice: why?

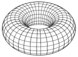
- Solid and well established tool to investigate wide variety of strong interaction phenomena $\longrightarrow$ QCD thermodynamics
- A priori method and exact in the continuum limit
- Technically and numerically challenging
- Rigorous and often involved data analysis mandatory
- Of course, everything should be done properly...

*«We would like numerical QCD to be so reliable that when one detects a numerically significant discrepancy between its prediction and experimental data, one can interpret it as evidence of new physics. »*

[H. Neuberger, Phys.Rev. D70 (2004)]

# QCD on the lattice: how?

$\mathcal{S}^{\text{cont.}} \longrightarrow \mathcal{S}^{\text{latt.}}$



$$\mathcal{S}^{\text{cont.}} = \mathcal{S}^{\text{latt.}} + c_1\, a + c_2\, a^2 + \mathcal{O}(a^3)$$

LATTICE SPACING

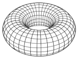
Wilson fermions

Staggered fermions

Many others

# QCD on the lattice: how?

$\mathcal{S}^{\text{cont.}} \longrightarrow \mathcal{S}^{\text{latt.}}$



$$\mathcal{S}[U] = \mathcal{S}_F + \mathcal{S}_G = \bar{\psi} \cdot \mathcal{D}[U] \cdot \psi + \mathcal{S}_G[U]$$

$$\langle O \rangle = \frac{\int D\bar{\psi} D\psi DU e^{-\mathcal{S}} O[U]}{\int D\bar{\psi} D\psi DU e^{-\mathcal{S}}} = \int DU\, O[U] \underbrace{\frac{\det \mathcal{D}[U]\, e^{-\mathcal{S}_G}}{\int DU \, \det \mathcal{D}[U]\, e^{-\mathcal{S}_G}}}_{\text{Prob. distr.} \Leftrightarrow \begin{cases} \det \mathcal{D} \in \mathbb{R} \\ \det \mathcal{D} \geqslant 0 \end{cases}}$$

**Algorithm**

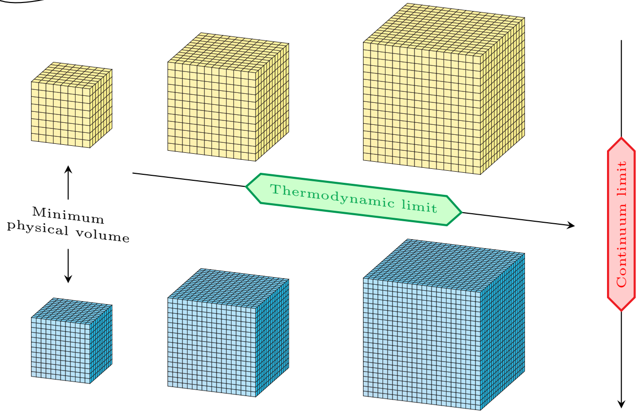
$\{U_1 \cdots U_N\}$

$$\langle O \rangle \approx \frac{1}{N} \sum_{h=1}^{N} O[U_h]$$

# LQCD thermodynamics

$$\frac{1}{T} = a(\beta) \cdot N_t$$

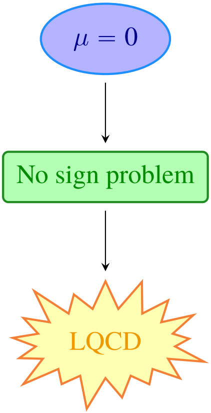
Lattice coupling
Lattice temporal extent
Lattice spacing

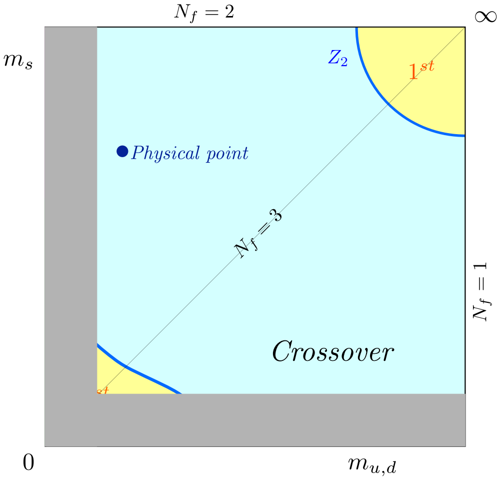


# Outline of the talk

# The Columbia Plot

Too small masses cannot be numerically reached...



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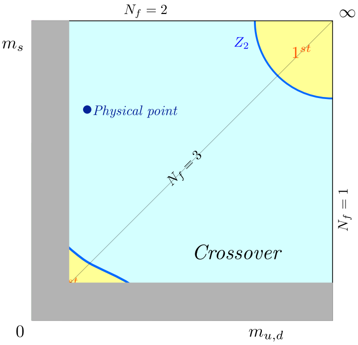
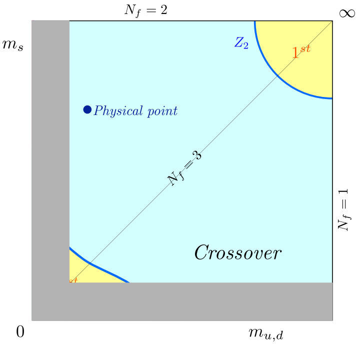


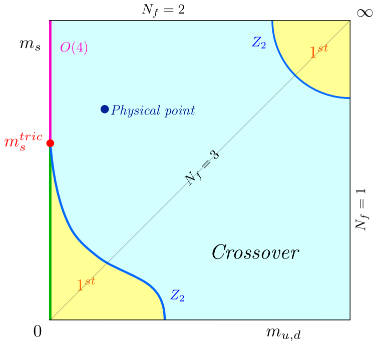



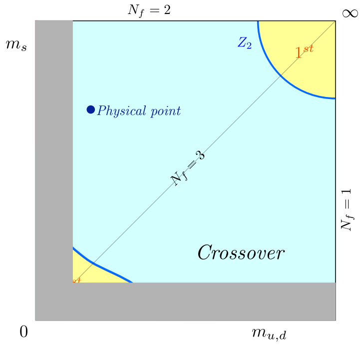

. . . and therefore several scenarios are still possible!

# The Columbia Plot

Too small masses cannot be numerically reached. . .

Second order scenario

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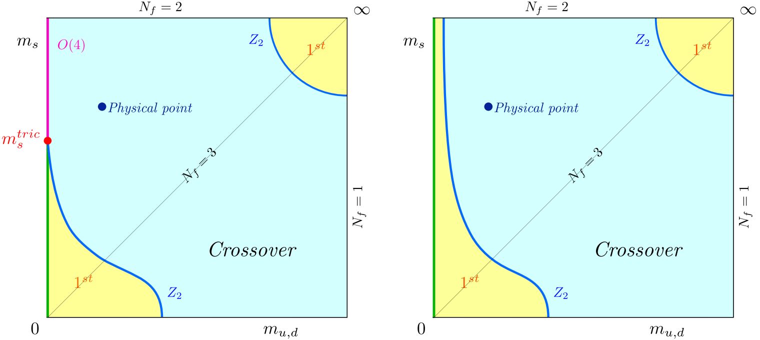
# The Columbia Plot

Too small masses cannot be numerically reached. . .

Second order scenario

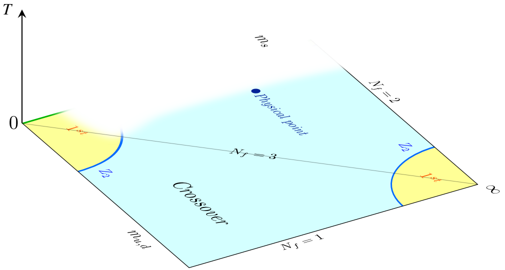
First order scenario




. . . and therefore several scenarios are still possible!

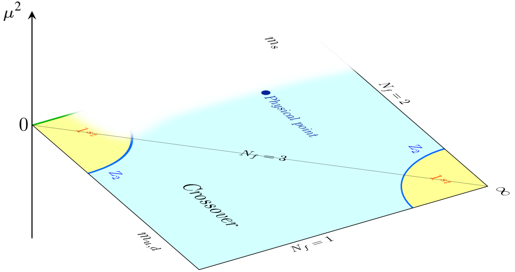
# The parameter space

$T - m_{u,d} - m_s$ and $\mu = 0$



# The parameter space

$T - m_{u,d} - m_s$ and $\mu \leqslant 0$



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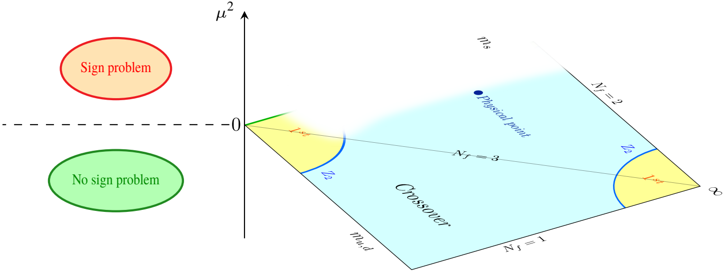
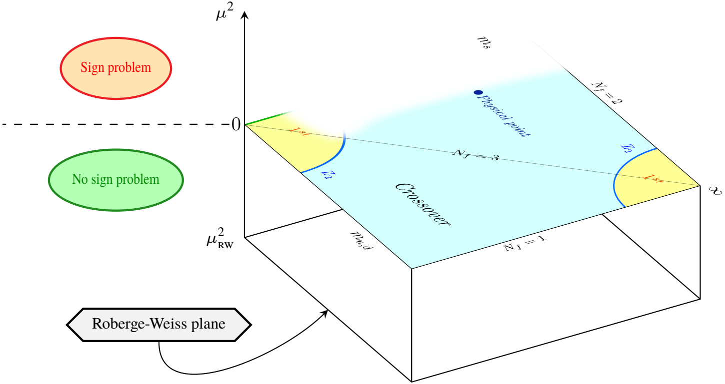



At purely imaginary chemical potential
standard numerical methods are safe [e.g. (R)HMC]

# The parameter space

$T - m_{u,d} - m_s$ and $\mu \lessgtr 0$

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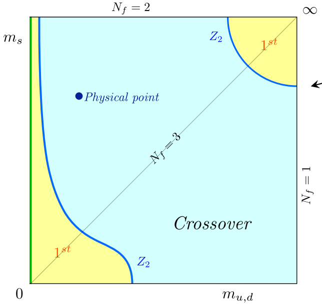
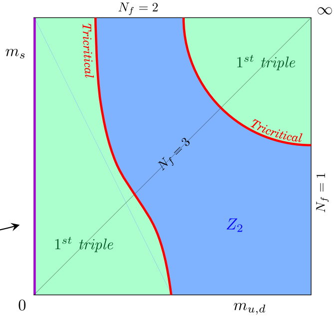
# The 3D Columbia Plot




$1^{st}$ order scenario

$\mu = 0$

$\mu = \mu_{\mathrm{RW}}$



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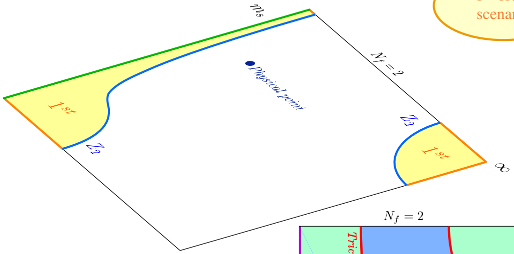


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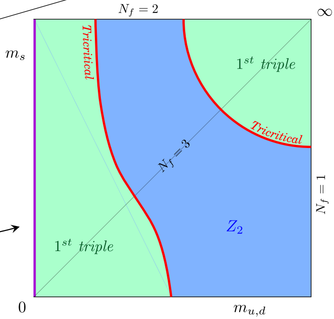

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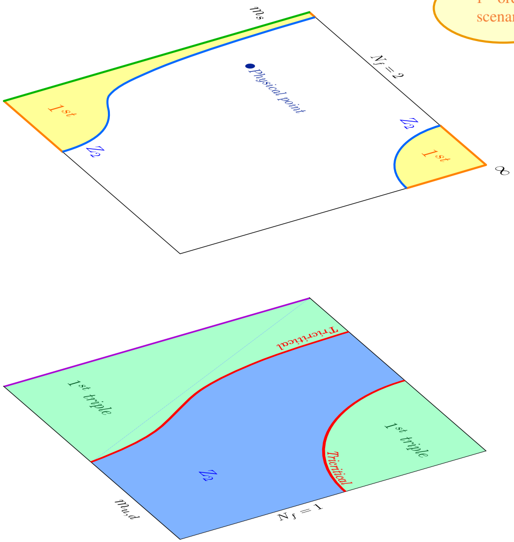

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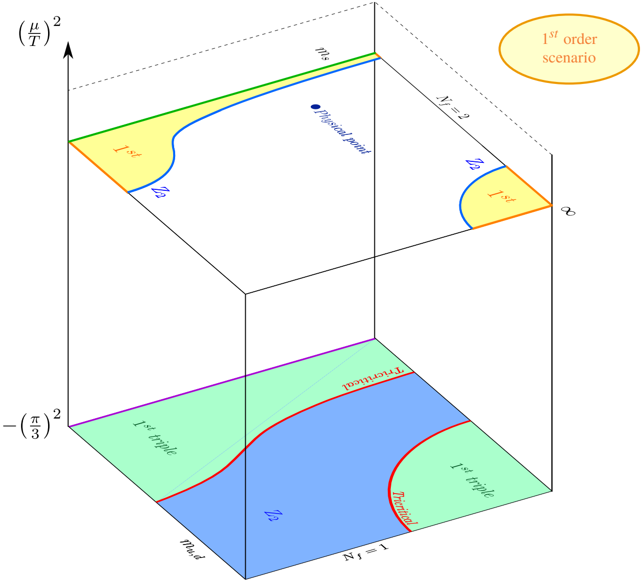

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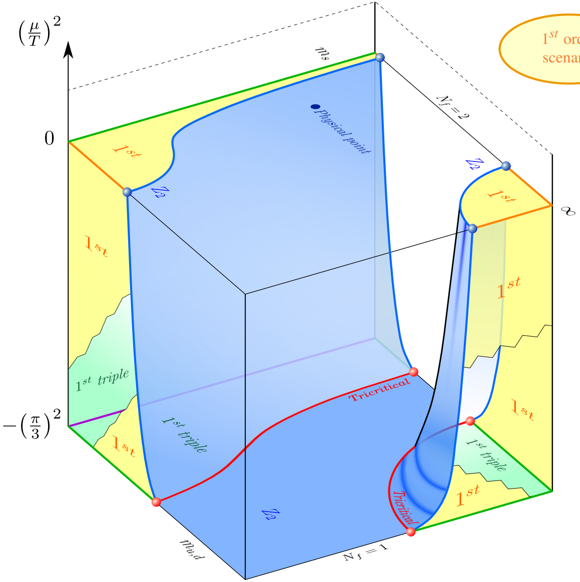


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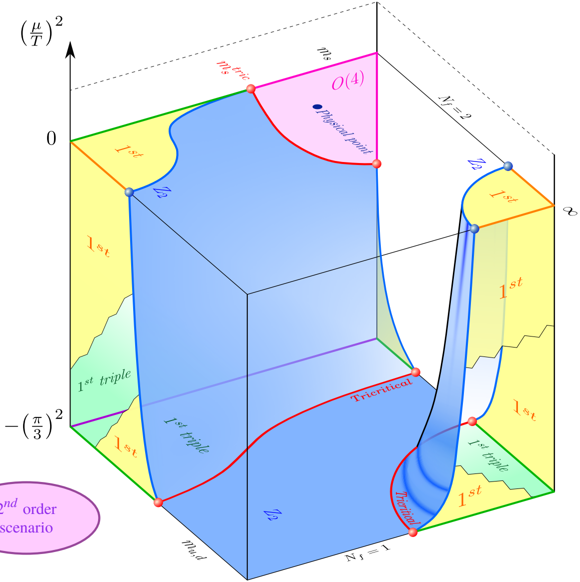


$2^{nd}$ order scenario

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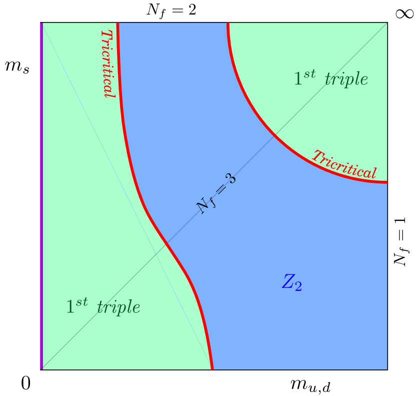
# Numeric setup

## To locate the tricritical mass values



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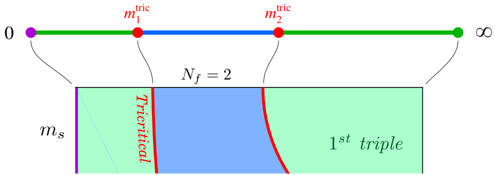


At fixed $N_t = 6$ and $\mu_I = \mu_I^{\text{RW}}$ and given a formulation:

```
for mass in ...; do          # 9 - 17 values (Wilson - Staggered)
   for Ns in ...; do         # at least 3 values >= 2*Nt
      for beta in ...; do    # at least 4 values around transition
         #Run 4 (R)HMC chains [CL2QCD → https://github.com/CL2QCD/cl2qcd]
         #When the statistics is high enough, stop simulation
      done
   done
done
```

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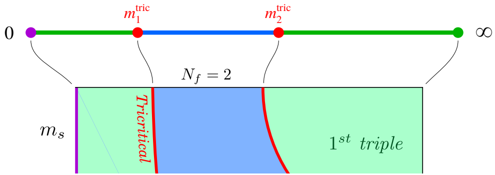


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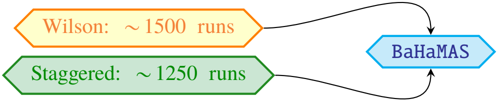
[A. Sciarra et al., Phys.Rev. D93 (2016)]




