# Extracting hadron masses from fixed topology simulations

Seminar "Field Theory on the Lattice and the Phenomenology of Elementary Particles", Humboldt Universität zu Berlin, Berlin, Germany


Marc Wagner

in collaboration with Arthur Dromard, Christopher Czaban


[A. Dromard and M. Wagner, PoS LATTICE **2013**, 339 (2013) [arXiv:1309.2483 [hep-lat]]]

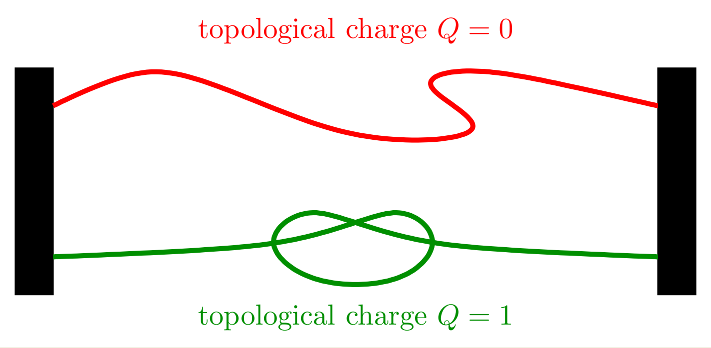
[C. Czaban and M. Wagner, PoS LATTICE **2013**, 465 (2013) [arXiv:1310.5258 [hep-lat]]]

[A. Dromard and M. Wagner, arXiv:1404.0247 [hep-lat]]

April 28, 2014

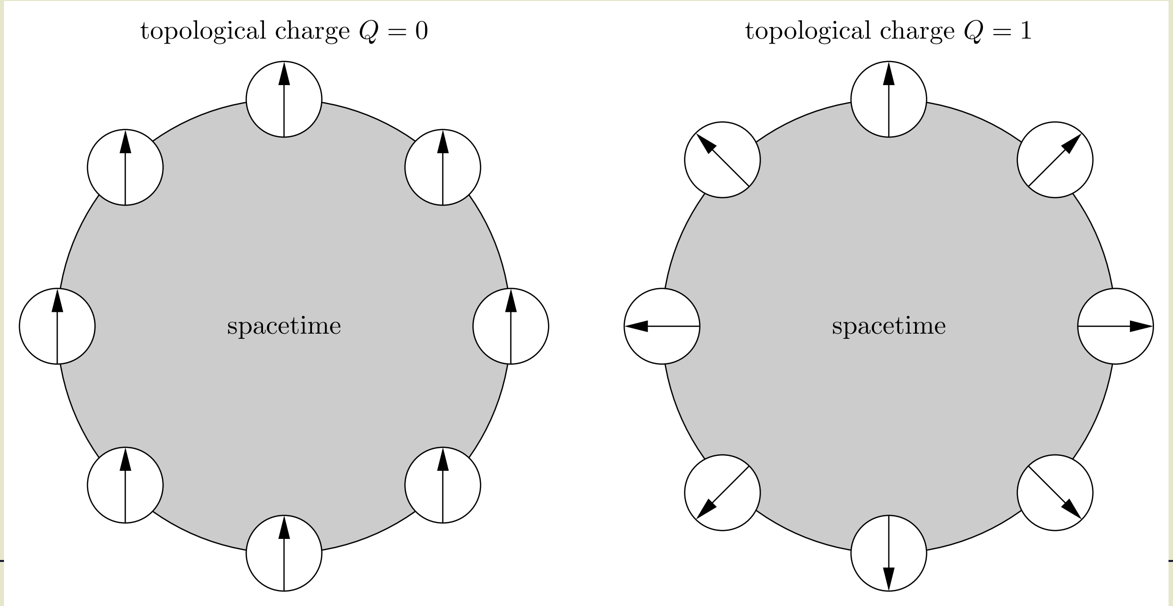
# Introduction, motivation (1)

- **Topological objects:** non-trivial structures in field configurations, which cannot be removed by continuous deformations, while keeping the action finite (their position can be changed and they can be deformed).
- Analogy: a knot in a rope.
- **Topological charge:** "number of topological objects" in a field configuration.



# Introduction, motivation (2)

- Examples of field theories, where topological objects/charge exist(s):
  - **1D QM on a circle**.
  - U(1) gauge theory and **the Schwinger model in 2D**.
  - **SU(2)**/SU(3) **Yang-Mills theory** and QCD **in 4D**.