[A. Sciarra, O. Philipsen, PoS LATTICE (2016)]

# Computational method

## To extract the critical exponent $\nu$

- Calculate kurtosis of the order parameter ($L_{\mathrm{Im}}$) distribution

$$B_4(\beta, N_s) = \frac{\langle (L_{\mathrm{Im}} - \langle L_{\mathrm{Im}} \rangle)^4 \rangle}{\langle (L_{\mathrm{Im}} - \langle L_{\mathrm{Im}} \rangle)^2 \rangle^2} \xrightarrow{N_s \to \infty} \begin{cases} 1 & \text{First order} \\ 1.5 & \text{First order triple} \\ 1.604 & \text{Second order} \\ 3 & \text{Crossover} \end{cases}$$

# Computational method

## To extract the critical exponent $\nu$

- Calculate kurtosis of the order parameter ($L_{\mathrm{Im}}$) distribution
- Finite size scaling via multi-branch fit to extract $\nu$

$$B_4(\beta, N_s) \simeq B_4(\beta_c, \infty) + a_1 \underbrace{(\beta - \beta_c)\, N_s^{1/\nu}}_{x} \quad \text{around } \beta_c$$

- Tricky fit due to unknown fit ranges (the region should be fixed in $x$ around $x_c = 0$)
  $\Rightarrow$ Fits in all possible $\beta$-ranges are performed + filtering

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- Tricky fit due to unknown fit ranges (the region should be fixed in $x$ around $x_c = 0$)
  $\Rightarrow$ Fits in all possible $\beta$-ranges are performed + filtering
- Obtain $\beta_c$ and $\nu$ *independently* attributing a quality $Q$ to the collapse plots!

$$Q(\bar{\beta}_c, \bar{\nu}, \Delta x) \equiv \frac{1}{\Delta x} \int_{x_{\min}}^{x_{\max}} \left\{ N_V \sum_{i=1}^{N_V} \Big[B_4\big(x(\bar{\beta}_c, \bar{\nu}, V_i)\big)\Big]^2 - \left[\sum_{i=1}^{N_V} B_4\big(x(\bar{\beta}_c, \bar{\nu}, V_i)\big)\right]^2 \right\} \mathrm{d}x$$

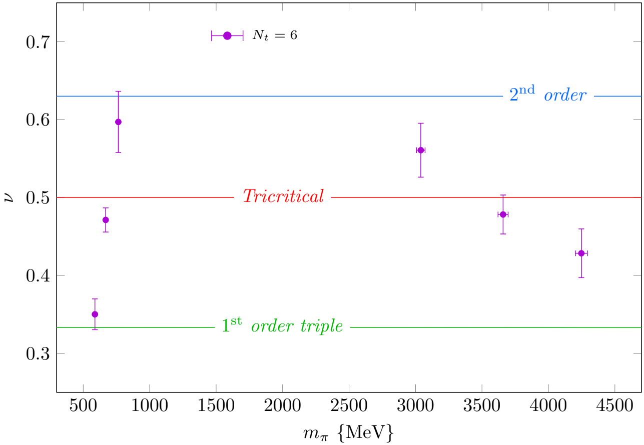
[M. Barkema, G. Newman, Phys.Rev. E53 (1996)]

Fixed $\Delta x$, minimise Q and find $(\bar{\beta}_c, \bar{\nu})$

Find $(\beta_c, \nu)$ extrapolating $(\bar{\beta}_c, \bar{\nu})$ to $\Delta x = 0$

# $N_t = 6$ with Wilson fermions

## Only brute force fit analysis



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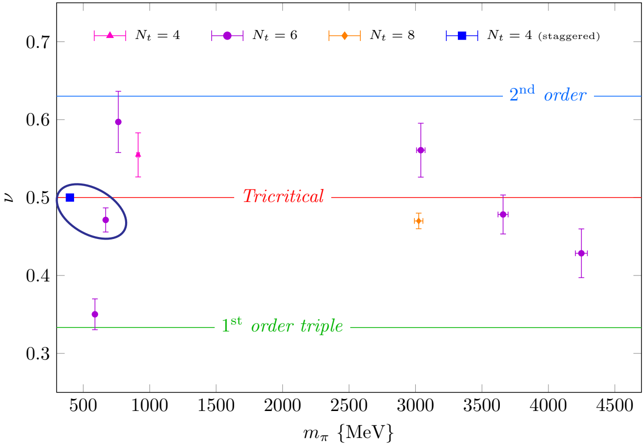


Still big cutoff effects on tricritical masses

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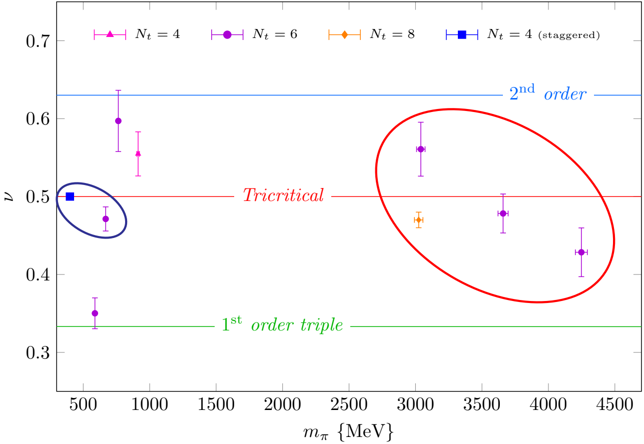
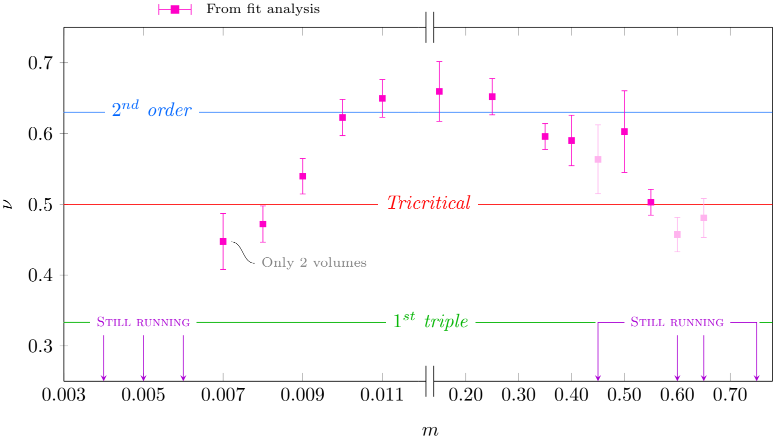



$a\, m_\pi > 1$

Still big cutoff effects on tricritical masses

# $N_t = 6$ with staggered fermions



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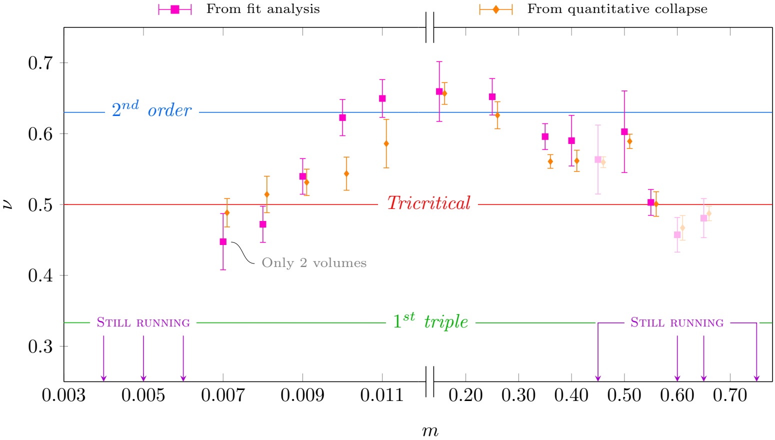


Two methods equivalent, but collapse more precise

Few more $m$ needed to constrain tricritical masses

# The tricritical points position

## On $N_t = 6$ lattices and $N_f = 2$

### Wilson fermions

$$\kappa^{\text{tric}}_{\text{light}} = 0.1625(25) \qquad \kappa^{\text{tric}}_{\text{heavy}} = 0.110(10)$$

$$m^{\text{tric}}_{\pi} = 669^{+95}_{-81}\,\text{MeV} \qquad m^{\text{tric}}_{\pi} = 3.7(6)\,\text{GeV}$$

### Staggered fermions

$$m^{\text{tric}}_{\text{light}} = 0.008^{+0.002}_{-0.003} \qquad m^{\text{tric}}_{\text{heavy}} = 0.55(10)$$

$$m^{\text{tric}}_{\pi} \approx 350\,\text{MeV} \qquad m^{\text{tric}}_{\pi} \approx 2.8\,\text{GeV}$$

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cutoff effects

$a\, m_\pi > 1$

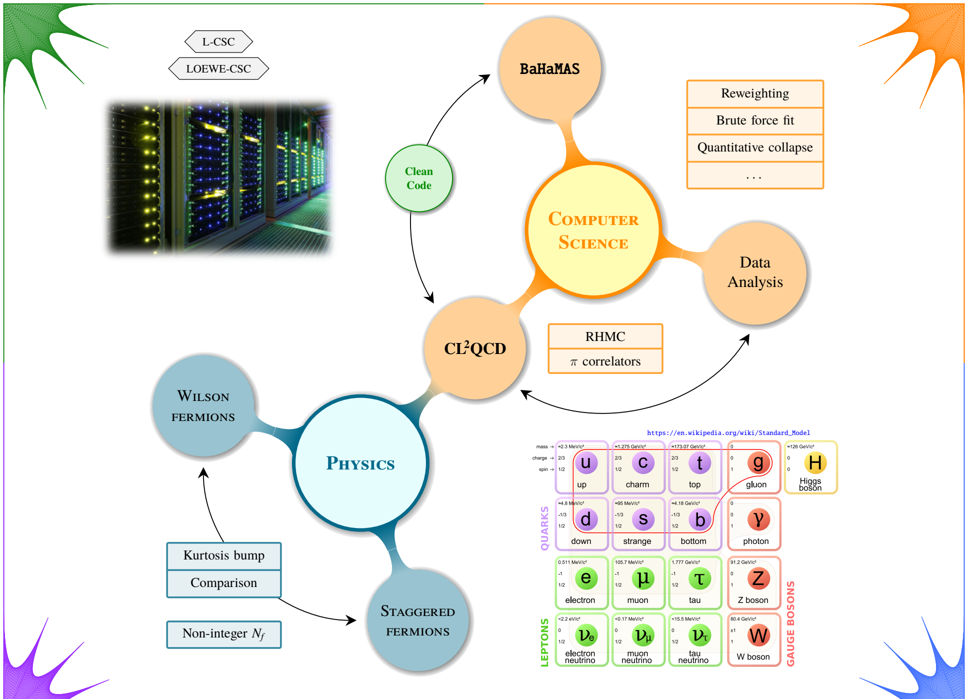
# Summary and perspectives

- The study of the QCD phase diagram is challenging both experimentally and theoretically
- Understanding the structure of the Columbia Plot would help to get insights about it
- Many aspects still unknown (e.g. the order of the transition in the $N_f = 2$ massless limit)
- Lattice QCD at purely imaginary $\mu$ is not affected by the sign problem
- It is possible to take advantage of scaling laws (e.g. tricritical scaling)

**In my Ph.D.**

- Implemented RHMC algorithm with staggered fermions in **CL$^2$QCD**
- Implemented series of tools missing but important (reweighting, **BaHaMAS**, etc.)
- Developed new, meticulous data analysis strategy (brute force fit, quantitative collapse)
- Located tricritical points in RW plane (two flavours, Wilson and staggered, $N_t = 6$)
- Developed analytic model to explain feature of data (Kurtosis bump)
- The data analysis strategy is now on a much more solid ground
- Still large cutoff effects $\Rightarrow$ finer lattices needed, extremely costly though!

*«Patience and diligence, like faith, remove mountains.»* – William Penn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# Kurtosis bump

# The Kurtosis bump

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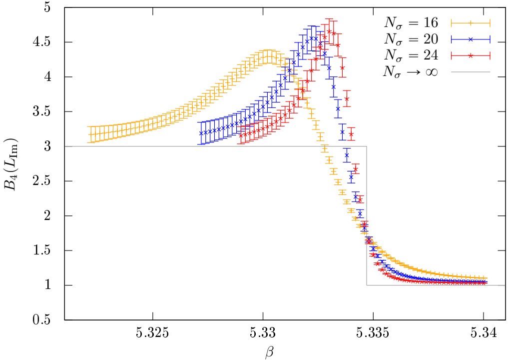
Back to overview

# The Kurtosis bump

$$B_4(\beta, N_s) = \frac{\langle (L_{\rm Im} - \langle L_{\rm Im}\rangle)^4\rangle}{\langle (L_{\rm Im} - \langle L_{\rm Im}\rangle)^2\rangle^2} \xrightarrow{N_s\to\infty} \begin{cases} 1 & \text{First order} \\ 1.5 & \text{First order triple} \\ 1.604 & \text{Second order} \\ 3 & \text{Crossover} \end{cases}$$

Wilson fermions: $N_f = 2$ $\mu_I = \mu_I^{\rm RW}$ $\kappa = 0.165$

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# A descriptive model

## Looking at the order parameter distribution

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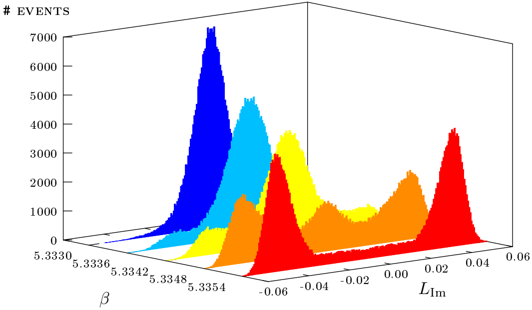
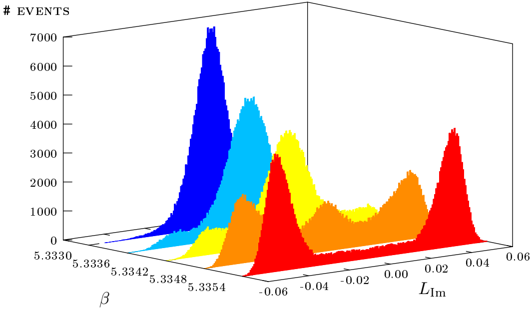


# A descriptive model

## Looking at the order parameter distribution

$$\mathcal{P}(x) \equiv w_o\, \mathcal{N}(-d,\sigma) + w_i\, \mathcal{N}(0,\sigma) + w_o\, \mathcal{N}(d,\sigma)$$

$$\mathcal{N}(\mu,\sigma) \equiv \frac{1}{\sigma\sqrt{2\pi}}\, e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

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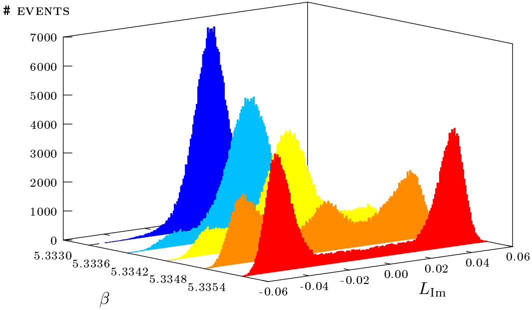
# A descriptive model

## Looking at the order parameter distribution

$$\mathcal{P}(x) \equiv w_o\,\mathcal{N}(-d,\sigma) + w_i\,\mathcal{N}(0,\sigma) + w_o\,\mathcal{N}(d,\sigma)$$

$$2w_o + w_i = 1$$

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# A descriptive model

## Looking at the order parameter distribution

$$\mathcal{P}(x) \equiv w_o\,\mathcal{N}(-d,\sigma) + w_i\,\mathcal{N}(0,\sigma) + w_o\,\mathcal{N}(d,\sigma)$$

$$2w_o + w_i = 1$$

$$\lim_{d\to 0} w_i(d) = 1 \qquad \lim_{d\to 0} w_o(d) = 0 \qquad \lim_{d\to \infty} w_i(d) = 0 \qquad \lim_{d\to \infty} w_o(d) = \frac{1}{2}$$

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# A descriptive model

## Looking at the order parameter distribution

$$\mathcal{P}(x) \equiv w_o\,\mathcal{N}(-d,\sigma) + w_i\,\mathcal{N}(0,\sigma) + w_o\,\mathcal{N}(d,\sigma)$$

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$$\lim_{d\to 0} w_i(d) = 1 \qquad \lim_{d\to 0} w_o(d) = 0 \qquad \lim_{d\to \infty} w_i(d) = 0 \qquad \lim_{d\to \infty} w_o(d) = \frac{1}{2}$$

$$w_i(d) = \frac{\frac{1}{\alpha d+1}}{\frac{1}{\alpha d+1} + 2\left(1 - \frac{1}{\frac{d}{\alpha}+1}\right)} = \frac{\alpha + d}{\alpha + 3d + 2\alpha d^2}$$

$$w_o(d) = \frac{1 - \frac{1}{\frac{d}{\alpha}+1}}{\frac{1}{\alpha d+1} + 2\left(1 - \frac{1}{\frac{d}{\alpha}+1}\right)} = \frac{d\,(1 + \alpha d)}{\alpha + 3d + 2\alpha d^2}$$

$\alpha > 0$ parameter to calibrate change of weights

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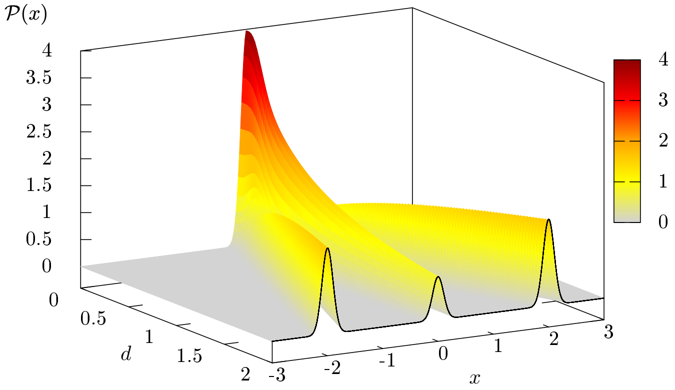
# A descriptive model

## Looking at the order parameter distribution

$\sigma = 0.1 \qquad \alpha = 1$



# Does it work?

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# Does it work?

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$$B_4\big[\mathcal{P}(x)\big] = \frac{\int_{-\infty}^{+\infty} x^4 \; \mathcal{P}(x) \; \mathrm{d}x}{\left[\int_{-\infty}^{+\infty} x^2 \; \mathcal{P}(x) \; \mathrm{d}x\right]^2}$$

$$\Downarrow$$

$$B_4\big[\mathcal{P}(x)\big] = 3 - \frac{2\,d^5\,(1+\alpha d)\,(4\alpha d^2+3d-\alpha)}{[2\,d^3\,(1+\alpha d)+\sigma^2\,(\alpha+3d+2\alpha d^2)]^2}$$

$$\Downarrow$$

$$B_4 > 3 \quad \Leftrightarrow \quad 0 < d < \frac{-3+\sqrt{9+16\alpha^2}}{8\alpha}$$

# Does it work?

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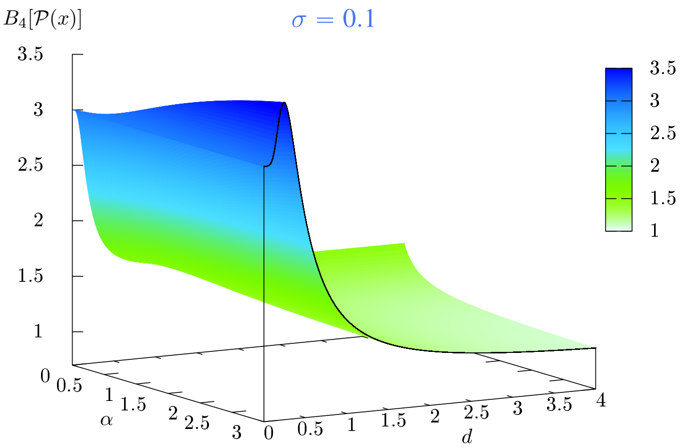
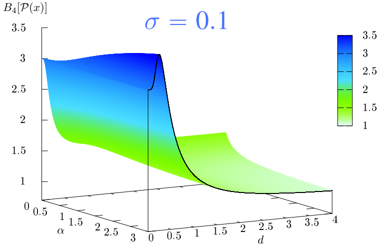
$\sigma = 0.1$



# Connection to physical parameters




- Clearly, it has to be $d = d(\beta)$
- The kurtosis has to stay on the value 3 for $\beta \ll \beta_c$
- The bump should occur at $\beta \lesssim \beta_c$ and it should be $B_4(\beta_c) = 1.5$
- The kurtosis has to stay on the value 1 for $\beta \gg \beta_c$
- The transition should happen faster for larger volumes

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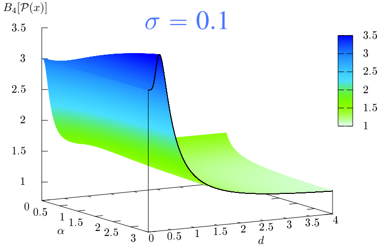
# Connection to physical parameters




$$d(\alpha, \beta) = \frac{e^{\alpha\beta} - 1}{e^{\alpha\beta_c} - 1}$$

$$\alpha \propto N_s$$

$$\sigma \propto \alpha^{-1}$$

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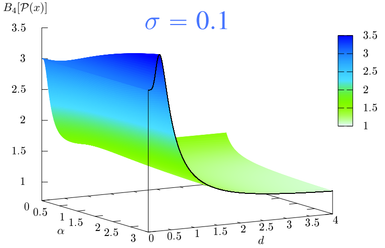
# Connection to physical parameters

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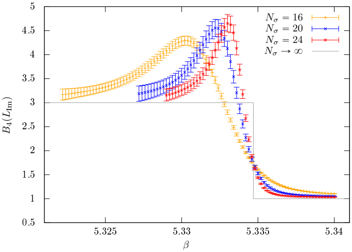


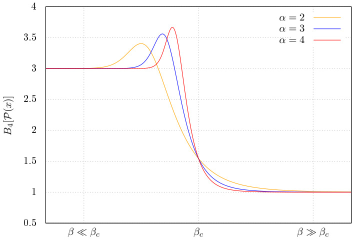


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# Connection to physical parameters

$$\lim_{\alpha\to\infty} B_4\left[\mathcal{P}(x)\right] = \begin{cases} 3 & \text{for} \quad \beta < \beta_c \\ 1 & \text{for} \quad \beta > \beta_c \end{cases}$$

$$\lim_{\alpha\to\infty} B_4\left[\mathcal{P}(x)\right]_{\beta=\beta_c} = 1.5$$

$$d(\alpha,\beta) = \frac{e^{\alpha\beta}-1}{e^{\alpha\beta_c}-1}$$

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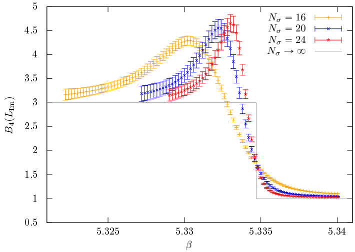


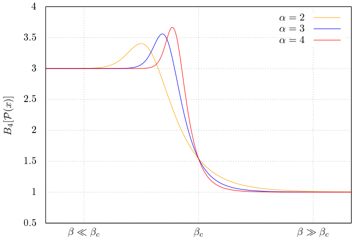

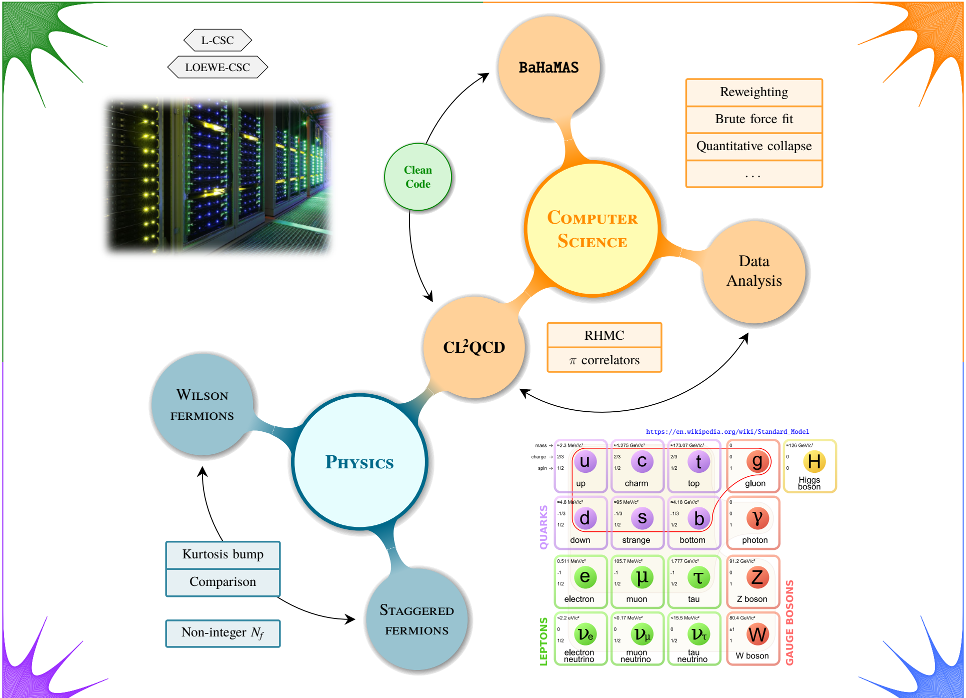
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muon
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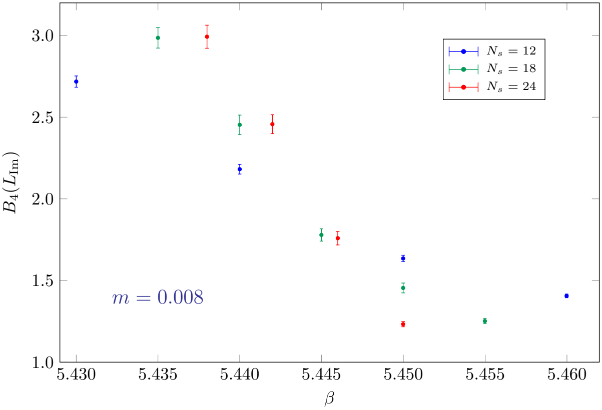
# Brute force fit

# The brute force fit: an example

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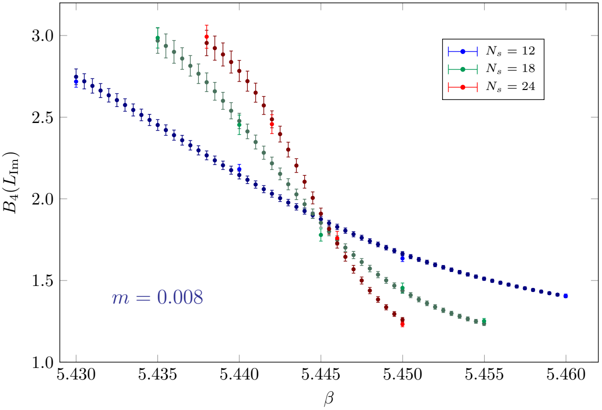
# The brute force fit: an example

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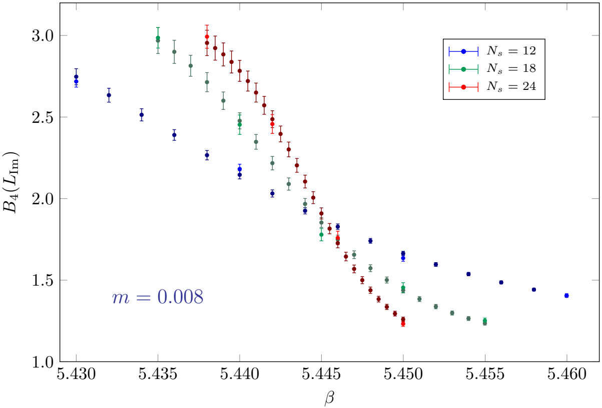
# The brute force fit: an example

$$B_4(\beta, N_s) \simeq B_4(\beta_c, \infty) + a_1 \underbrace{(\beta - \beta_c) N_s^{1/\nu}}_{x} \quad \text{around } \beta_c$$

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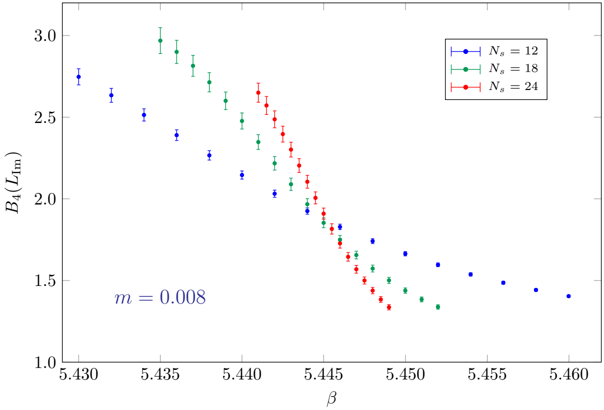
# The brute force fit: an example

$$B_4(\beta, N_s) \simeq {\color{red}B_4(\beta_c, \infty)} + {\color{red}a_1} \underbrace{(\beta - {\color{red}\beta_c})\, N_s^{1/{\color{red}\nu}}}_{x} \quad \text{around } \beta_c$$

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# The brute force fit: an example

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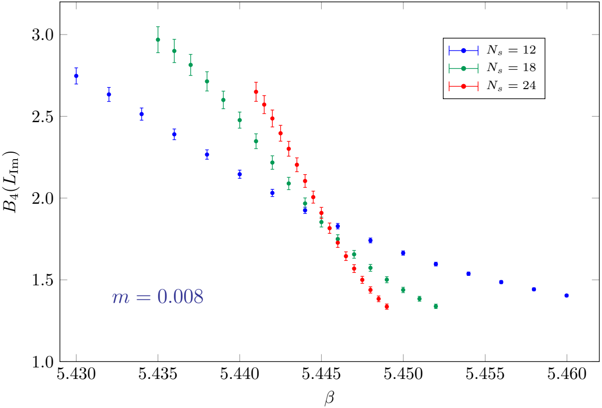


17 points

19 points

18 points

In total $136 \times 171 \times 153 = 3\,558\,168$ possible fits!

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# The brute force fit: an example

$$B_4(\beta, N_s) \simeq B_4(\beta_c, \infty) + a_1 \underbrace{(\beta - \beta_c) N_s^{1/\nu}}_{x} \quad \text{around } \beta_c$$

Typically $\mathcal{O}(10^6)$ possible fits, but not all have to be performed:

- At least 2 points per volume have to be used
- $N_{s_1} < \ldots < N_{s_n} \quad \Rightarrow \quad I_1 \supseteq \cdots \supseteq I_n$

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3 558 168 → 250 098 fits

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3 558 168 → 250 098 fits

After having done the remaining fits, filter the results:

- $1 - \delta < \chi^2 < 1 + \delta$ (typically $\delta \approx 0.2$)
- Minimum overlap of intervals in variable $x$ has to be 80%
- The fit with highest minimum symmetry percentage (in $x$ around 0) is picked

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Usually the final choice is made out a small bunch of fits

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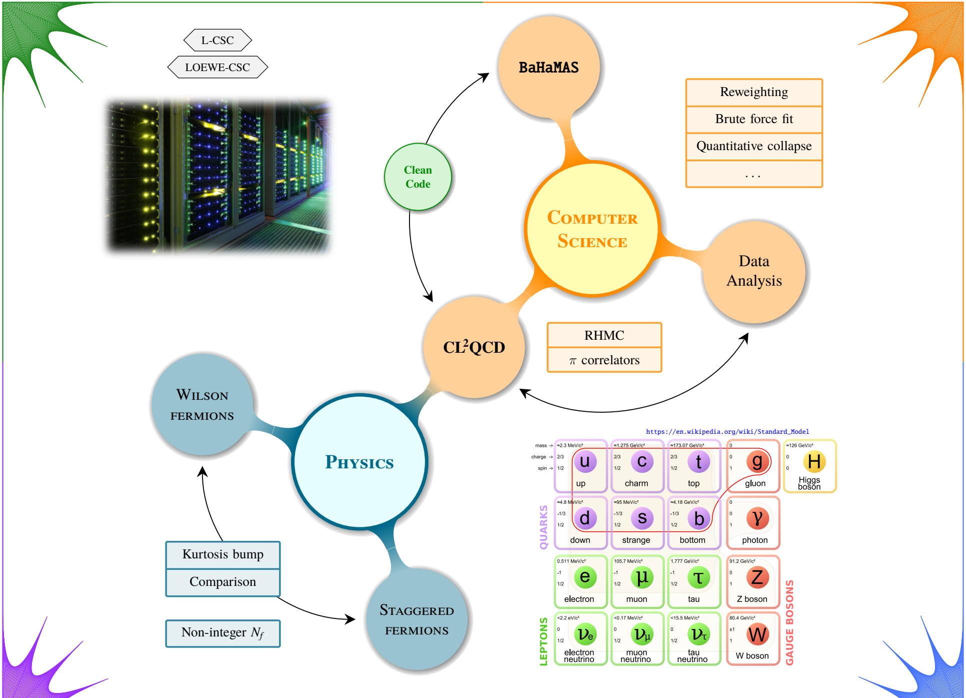
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W boson
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# Quantitative collapse

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# The data collapse

## A quantitative approach

$$B_4 = g\left(t\,N_s^{1/\nu}\right)$$

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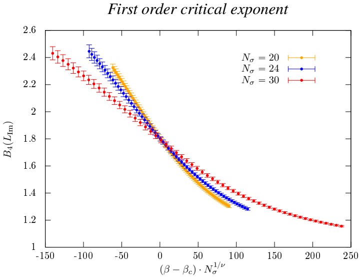
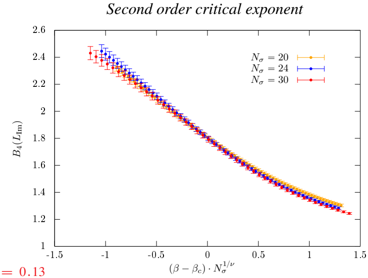


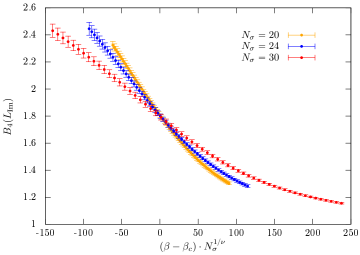

$\kappa = 0.13$

# The data collapse

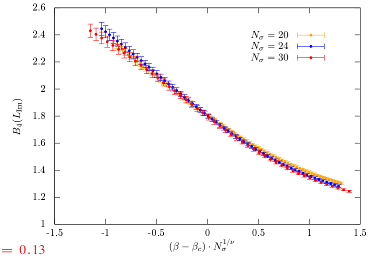
## A quantitative approach

$$B_4 = g\left(t\, N_s^{1/\nu}\right)$$

*First order critical exponent*




*Second order critical exponent*




$\kappa = 0.13$

Judgement by eye is only qualitative, how to estimate $\nu$?