# Introduction, motivation (3)

- Typical lattice simulation algorithms might have difficulties changing the topological charge/sector ($\rightarrow$ topology freezing).
- Reasons:
  - Field configurations are updated in a nearly continuous way.
  - Topological sectors are separated by large action barriers (in the continuum by infinite barriers).
- Topology changes are strongly suppressed, when
  - using overlap sea quarks,

    [S. Aoki *et al.* [JLQCD Collaboration], Phys. Rev. D **78**, 014508 (2008) [arXiv:0803.3197 [hep-lat]]]
    [S. Aoki *et al.*, PTEP **2012**, 01A106 (2012)]
  - the lattice spacing is small ($a \lesssim 0.05\,\text{fm}$, i.e. close to the continuum).

    [M. Lüscher and S. Schaefer, JHEP **1107**, 036 (2011) [arXiv:1105.4749 [hep-lat]]]
    [S. Schaefer, PoS LATTICE **2012**, 001 (2012) [arXiv:1211.5069 [hep-lat]]]

# Introduction, motivation (4)

- The simulation of a path integral requires averaging over field configurations from all topological sectors,

$$Z_V \equiv \int DA\, D\psi\, D\bar{\psi}\, e^{-S_E[A,\bar{\psi},\psi]} \quad , \quad \ldots$$

- When topology is fixed,

$$Z_{Q,V} \equiv \int DA\, D\psi\, D\bar{\psi}\, \delta_{Q,Q[A]} e^{-S_E[A,\bar{\psi},\psi]} \quad , \quad \ldots ,$$

  results exhibit systematic errors; in particular two-point correlation functions are not proportional $e^{-M_H t}$ for large temporal separations $t$.

- These errors are proportional to $1/V$ ($V$: spacetime volume); their behavior can be calculated as a power series in $1/V$; using the results one can determine physical quantities, e.g. hadron masses, from correlation functions from fixed topology simulations.

# Introduction, motivation (5)

- There are also cases, where one might fix topology on purpose.
- Example: using a mixed action setup of high quality overlap quarks and computationally inexpensive Wilson (tm) quarks at light quark masses ...
  - ... at light quark masses and $Q \neq 0$ the valence overlap Dirac matrix has near zero modes (Atiyah-Singer index theorem) ...
  - ... which are not present (and, therefore, compensated) in the sea Wilson (tm) Dirac matrix ...
  - ... the consequence is an ill-behaved continuum limit.

[K. Cichy, G. Herdoiza and K. Jansen, Nucl. Phys. B **847**, 179 (2011) [arXiv:1012.4412 [hep-lat]]]
[K. Cichy *et al.*, Nucl. Phys. B **869**, 131 (2013) [arXiv:1211.1605 [hep-lat]]]

- A possible solution to this problem might be to fix topology to $Q = 0$,where also the valence overlap Dirac matrix has no near zero modes.

# Introduction, motivation (6)

- Topology can be fixed by
  - either **sorting the generated field configurations according to their topological charge**
  - or by employing topology fixing actions.

    [H. Fukaya *et al.*, Phys. Rev. D **73**, 014503 (2006) [hep-lat/0510116]]
    [W. Bietenholz *et al.*, JHEP **0603**, 017 (2006) [hep-lat/0511016]]
    [F. Bruckmann *et al.*, Eur. Phys. J. A **43**, 303 (2010) [arXiv:0905.2849 [hep-lat]]]

# Part 1

# The behavior of two-point correlation functions at fixed topology

# Literature

- Idea:
  - Topology fixing causes systematic errors, which are finite volume corrections.
  - Expand two-point correlation functions at fixed topology $C_{Q,V}(t)$ (which are used to determine hadron masses) as a power series in $1/V$.
- Seminal paper: expansion of $C_{Q,V}(t)$ up to $\mathcal{O}(1/V)$ and in part up to $\mathcal{O}(1/V^2)$.

  [R. Brower, S. Chandrasekharan, J. W. Negele and U. J. Wiese, Phys. Lett. B **560**, 64 (2003) [hep-lat/0302005]]
- General discussion of $n$-point functions at fixed topology including also higher orders in $1/V$.

  [S. Aoki, H. Fukaya, S. Hashimoto and T. Onogi, Phys. Rev. D **76**, 054508 (2007) [arXiv:0707.0396 [hep-lat]]]
- Our contribution: expansion of $C_{Q,V}(t)$ up to $\mathcal{O}(1/V^3)$.