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# The data collapse

## A quantitative approach

[M. Barkema, G. Newman, Phys.Rev. E53 (1996)]

$$Q(\bar{\beta}_c, \bar{\nu}, \Delta x) \equiv \frac{1}{\Delta x} \int_{x_{\min}}^{x_{\max}} \left\{ N_V \sum_{i=1}^{N_V} \Big[ B_4\big(x(\bar{\beta}_c, \bar{\nu}, V_i)\big) \Big]^2 - \left[ \sum_{i=1}^{N_V} B_4\big(x(\bar{\beta}_c, \bar{\nu}, V_i)\big) \right]^2 \right\} \mathrm{d}x$$

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# The data collapse

## A quantitative approach

[M. Barkema, G. Newman, Phys.Rev. E53 (1996)]

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- Functional form of $B_4(x)$ is unknown
- Interpolating reweighted points (per each $N_s$), it is possible to get $Q$ numerically
- At fixed $\Delta x$, $\bar{\nu}$ and $\bar{\beta}_c$ are estimated minimising $Q(\bar{\beta}_c, \bar{\nu}, \Delta x)$
- $\Delta x$ must contain data from all volumes (no extrapolation!)
- Attribute an uncertainty to $\nu$ and $\beta_c$ repeating the steps above per each bootstrap estimator obtained reweighting the data
- Width of scaling region around critical temperature unknown $\Rightarrow$ extrapolate to $\Delta x \to 0$

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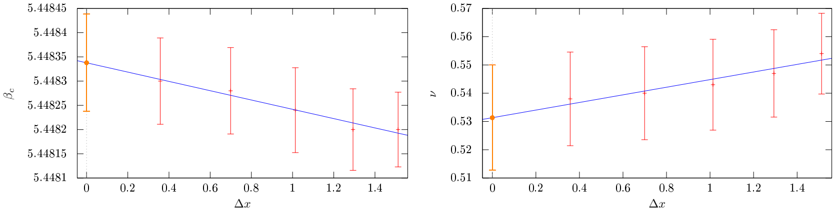
# The data collapse

## A quantitative approach

[M. Barkema, G. Newman, Phys.Rev. E53 (1996)]

$$Q(\bar{\beta}_c, \bar{\nu}, \Delta x) \equiv \frac{1}{\Delta x} \int_{x_{\min}}^{x_{\max}} \left\{ N_V \sum_{i=1}^{N_V} \Big[ B_4\big(x(\bar{\beta}_c, \bar{\nu}, V_i)\big) \Big]^2 - \left[ \sum_{i=1}^{N_V} B_4\big(x(\bar{\beta}_c, \bar{\nu}, V_i)\big) \right]^2 \right\} \mathrm{d}x$$




**Extraction of $\nu$ does not require arbitrary decisions!**

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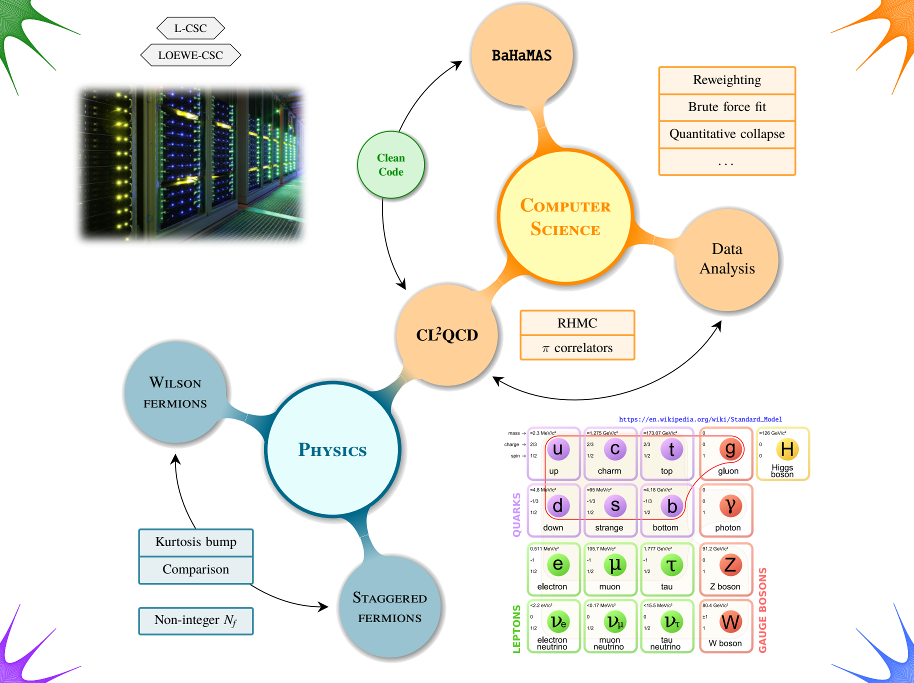
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# Reweighting

# The multiple histogram method

- Applicable whenever $\mathcal{S}$ is linear in reweighting parameter (e.g. $\beta$)
- Based on best estimate of density of states from a set of different simulations
- Interpolation of (not too distant) parameters preferred to extrapolation
- Not straightforward to be implemented, but very powerful tool
- It is possible to reweight a probability distribution of an observable
- Generalisation to multiple parameters is straightforward

$$\langle Q(\beta)\rangle = \frac{1}{\mathcal{Z}(\beta)} \sum_{i,s} \frac{Q_s(\beta_i)}{\sum_j n_j\, \mathcal{Z}^{-1}(\beta_j)\, e^{(\beta-\beta_j)\cdot E_s(\beta_i)}}$$

$$\mathcal{Z}(\beta_j) = \sum_{i,s} \frac{1}{\sum_k n_k\, \mathcal{Z}^{-1}(\beta_k)\, e^{(\beta_j-\beta_k)\cdot E_s(\beta_i)}}$$

$$\mathcal{Z}(\beta) = \sum_{i,s} \frac{1}{\sum_k n_k\, \mathcal{Z}^{-1}(\beta_k)\, e^{(\beta-\beta_k)\cdot E_s(\beta_i)}}$$

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LOEWE-CSC

Clean Code

**BaHaMAS**

| |
|---|
| Reweighting |
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| ... |

COMPUTER SCIENCE

Data Analysis

CL²QCD

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| RHMC |
| $\pi$ correlators |

WILSON FERMIONS

PHYSICS

STAGGERED FERMIONS

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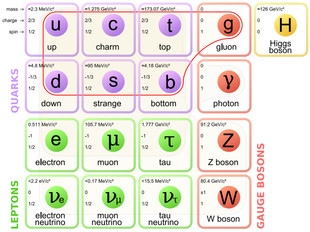
| Kurtosis bump |
| Comparison |

Non-integer $N_f$

https://en.wikipedia.org/wiki/Standard_Model



# BaHaMAS

# Daily finite temperature lattice QCD

## Running simulations on a supercomputer

- A job scheduler controls the execution of programs on the cluster
- To run a simulation, a job-script file has to be produced
- The application often needs an input file as well with physical parameters
- To produce the required files by hand is the most error-prone way to proceed
- To continue a (maybe crashed) simulation is often needed
- Resuming simulations from previous checkpoints requires cleaning operations
- Working by hand is *deadly* uncomfortable and inefficient!

Wilson: $\sim 1500$ runs

[A. Sciarra et al., Phys.Rev. D93 (2016)]

Staggered: $\sim 1250$ runs

[A. Sciarra, O. Philipsen, PoS LATTICE (2016)]

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# BaHaMAS

A Bash Handler to Monitor and Administrate Simulations

- Every operation is automatised: just run a script with command line options!
- Physical parameters contained in folders path and in $\beta$-file
- Thermalisation handled automatically using fixed naming scheme of folders
- Job-script parameters given as command line option (e.g. walltime)
- Starting, continuing and resuming simulations is straightforward
- Monitor status of simulations at fixed $N_s$ with few keystrokes (`-l` option)
- Monitor status of ALL simulations using database functionality

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# BaHaMAS

## A Bash Handler to Monitor and Administrate Simulations

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- Thermalisation handled automatically using fixed naming scheme of folders
- Job-script parameters given as command line option (e.g. walltime)
- Starting, continuing and resuming simulations is straightforward
- Monitor status of simulations at fixed $N_s$ with few keystrokes (`-l` option)
- Monitor status of ALL simulations using database functionality

Time to handle $\mathcal{O}(10^2)$ simulations

- Before `BaHaMAS`: $\sim 1\,d$
- Before database: $\sim 2\,h$
- With database: $\sim 20\,min$

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# BaHaMAS at work

## Monitor the status of the simulations in real time

| Beta | Traj. Done | (Acc.) | [Last 1000] | int0-1-2-kmp | Status | Max DS | Last tr. finished | Tr: # |
|---|---|---|---|---|---|---|---|---|
| 5.4330_s4330_NC | 60000 | (84.54 %) | [80.00 %] | 10-17 | PENDING | 4.24899 | ------ sec. ago | 64999 |
| 5.4330_s4330_fC | 4000 | (97.67 %) | [98.30 %] | 10-29 | notQueued | 0.262304 | ------ sec. ago | 4999 |
| 5.4330_s5441_NC | 60000 | (84.82 %) | [82.60 %] | 10-17 | PENDING | 5.007 | ------ sec. ago | 64999 |
| 5.4330_s6552_NC | 60000 | (84.37 %) | [80.50 %] | 10-17 | PENDING | 5.01998 | ------ sec. ago | 64999 |
| 5.4330_s7663_NC | 60000 | (84.50 %) | [76.30 %] | 10-17 | PENDING | 4.34834 | ------ sec. ago | 64999 |
| 5.4350_s4350_fH | 1000 | (97.50 %) | [97.50 %] | 10-32 | notQueued | 4.0071 | ------ sec. ago | 999 |
| 5.4360_s4360_NC | 66709 | (86.54 %) | [86.00 %] | 10-17 | RUNNING | 3.8505 | 29 sec. ago | 71708 |
| 5.4360_s4360_fC | 4000 | (97.90 %) | [97.90 %] | 10-29 | notQueued | 0.213323 | ------ sec. ago | 4999 |
| 5.4360_s5471_NC | 67189 | (85.98 %) | [79.90 %] | 10-17 | RUNNING | 4.17417 | 20 sec. ago | 72188 |
| 5.4360_s6582_NC | 66165 | (86.06 %) | [80.30 %] | 10-17 | RUNNING | 4.67013 | 12 sec. ago | 71164 |
| 5.4360_s7693_NC | 66726 | (86.13 %) | [81.10 %] | 10-17 | RUNNING | 3.94837 | 9 sec. ago | 71725 |
| 5.4390_s4390_NC | 69317 | (82.40 %) | [78.70 %] | 10-16 | RUNNING | 6.72853 | 11 sec. ago | 74316 |
| 5.4390_s4390_fC | 4000 | (98.00 %) | [97.60 %] | 10-29 | notQueued | 0.234035 | ------ sec. ago | 4999 |
| 5.4390_s5401_NC | 69567 | (82.69 %) | [79.90 %] | 10-16 | RUNNING | 27.41427 | 36 sec. ago | 74566 |
| 5.4390_s6512_NC | 69529 | (84.67 %) | [83.70 %] | 10-17 | RUNNING | 6.50622 | 23 sec. ago | 74528 |
| 5.4390_s7623_NC | 67410 | (81.57 %) | [74.60 %] | 10-16 | RUNNING | 6.63593 | 31 sec. ago | 72409 |
| 5.4400_s4400_fH | 1000 | (96.80 %) | [96.80 %] | 10-32 | notQueued | 11.2124 | ------ sec. ago | 999 |
| 5.4420_s4420_NC | 60000 | (81.50 %) | [83.60 %] | 10-16 | RUNNING | 7.31466 | 1025 sec. ago | 64999 |
| 5.4420_s5531_NC | 59443 | (80.92 %) | [66.80 %] | 10-16 | RUNNING | 7.06359 | 28 sec. ago | 64442 |
| 5.4420_s6642_NC | 59946 | (81.36 %) | [91.00 %] | 10-17 | RUNNING | 7.90988 | 1 sec. ago | 64945 |
| 5.4420_s7753_NC | 59392 | (80.49 %) | [78.00 %] | 10-16 | RUNNING | 6.51365 | 13 sec. ago | 64391 |
| 5.4450_s4450_NC | 36555 | (81.35 %) | [82.60 %] | 10-16 | RUNNING | 5.67753 | 32 sec. ago | 41554 |
| 5.4450_s4450_fH | 1000 | (98.00 %) | [98.00 %] | 10-32 | notQueued | 8.78924 | ------ sec. ago | 999 |
| 5.4450_s5561_NC | 37272 | (82.83 %) | [88.40 %] | 10-16 | RUNNING | 6.22743 | 12 sec. ago | 42271 |
| 5.4450_s6672_NC | 36562 | (81.54 %) | [76.40 %] | 10-16 | RUNNING | 4.89611 | 5 sec. ago | 41561 |
| 5.4450_s7783_NC | 34850 | (81.70 %) | [85.50 %] | 10-16 | RUNNING | 6.07066 | 14 sec. ago | 39849 |

*Column containing the time needed to perform one trajectory omitted for readability reasons*

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# BaHaMAS at work

## The database report of the simulations

```
AUTOMATIC REPORT FROM DATABASE (status on 26.08.2016 at 08:16)

                    Simulations on  broken GPU:    1
  Simulations with too low acceptance - last 1k:    0  -    1  [  0%,  68% )
      Simulations with low acceptance - last 1k:    0  -    1  [ 68%,  70% )
  Simulations with optimal acceptance - last 1k:   28  -   52  [ 70%,  78% ]
     Simulations with high acceptance - last 1k:  401  -  373  ( 78%,  90% ]
 Simulations with too high acceptance - last 1k:  111  -  113  ( 90%, 100% ]
                         Simulations  running:  113
                         Simulations  pending:    0
              Simulations  stuck (or finished):   10
                     Simulations  running fine:  103
                   Output files  to be cleaned:    0

     Use -ds | --dataBase --show option to display set of simulations.
```

To understand which simulations are problematic cannot be easier!

Upgrade and release planned for next Lattice conference!

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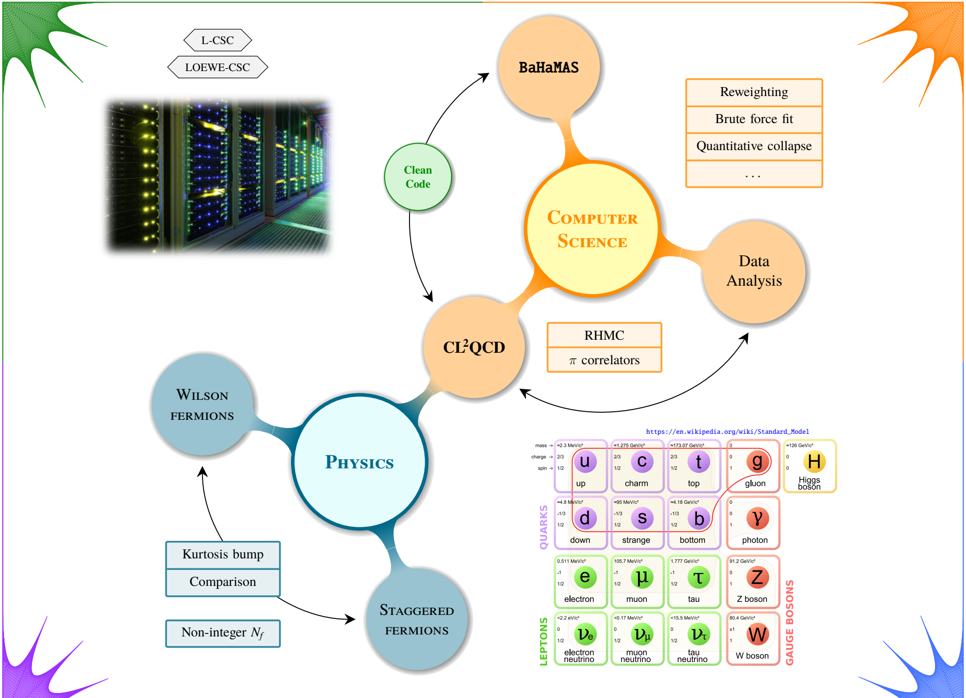
L-CSC
LOEWE-CSC
BaHaMAS
Clean Code
Computer Science
Reweighting
Brute force fit
Quantitative collapse
. . .
Data Analysis
CL²QCD
RHMC
π correlators
Wilson fermions
Physics
Staggered fermions
Kurtosis bump
Comparison
Non-integer N_f
https://en.wikipedia.org/wiki/Standard_Model
mass
charge
spin
QUARKS
LEPTONS
GAUGE BOSONS
u up
c charm
t top
g gluon
H Higgs boson
d down
s strange
b bottom
γ photon
e electron
μ muon
τ tau
Z Z boson
νe electron neutrino
νμ muon neutrino
ντ tau neutrino
W W boson

# CL$^2$QCD: A short overview



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# CL$^2$QCD: A short overview

# Why do we need a fast code?

## Just to give an idea of how costly it is

```
for Nt in ...; do                        # ~3 values
    for mu in ...; do                    # ~6 values
        for mass in ...; do              # ~6 values
            for Ns in ...; do            # ~3 values >= 3*Nt
                for T in ...; do         # ~5 values
                  echo "Run the (R)HMC for >50k trajectories"
                  # ...
                done
            done
        done    # Consider that the typical time of a
    done        # simulation varies from weeks to months
done
```

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# Why do we need a fast code?

## Just to give an idea of how costly it is

```
for Nt in ...; do                              # ~3 values
    for mu in ...; do                          # ~6 values
        for mass in ...; do                    # ~6 values
            for Ns in ...; do                  # ~3 values >= 3*Nt
                for T in ...; do               # ~5 values
                  echo "Run the (R)HMC for >50k trajectories"
                  # ...
                done
            done
        done    # Consider that the typical time of a
    done        # simulation varies from weeks to months
done
```

**Considering 3 months as average time of a single simulation**

- For loop in order as above $\longrightarrow$ 405 years
- Inner three for loop parallel $\longrightarrow$ 4.5 years

$\times$ (roughly 1.5) STRETCH FACTOR (feedback, technical)

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# CL$^2$QCD: A short overview

# Why GPUs?


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# Why GPUs?



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# Why GPUs?