  [A. Dromard and M. Wagner, arXiv:1404.0247 [hep-lat]]

# $Z_{Q,V}$ ($Z$ at fixed $Q$ and finite $V$) (1)

- In the following: expansion of

$$Z_{Q,V} \equiv \int DA\, D\psi\, D\bar{\psi}\, \delta_{Q,Q[A]} e^{-S_E[A,\bar{\psi},\psi]},$$

the partition function at fixed topological charge $Q$ and spacetime volume $V$, in powers of $1/V$ (QCD at fixed topology is not a quantum theory).

- $Z_{Q,V}$ is the Fourier transform of $\mathcal{Z}_{\theta,V}$, the partition function at vacuum angle $\theta$ ($S_{E,\theta}[A,\bar{\psi},\psi] \equiv S_E[A,\bar{\psi},\psi] + i\theta Q[A]$; $\theta = 0 \leftrightarrow$ ordinary QCD):

$$Z_{Q,V} = \int DA\, D\psi\, D\bar{\psi} \left(\frac{1}{2\pi}\int_{-\pi}^{+\pi} d\theta\, e^{i(Q-Q[A])\theta}\right) e^{-S_E[A,\bar{\psi},\psi]} =$$

$$= \frac{1}{2\pi}\int_{-\pi}^{+\pi} d\theta\, e^{iQ\theta} \underbrace{\int DA\, D\psi\, D\bar{\psi}\, e^{-S_{E,\theta}[A,\bar{\psi},\psi]}}_{\equiv \mathcal{Z}_{\theta,V}} = \frac{1}{2\pi}\int_{-\pi}^{+\pi} d\theta\, e^{iQ\theta}\, \mathcal{Z}_{\theta,V}.$$

(QCD at $\theta \neq 0$ is a quantum theory, e.g. a Hamiltonian and states exist, ...).

# $Z_{Q,V}$ ($Z$ at fixed $Q$ and finite $V$) (2)

- One can show $E_n(+\theta, V_s) = E_n(-\theta, V_s)$; it implies $(d/d\theta) E_n(\theta, V_s)|_{\theta=0} = 0$.
- One can show $\chi_t = e_0^{(2)}(\theta)|_{\theta=0}$ (the second derivative of the vacuum energy density at $\theta = 0$),

$$\begin{aligned} \chi_t &\equiv \lim_{V\to\infty} \frac{\langle Q^2 \rangle}{V} = -\lim_{V\to\infty} \frac{1}{\mathcal{Z}_{\theta,V} V} \frac{d^2}{d\theta^2} \mathcal{Z}_{\theta,V}\Big|_{\theta=0} = \\ &= -\lim_{V\to\infty} \frac{1}{\mathcal{Z}_{\theta,V} V} \frac{d^2}{d\theta^2} \sum_n e^{-E_n(\theta,V_s)T}\Big|_{\theta=0} = \\ &= \lim_{V\to\infty} \frac{1}{\mathcal{Z}_{\theta,V} V_s} \sum_n \frac{d^2 E_n(\theta, V_s)}{d\theta^2} e^{-E_n(\theta,V_s)T}\Big|_{\theta=0} = \\ &= \lim_{V_s\to\infty} \frac{E_0^{(2)}(\theta, V_s)}{V_s}\Big|_{\theta=0} = e_0^{(2)}(\theta)\Big|_{\theta=0} \end{aligned}$$

(ordinary finite size effects neglected, e.g. $E_0(\theta, V_s) = e_0(\theta) V_s$).

- This calculation explains the appearance of $\chi_t$ in the following equations.

# $Z_{Q,V}$ ($Z$ at fixed $Q$ and finite $V$) (3)

- $\mathcal{Z}_{\theta,V}$ is dominated by the vacuum at large temporal extension $T$,

$$Z_{Q,V} = \frac{1}{2\pi}\int_{-\pi}^{+\pi} d\theta\, e^{iQ\theta} \mathcal{Z}_{\theta,V} = \\ = \frac{1}{2\pi}\int_{-\pi}^{+\pi} d\theta\, e^{iQ\theta} e^{-E_0(\theta,V_s)T}\Big(1 + \mathcal{O}(e^{-\Delta E(\theta)T})\Big). \quad (1)$$

- The vacuum energy $E_0(\theta, V_s)$ can be written as a power series in $\theta$,