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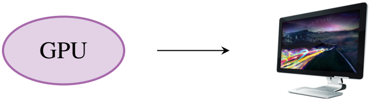
# GPGPU

## General Purpose Graphics Processing Unit

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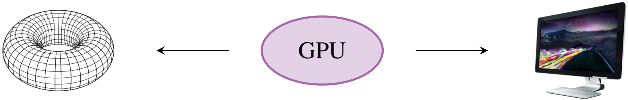
# GPGPU

## General Purpose Graphics Processing Unit

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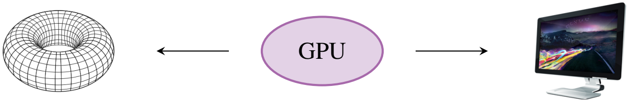
# GPGPU

## General Purpose Graphics Processing Unit




| Card | Chip | Memory {GB} | Peak DP {GFLOPS} | Peak BW {GB/s} | Clock {MHz} | Year |
|---|---|---|---|---|---|---|
| AMD Radeon HD 5870 | Cypress | 1 | 544 | 154 | 850 | 2009 |
| AMD Radeon HD 7970 | Tahiti | 3 | 947 | 264 | 925 | 2012 |
| AMD FirePro S10000 | Tahiti Pro GL | $2\times 3$ - 6 | $2\times 1480$ | $2\times 240$ | 825 | 2012 |
| AMD FirePro S9050 | Thaiti | 12 | 806 | 264 | 900 | 2014 |
| AMD FirePro S9150 | Hawaii | 16 | 2530 | 320 | 900 | 2014 |
| AMD FirePro S9170 | Grenada | 32 | 2620 | 320 | 930 | 2015 |
| AMD FirePro S9300 | Capsaicin | $2\times 4$ (HBM) | 868 | $2\times 512$ | 850 | 2016 |
| NVIDIA GeForce GTX 680 | Kepler | 2 - 4 | 129 | 192 | 1006 | 2012 |
| NVIDIA Tesla K40 | Kepler | 12 | 1680 | 288 | 745 | 2013 |
| NVIDIA Tesla K80 | Kepler | $2\times 12$ | 2912 | $2\times 240$ | 560 | 2014 |

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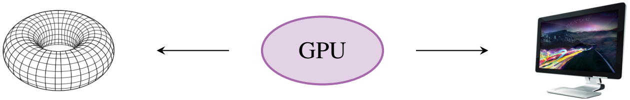
# GPGPU

## General Purpose Graphics Processing Unit

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| AMD FirePro S9170 | Grenada | 32 | 2620 | 320 | 930 | 2015 |
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| NVIDIA Tesla K80 | Kepler | $2\times12$ | 2912 | $2\times240$ | 560 | 2014 |

$$\rho = \frac{\text{Number of FLOPs}}{\text{Number of Bytes to read and write}}$$

**Wilson fermions** $\rho(\not{D}) \sim 0.57$

**Staggered fermions** $\rho(D_{KS}) \sim 0.35$

*«FLOPS do not count.»* – Clark

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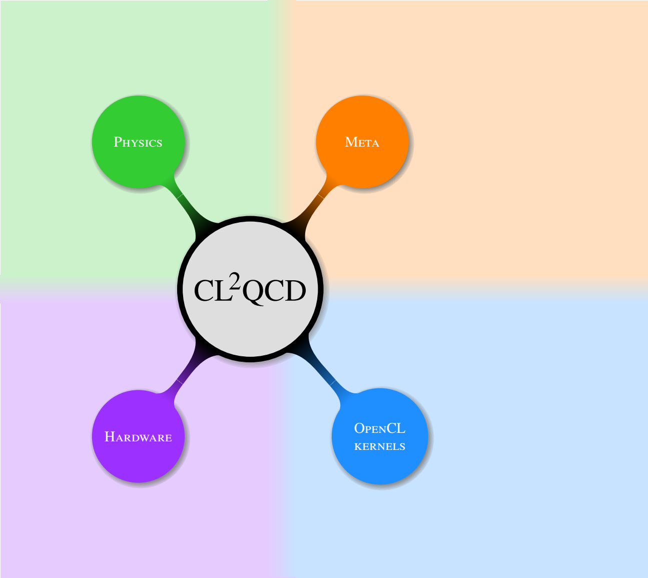
# CL$^2$QCD: A short overview

# Structure of the code

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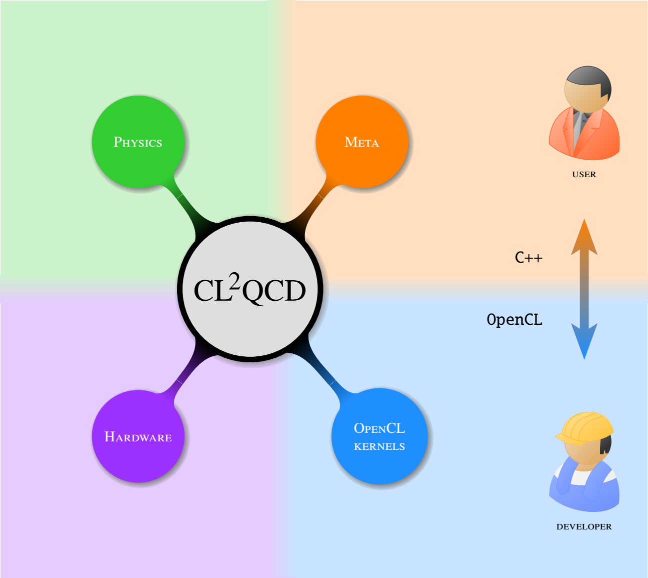
# Structure of the code

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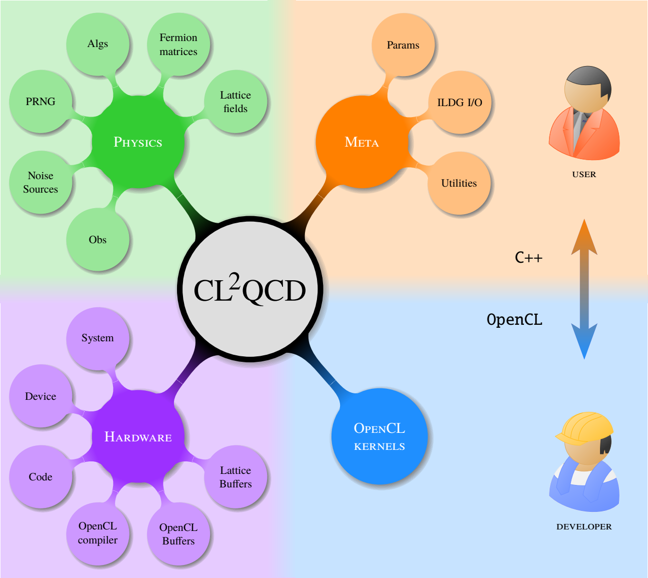
# Structure of the code

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# CL$^2$QCD: A short overview



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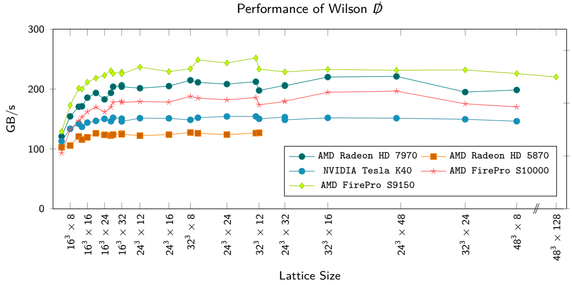
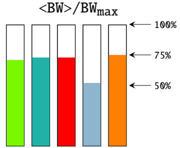
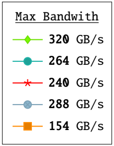
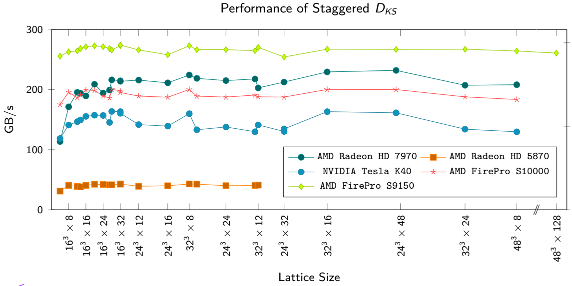
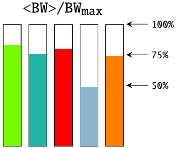
# The Dirac operator kernel

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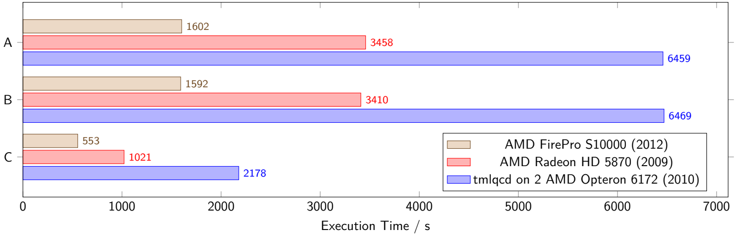
# CL$^2$QCD **VS** tmLQCD (in 2013)




| SETUP | $m_\pi$ {MeV} |
|---|---|
| A | 260 |
| B | 310 |
| C | 520 |

$$\beta = 3.9$$
$$\kappa_c = 0.160856$$
$$N_\tau = 8$$
$$N_\sigma = 24$$

AT MAXIMAL TWIST

- Runs done on LOEWE-CSC
- tmLQCD has been run on a whole node (24 cores)
- Price per flop for GPUs much lower than for CPUs

[M. Bach et al., PoS LATTICE (2013)]

1 GPU $\approx$ 4 CPU

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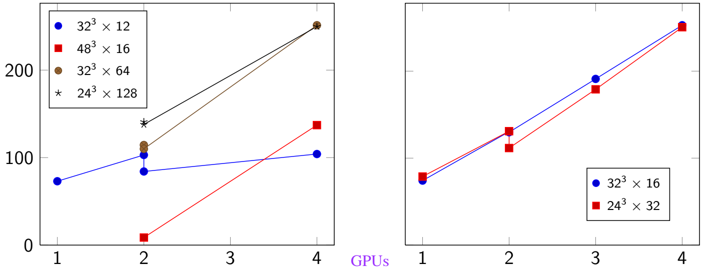
# Multi-GPU scaling

- At the moment, the lattice can be divided *only* in the temporal direction
- CL$^2$QCD can use multiple GPUs *within the same node*
- Tested on SANAM (AMD FirePro S10000, in 2013), 4 GPUs per node

Solver performance {GFLOPs}




**Hard scaling:**

The total lattice size is kept constant

**Weak scaling:**

The local lattice size is kept constant

# CL$^2$QCD: A short overview



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# Should a code *just* work?

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# Should a code *just* work?

## Absolutely no!

Any code in principle should be:

- Readable
- Maintainable
- Easy to extend
- Easy to use
- Hard to break
- Testable

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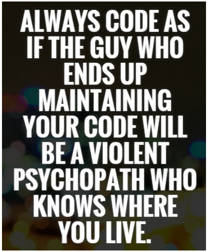


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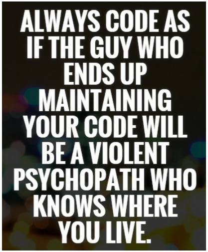


$\mathrm{CL}^2\mathrm{QCD}$

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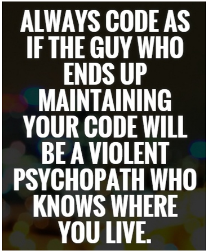


Lattice QCD with Open CL

CL$^2$QCD

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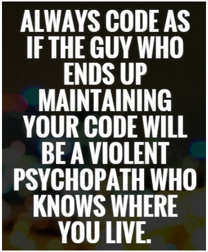


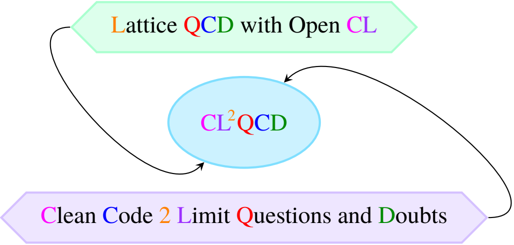


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# Unit tests and maintainability

- Robert C. Martin (2009), «*Clean Code*»
- Kent Beck (2002), «*Test Driven Development: By Example*»

# Unit tests and maintainability

Robert C. Martin (2009), «*Clean Code*»

Kent Beck (2002), «*Test Driven Development: By Example*»

- Test each single part of code on its own
- Unit tests implemented using `BOOST` and `CMake` unit test frameworks
- Regression tests for the Open CL parts are **absolutely mandatory**
- LQCD functions are local $\rightarrow$ analytic results to test against can be calculated
- Avoid dependence of the tests on specific environments $\rightarrow$ PORTABILITY!

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# Unit tests and maintainability

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Kent Beck (2002), «*Test Driven Development: By Example*»

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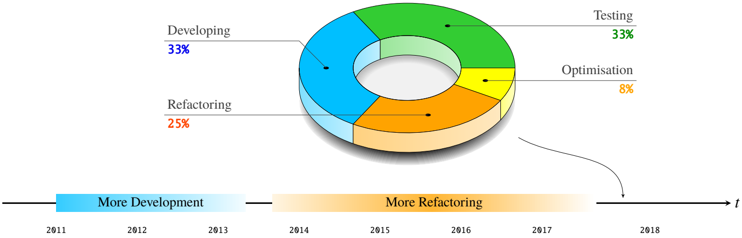


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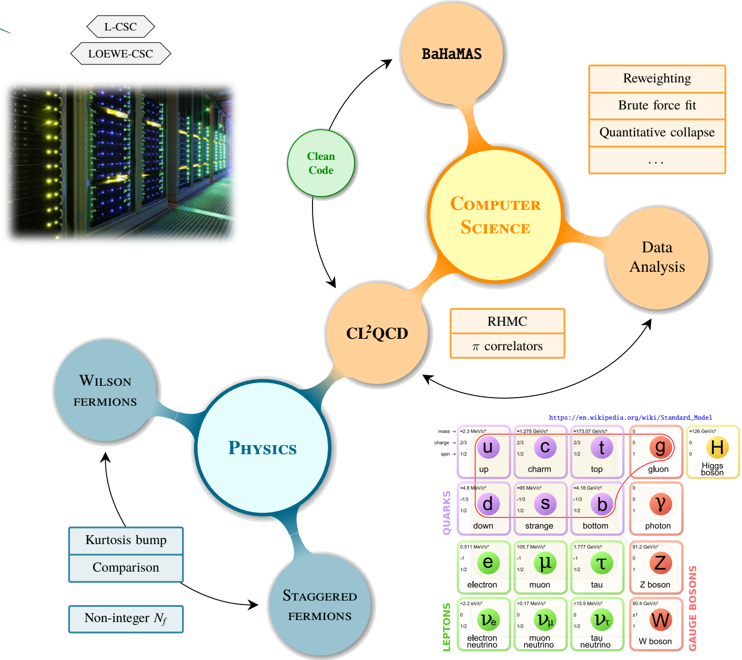
L-CSC
LOEWE-CSC
BaHaMAS
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Computer Science
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...
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RHMC
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Kurtosis bump
Comparison
Non-integer N_f
https://en.wikipedia.org/wiki/Standard_Model
mass
charge
spin
u up
c charm
t top
g gluon
H Higgs boson
d down
s strange
b bottom
γ photon
e electron
μ muon
τ tau
Z Z boson
ν_e electron neutrino
ν_μ muon neutrino
ν_τ tau neutrino
W W boson
QUARKS
LEPTONS
GAUGE BOSONS

# Something more about physics

# Something more about physics



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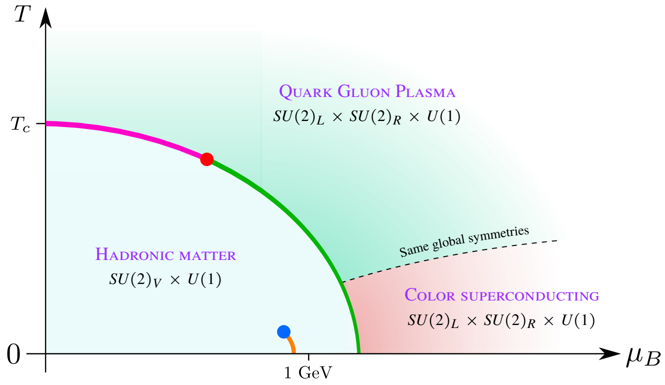
# Two-flavour QCD phase diagram

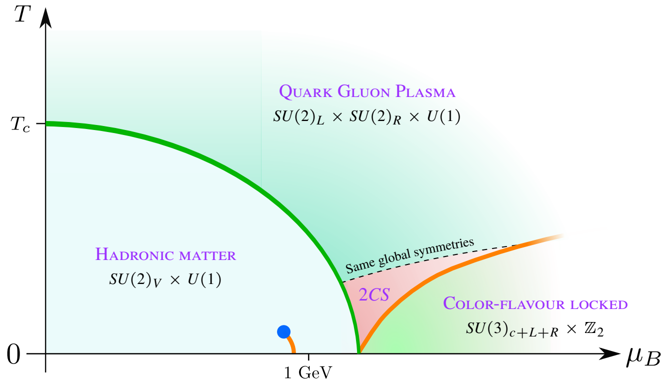
## Massless up and down quarks




In the 2$SC$ phase: $SU(3)_{colour} \rightarrow SU(2)_{rg}$

# QCD phase diagram → $N_f = 2+1$

Massless up and down, physical strange quark




Introducing physical masses for up and down quarks breaks chiral symmetry explicitly!

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# Something more about physics



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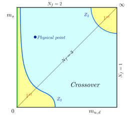
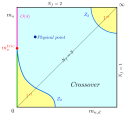
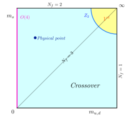
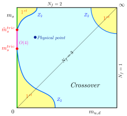
# The Columbia plot

## A bit of speculation

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# The Columbia plot

## A bit of speculation

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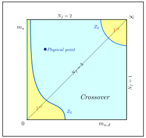


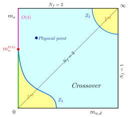


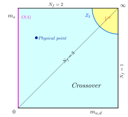


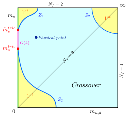


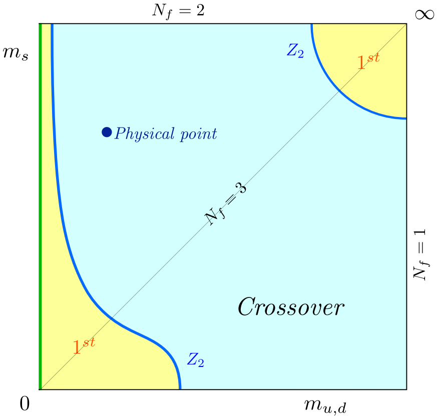


3D

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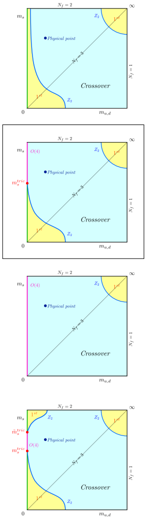
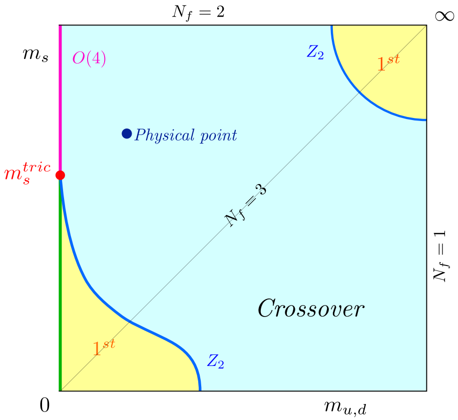
# The Columbia plot

## A bit of speculation

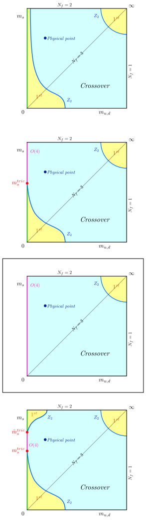


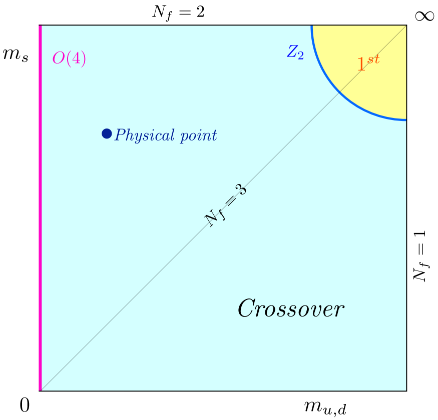




▸ 3D

# The Columbia plot

## A bit of speculation

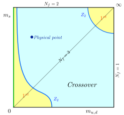


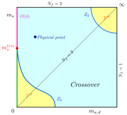



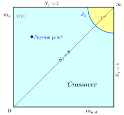

3D

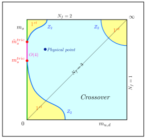
# The Columbia plot

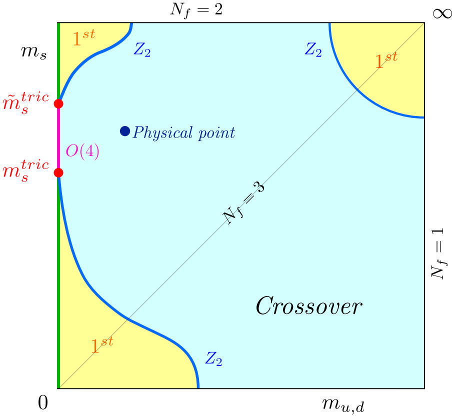
## A bit of speculation









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# The Columbia plot

## A bit of speculation

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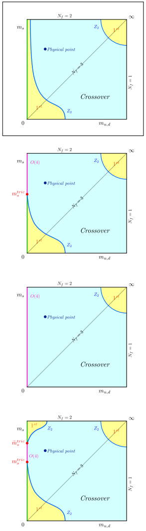


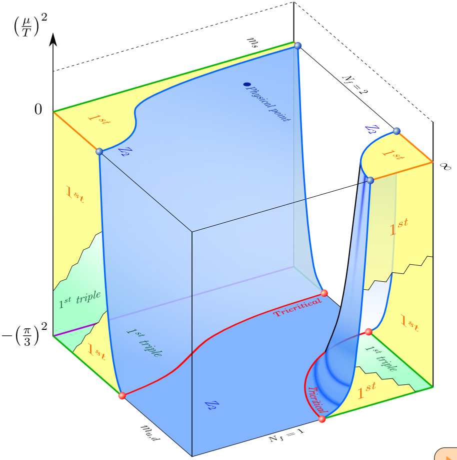


2D

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# The Columbia plot

## A bit of speculation

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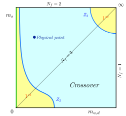


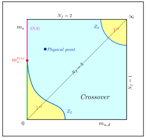


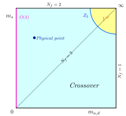


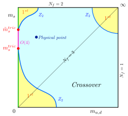


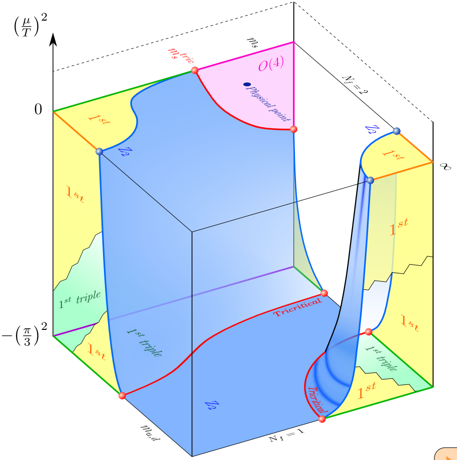


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# The Columbia plot

## A bit of speculation

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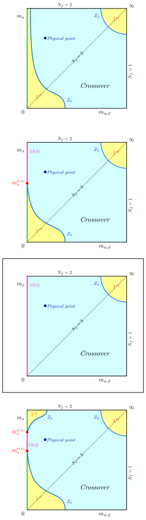


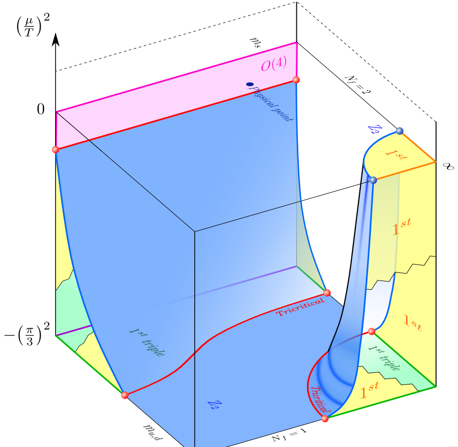


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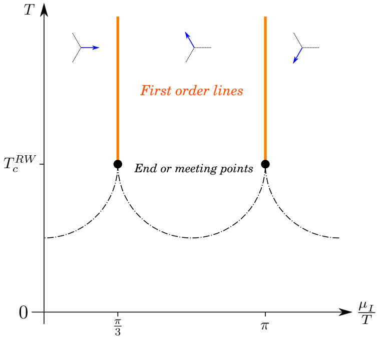
2D

# Something more about physics

# The Roberge-Weiss symmetry

## Extended centre symmetry

[Roberge & Weiss, Nucl. Phys. B275 (1986)]




$$\mathcal{Z}\left(\frac{\mu}{T}\right) = \mathcal{Z}\left(\frac{\mu}{T} + \imath\frac{2\pi N}{N_c}\right)$$

$$\mu_I^c = \frac{\pi T}{N_c}(2n+1) \qquad \boxed{n \in \mathbb{Z}}$$

Varying $\mu_I$ at fixed $T$ $\begin{cases} \text{High T} \rightarrow 1^{st}\,\textit{order} \\ \text{Low T} \rightarrow \textit{crossover} \end{cases}$

[P. de Forcrand, O. Philipsen, Nucl. Phys. B534 (2002)]
[M. D'Elia, M.-P. Lombardo, Phys. Rev. D67 (2003)]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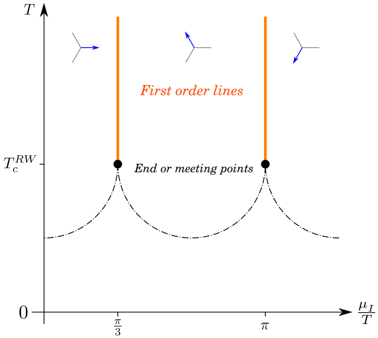
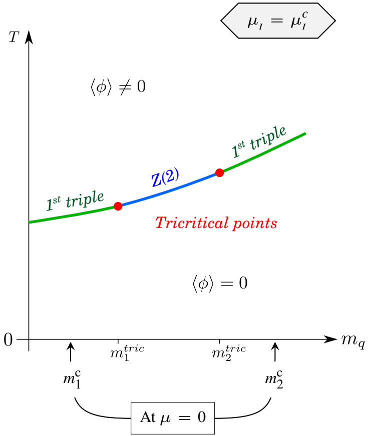
# The Roberge-Weiss symmetry

## Extended centre symmetry

[Roberge & Weiss, Nucl. Phys. B275 (1986)]




The temperature and the nature of RW points depend on quark masses

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# The Roberge-Weiss endpoints

## How their nature changes as function of $m_q$

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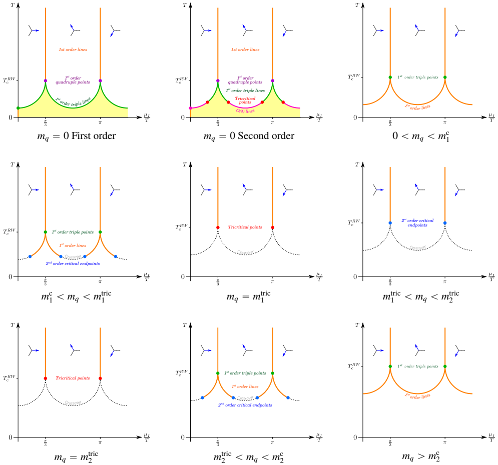


*$m_1^c$ and $m_2^c$ are the critical masses at the $Z_2$ lines in the Columbia plot ($\mu = 0$)*

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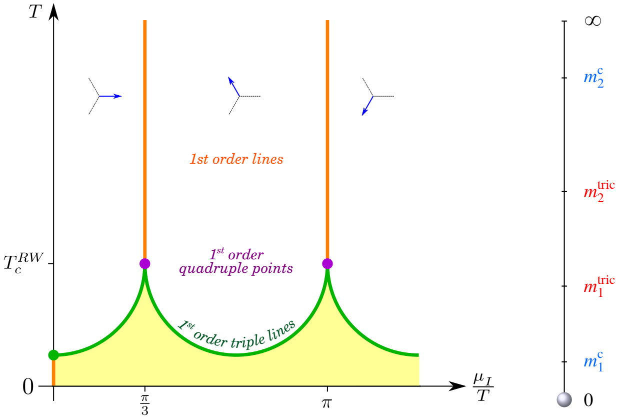
# The Roberge-Weiss endpoints

## How their nature changes as function of $m_q$

First order scenario

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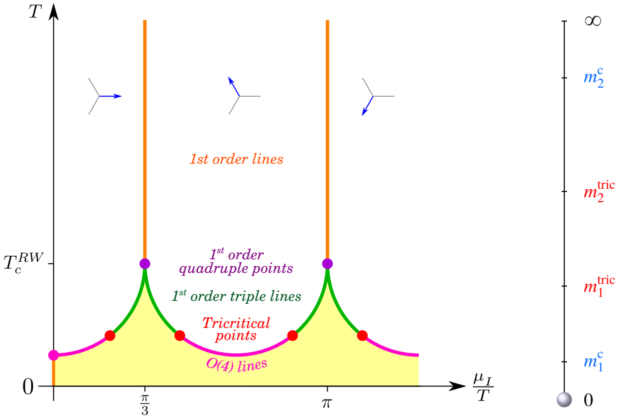
# The Roberge-Weiss endpoints

## How their nature changes as function of $m_q$

Second order scenario




*$m_1^c$ and $m_2^c$ are the critical masses at the $Z_2$ lines in the Columbia plot ($\mu = 0$)*

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# The Roberge-Weiss endpoints

## How their nature changes as function of $m_q$

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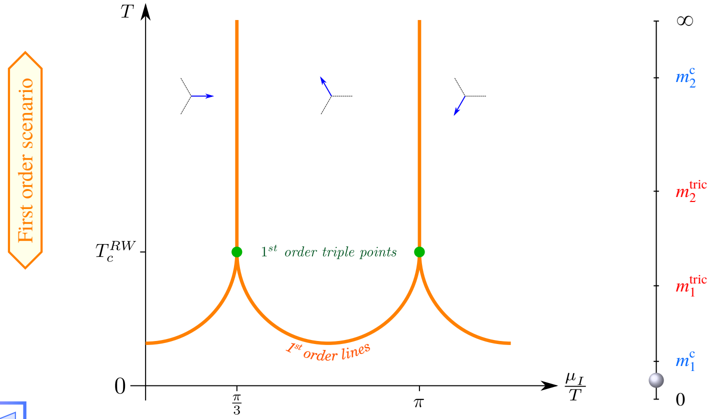


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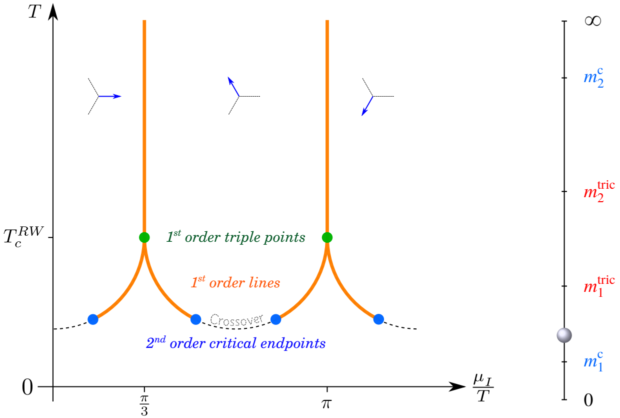


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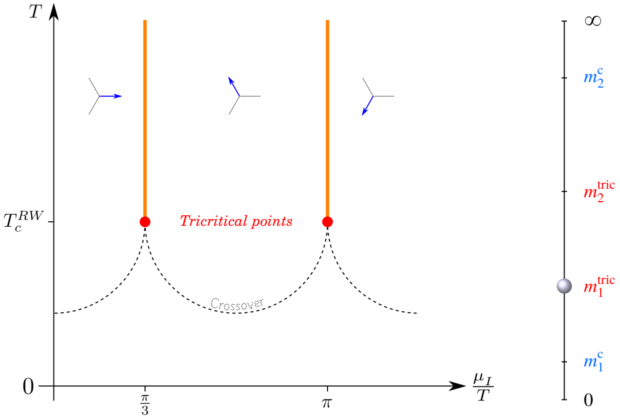


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## How their nature changes as function of $m_q$

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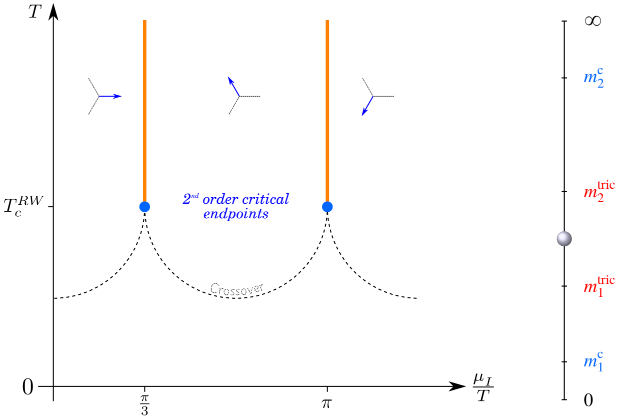


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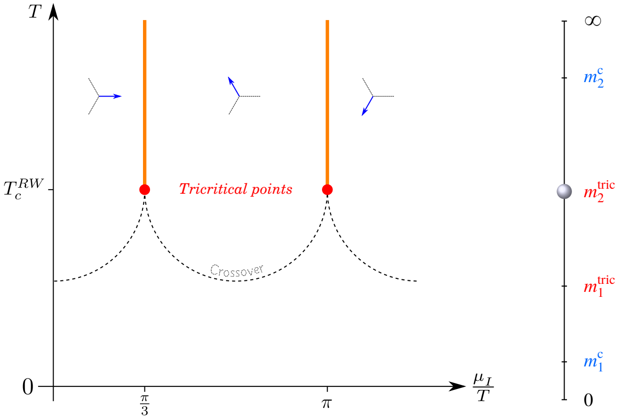


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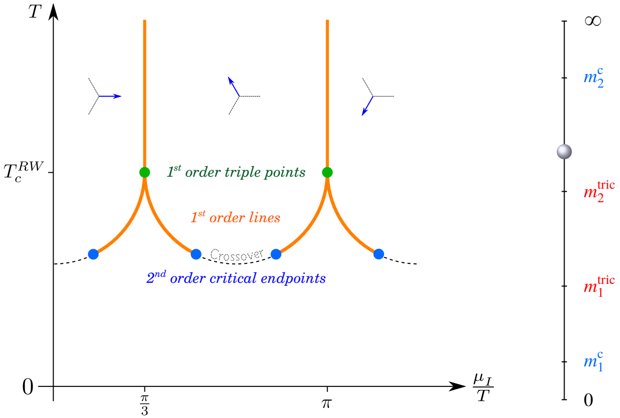


*$m_1^c$ and $m_2^c$ are the critical masses at the $Z_2$ lines in the Columbia plot ($\mu = 0$)*

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# The Roberge-Weiss endpoints

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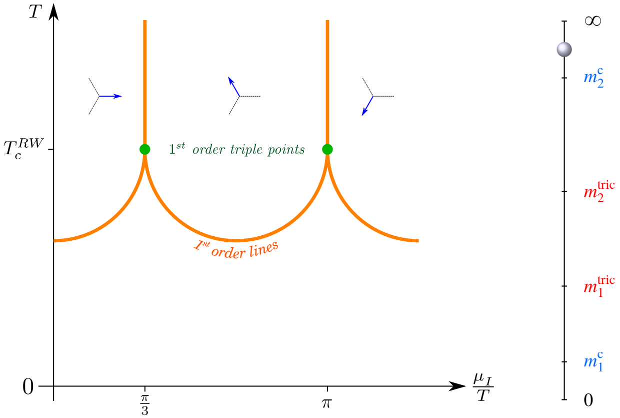
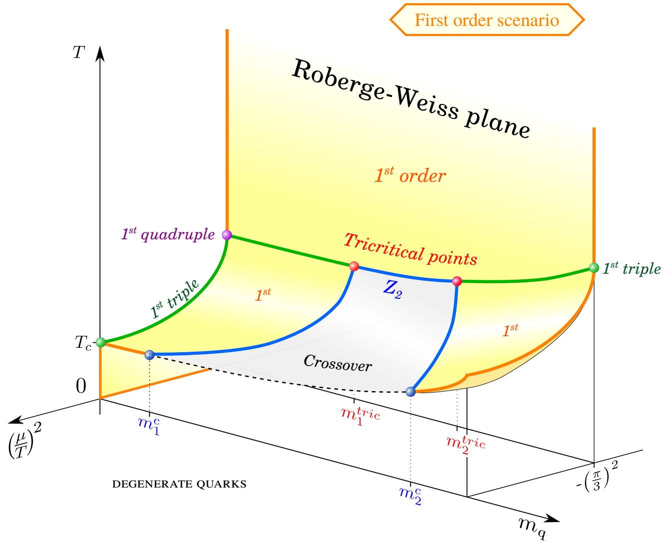


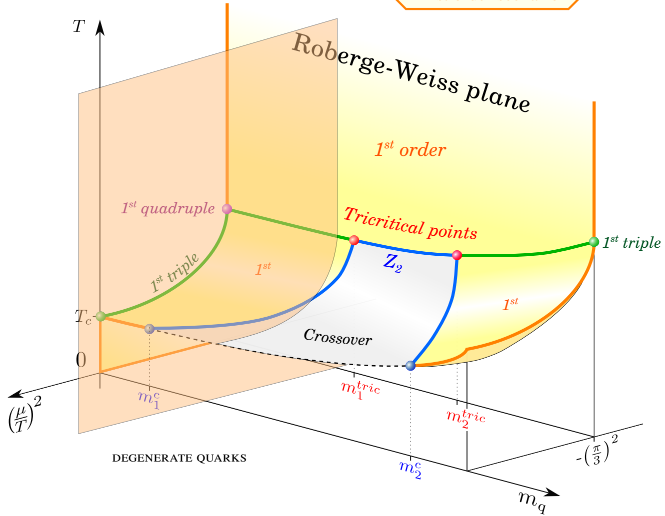

*$m_1^c$ and $m_2^c$ are the critical masses at the $Z_2$ lines in the Columbia plot ($\mu = 0$)*

# The $(T,\ \mu,\ m_q)$ phase diagram



# The $(T,\ \mu,\ m_q)$ phase diagram

First order scenario

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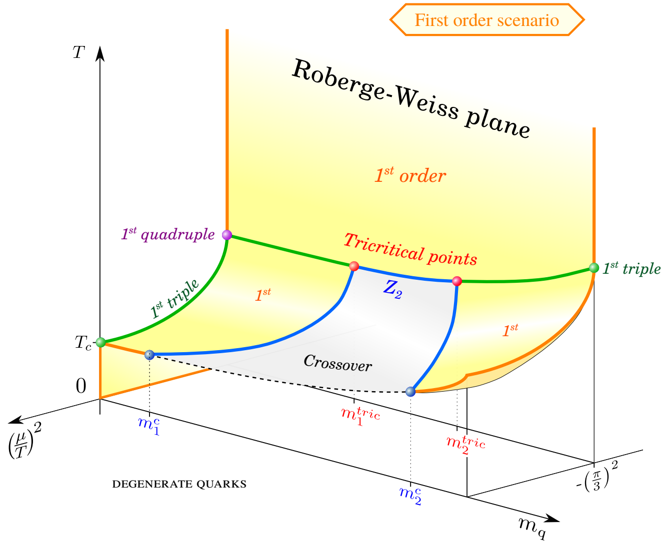
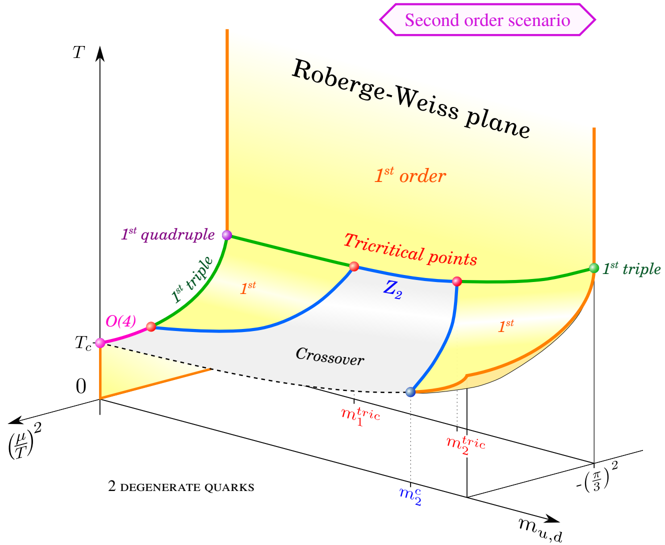
# The $(T,\,\mu,\,m_q)$ phase diagram



# The $(T,\, \mu,\, m_q)$ phase diagram

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# Something more about physics



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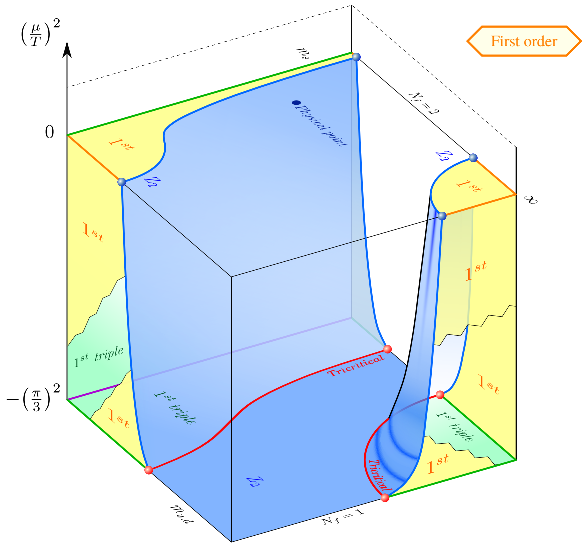
# The back-plane for $N_f = 2$

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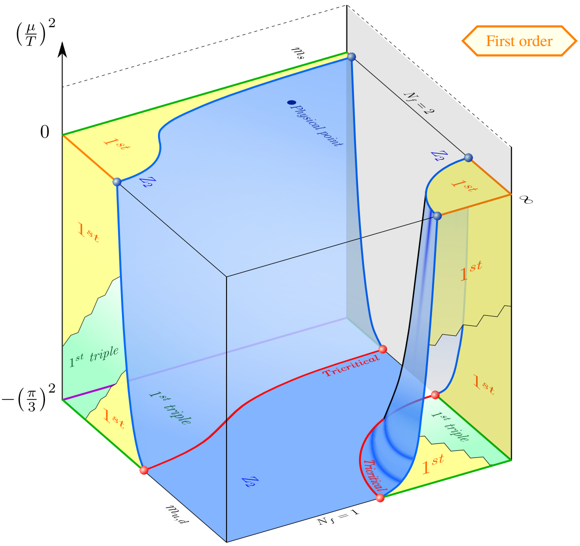
# The back-plane for $N_f = 2$

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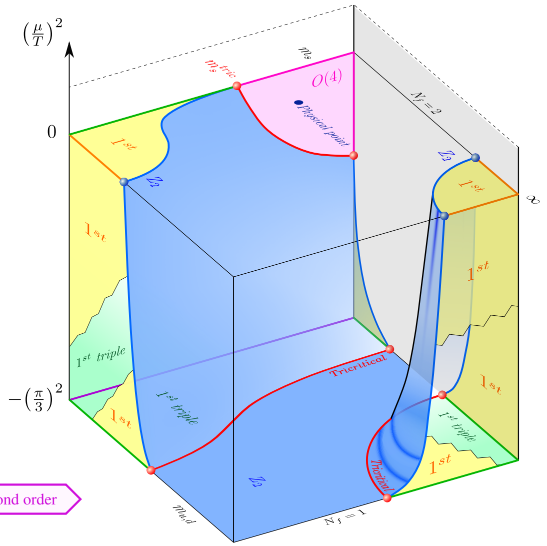
# The back-plane for $N_f = 2$




Second order

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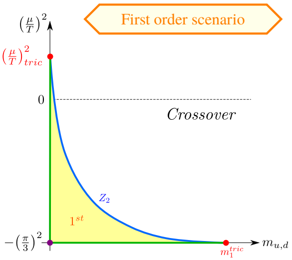
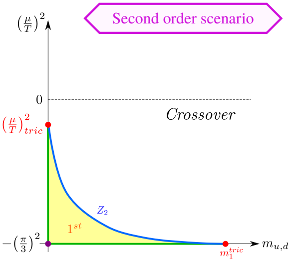
# How to use the tricritical scaling



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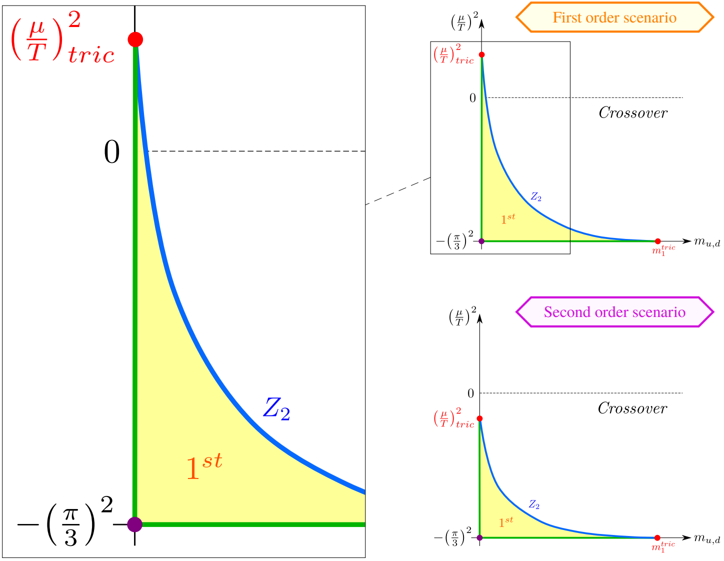


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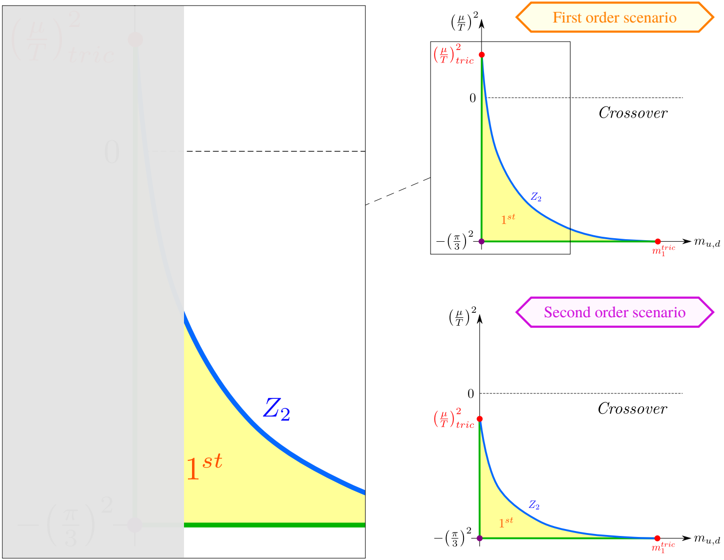
# How to use the tricritical scaling

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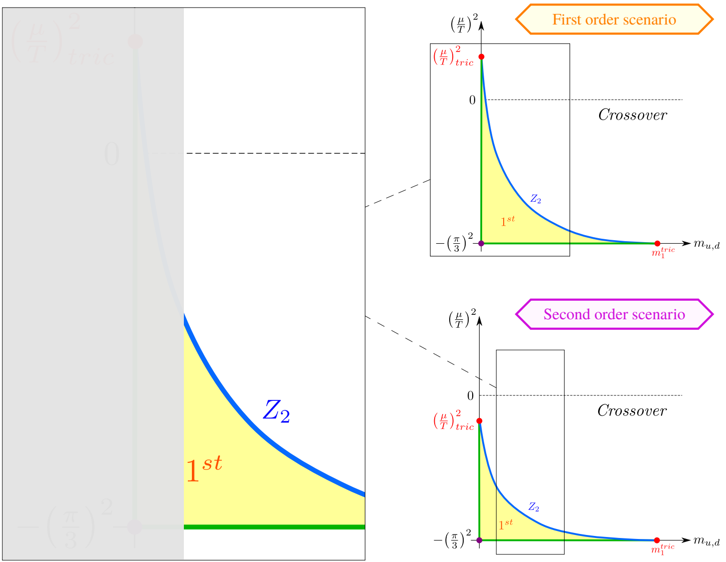
# How to use the tricritical scaling



# How to use the tricritical scaling

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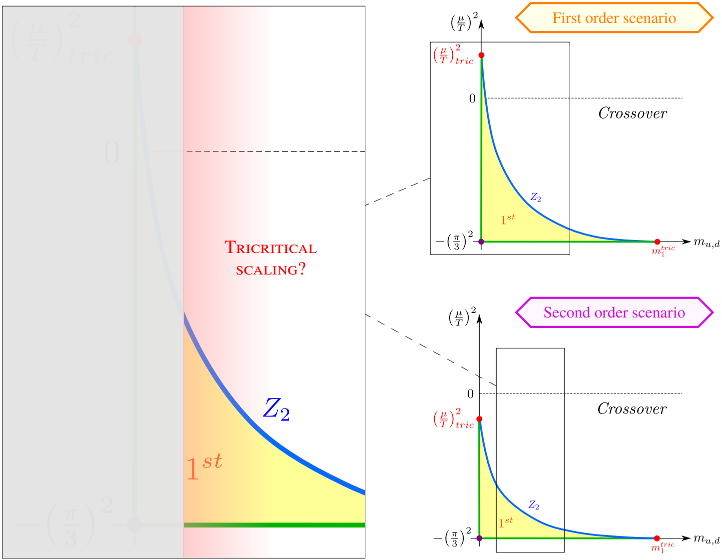


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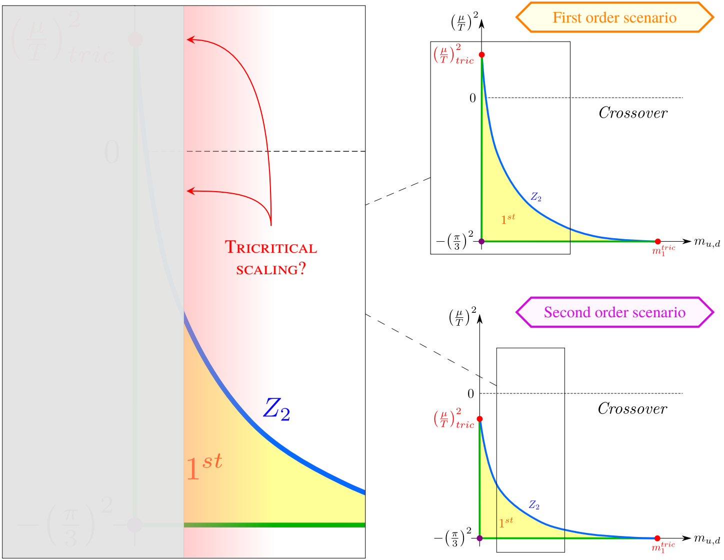
# How to use the tricritical scaling



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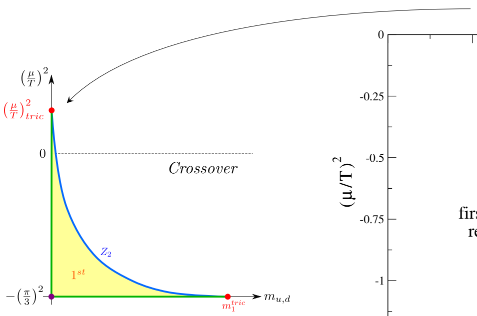
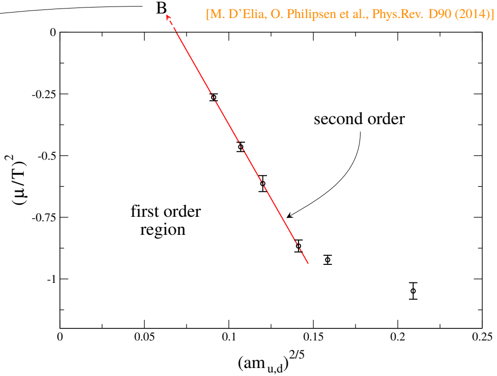
# Results on $N_t = 4$ lattices

## Successfully done with unimproved staggered fermions

[M. D'Elia, O. Philipsen et al., Phys.Rev. D90 (2014)]

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# Results on $N_t = 4$ lattices

## Successfully done with unimproved Wilson fermions

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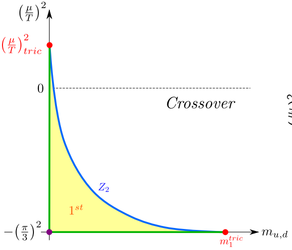
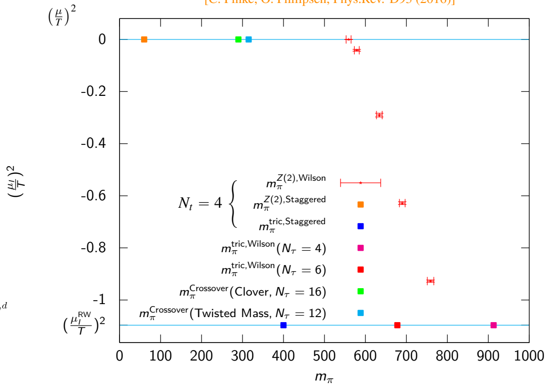



[C. Pinke, O. Philipsen, Phys.Rev. D93 (2016)]

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# Results on $N_t = 4$ lattices

## Successfully done with unimproved Wilson fermions

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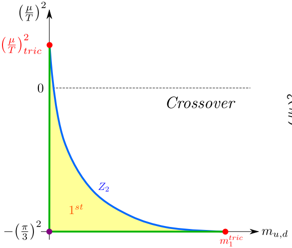
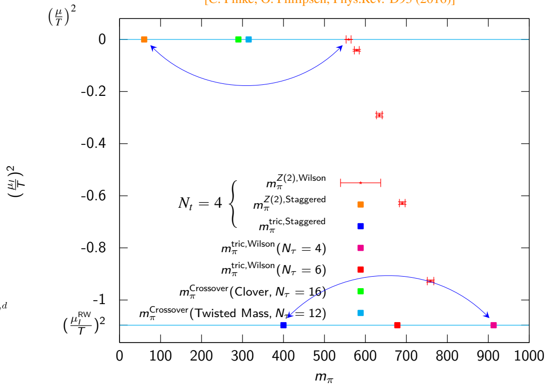
[C. Pinke, O. Philipsen, Phys.Rev. D93 (2016)]




What about finer lattices?

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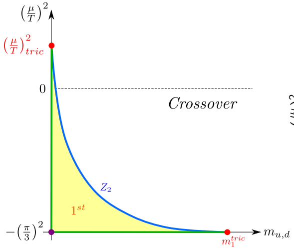
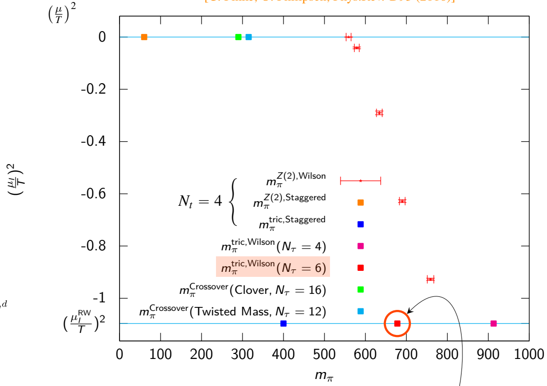
# Results on $N_t = 4$ lattices

## Successfully done with unimproved Wilson fermions




[C. Pinke, O. Philipsen, Phys.Rev. D93 (2016)]




What about finer lattices?

[A. Sciarra et al., Phys.Rev. D93 (2016)]

Working at first in RW plane

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# Something more about physics



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# Lattice spectroscopy

$$\langle O(n_t)\,\bar{O}(0)\rangle$$

*hadron interpolators*

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# Lattice spectroscopy

$$\langle O(n_t)\,\bar{O}(0)\rangle = \sum_k \langle 0|\,\hat{O}\,|k\rangle\,\langle k|\,\hat{O}^\dagger\,|0\rangle\,e^{-n_t\,a\,E_k}$$

*hadron interpolators*

# Lattice spectroscopy

$$\langle O(n_t)\,\bar{O}(0)\rangle = A\,e^{-n_t\,a\,E_H}\left[1+\mathcal{O}\left(e^{-n_t\,a\,\Delta E}\right)\right]$$

*hadron interpolators*

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# Lattice spectroscopy

$n_t \gg 1$

$$\left\langle O(n_t)\, \bar{O}(0) \right\rangle = A\, e^{-n_t\, a\, E_H} \left[ 1 + \mathcal{O}\left( e^{-n_t\, a\, \Delta E} \right) \right]$$

*hadron interpolators*

$$\approx A\, e^{-n_t\, a\, E_H}$$

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# Lattice spectroscopy

$n_t \gg 1$

$$\langle O(n_t)\,\bar{O}(0)\rangle = A\, e^{-n_t\, a\, E_H}\left[1 + \mathcal{O}\left(e^{-n_t\, a\, \Delta E}\right)\right]$$

$$\approx A\, e^{-n_t\, \hat{m}_H}$$

*hadron interpolators*

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# Lattice spectroscopy

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*hadron interpolators*

$$\approx A\,e^{-n_t\,\hat{m}_H} \longrightarrow \textit{hadron mass in lattice units}$$

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# Lattice spectroscopy

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For mesons: $O_M(n) = \bar{\psi}^{(f_1)}(n)\,\Gamma\,\psi^{(f_2)}(n)$

monomial of $\gamma$ matrices

# Lattice spectroscopy

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monomial of $\gamma$ matrices

For mesons: $O_M(n) = \bar{\psi}^{(f_1)}(n)\,\Gamma\,\psi^{(f_2)}(n)$

- Choose an interpolator with desired quantum numbers
- Compute Grassmann integrals hidden in $\langle \dots \rangle$ analytically
- Use appropriate sources to evaluate inverse of Dirac operator
- Compute gauge integral remained in $\langle \dots \rangle$ numerically
- Extract final particle mass fitting the correlation function

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# Pion mass measurement on the lattice

## With two degenerate flavours

$$C(n_t) \equiv \langle O(n_t)\,\bar{O}(0)\rangle \approx A\,e^{-n_t\,\hat{m}_H}$$

$$O_{\pi^+}(n) = \bar{d}(n)\,\gamma_5\,u(n)$$
$$O_{\pi^-}(n) = \bar{u}(n)\,\gamma_5\,d(n)$$
$$O_{\pi^0}(n) = \frac{1}{\sqrt{2}}\left[\bar{u}(n)\,\gamma_5\,u(n) - \bar{d}(n)\,\gamma_5\,d(n)\right]$$

**Wilson fermions**

$$C_g^W(n_t) = -\sum_{\substack{\vec{x},\alpha,\beta\\ c,d}} \left|D^{-1}(\vec{x}\mid 0)^{\alpha\beta}_{cd}\right|^2$$

few *lines* of algebra

**Staggered fermions**

$$C_g^S(n_t) = -64\cdot(-1)^{n_t}\sum_{\vec{x},c,d}\left|D^{-1}(\vec{x}\mid 0)_{cd}\right|^2$$

few *pages* of algebra

*spin* $\otimes$ *taste* ⚠ taste symmetry

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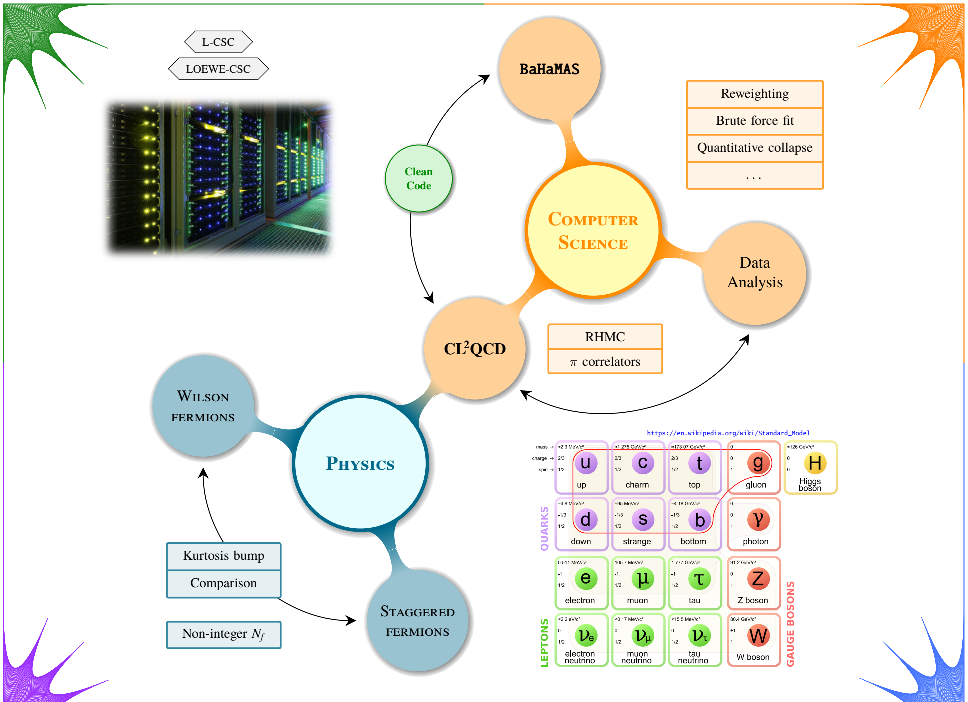
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muon neutrino
tau neutrino
W boson
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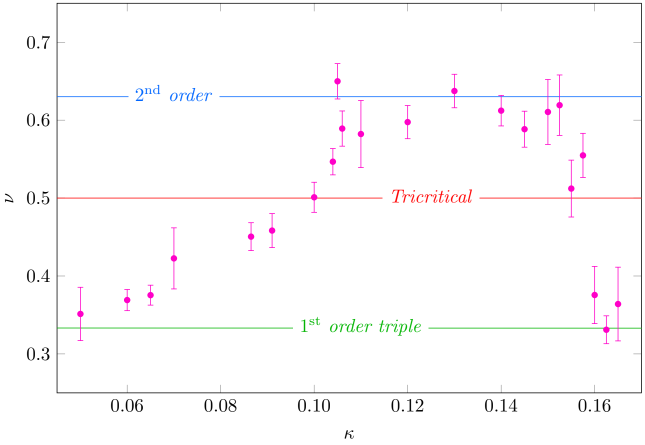
# Wilson Fermions

# Some more results

$\mu_I = \mu_I^{\text{RW}} \quad N_t = 4$

[C. Pinke, O. Philipsen, Phys.Rev. D89 (2014)]

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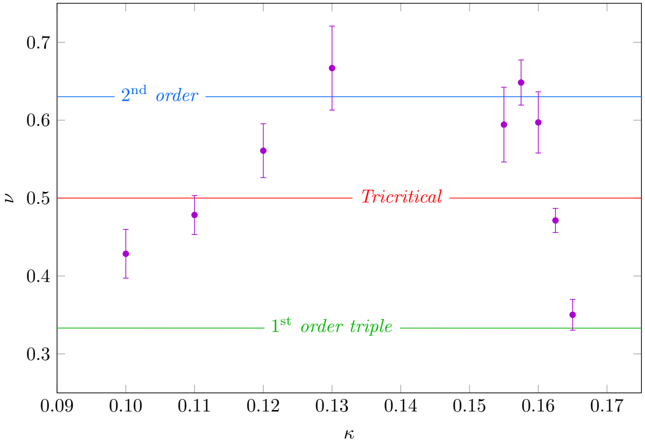
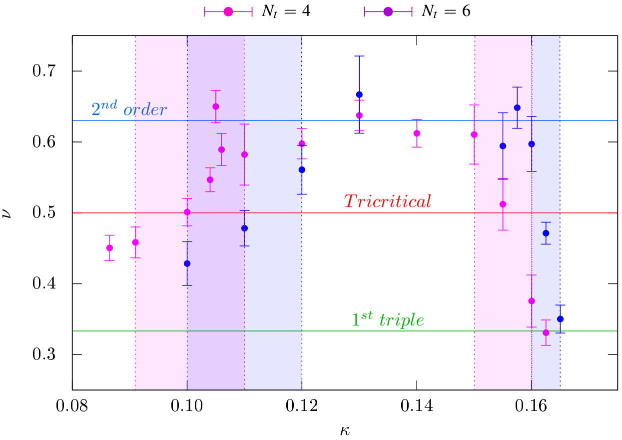
# Some more results

$\mu_I = \mu_I^{\text{RW}} \quad N_t = 6$



# Some more results

$\mu_I = \mu_I^{\mathrm{RW}} \quad N_t = 4$ vs $N_t = 6$

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# Multiple chains technique

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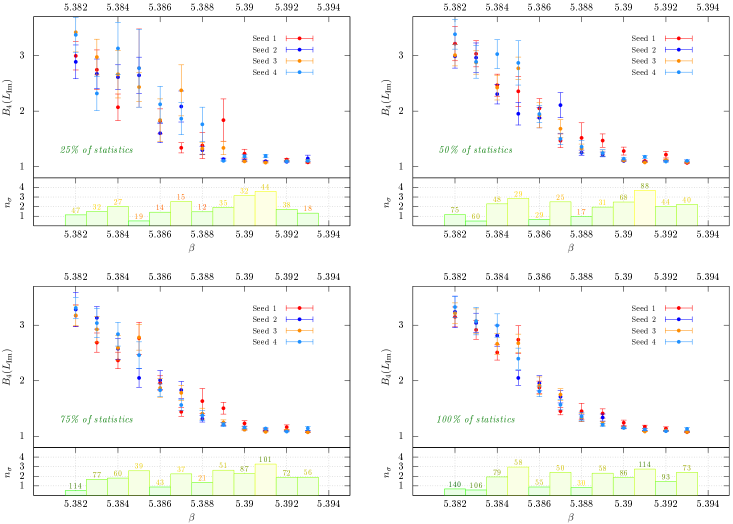

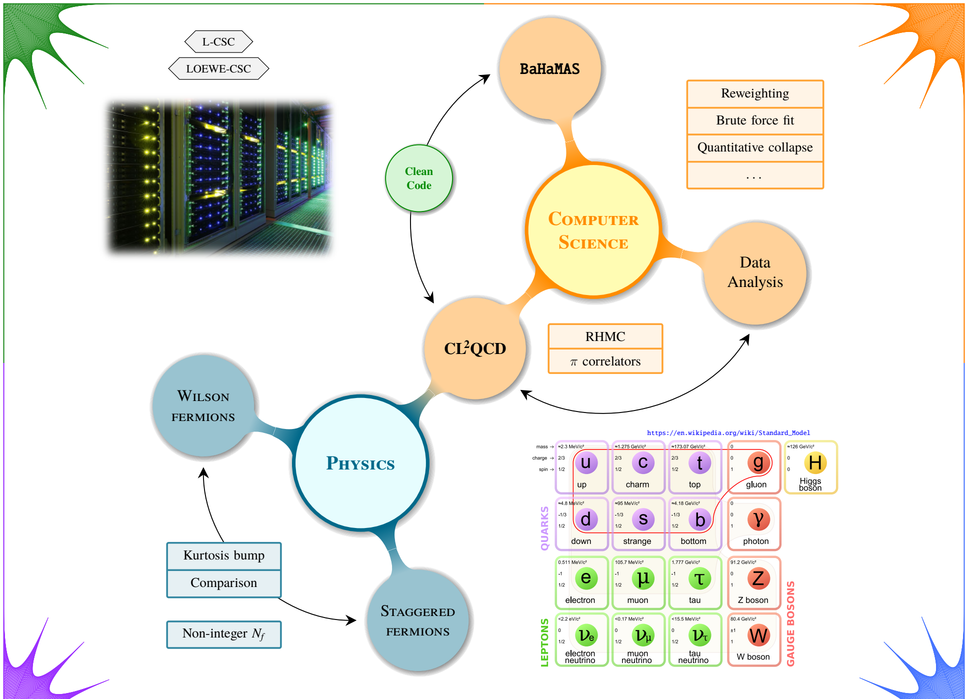
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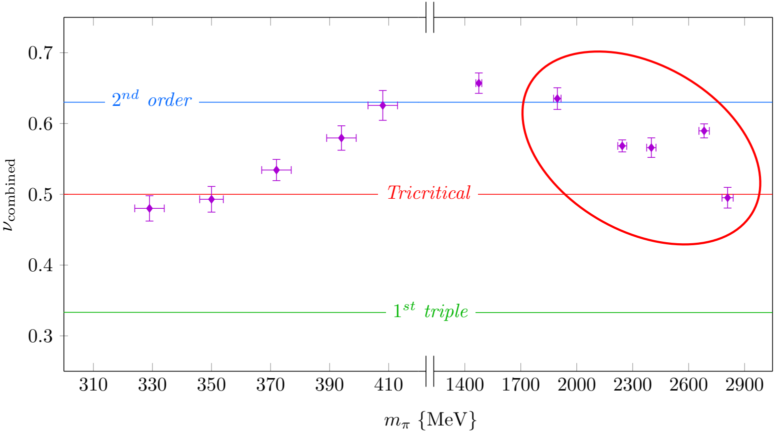
# Staggered Fermions

# Some more results

## Few more *m* needed to constrain tricritical masses




$a\,m_\pi > 1$

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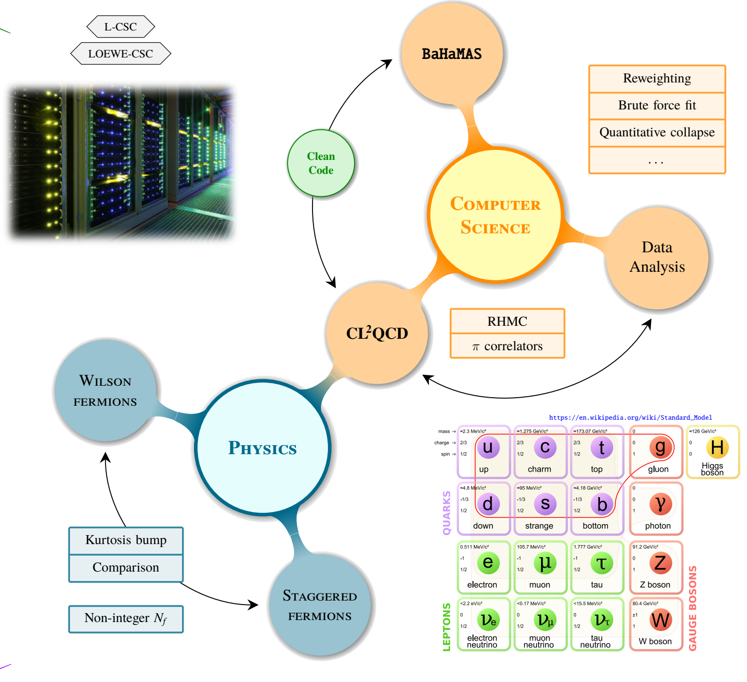

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