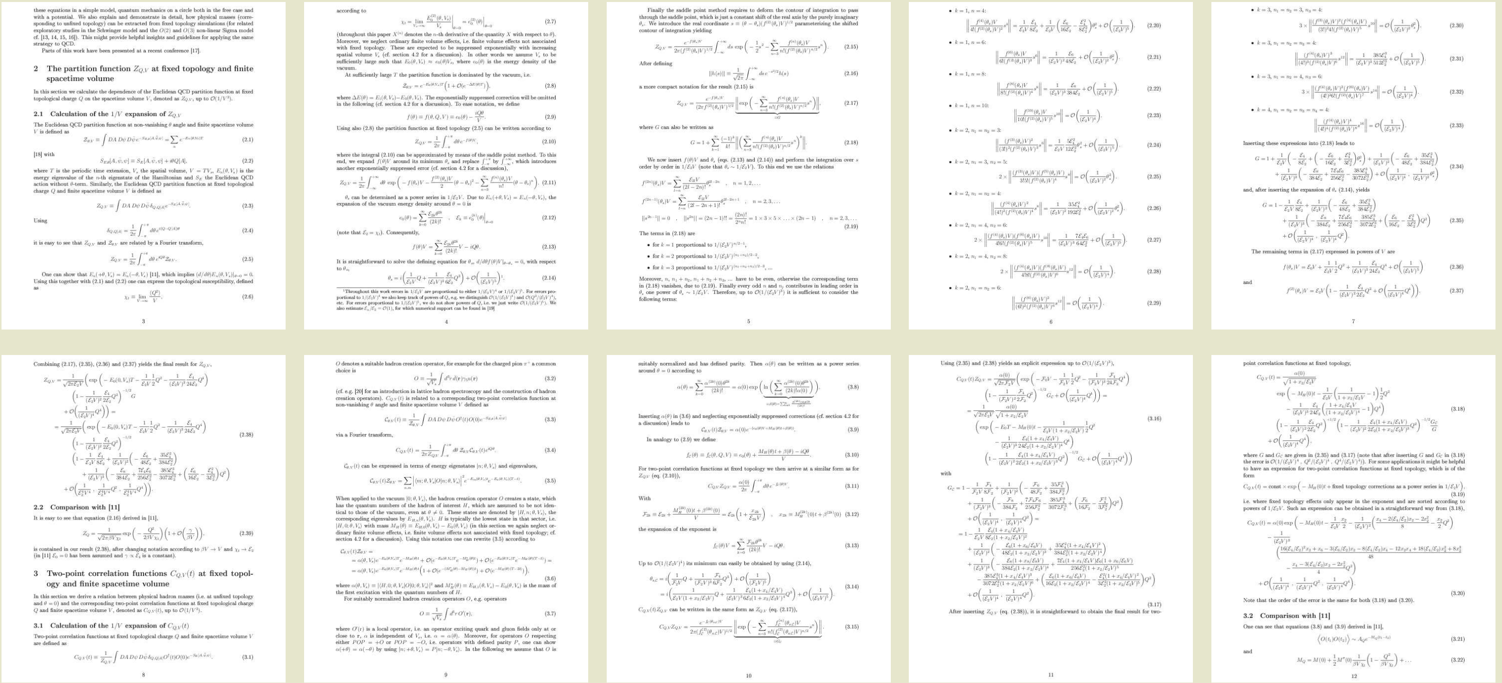
$$E_0(\theta, V_s)T = e_0(\theta)V = \left(\sum_{n=0}^{\infty} \frac{\mathcal{E}_{2n}}{(2n)!}\theta^{2n}\right)V,$$

where $\mathcal{E}_n \equiv e_0^{(n)}(\theta)\Big|_{\theta=0}$, in particular $\mathcal{E}_2 = \chi_t$.

- The integral in (1) can be solved (calculating order by order in $1/V$) using standard techniques: $\int_{-\pi}^{+\pi} d\theta \to \int_{-\infty}^{+\infty} d\theta$ (exponentially suppressed errors) ... residue theorem ... Gaussian integrals ("saddle point approximation") ...

# $Z_{Q,V}$ ($Z$ at fixed $Q$ and finite $V$) (4)

- The calculation is lengthy ... details not suited for a talk ...



# $Z_{Q,V}$ ($Z$ at fixed $Q$ and finite $V$) (5)

- Result for $Z_{Q,V}$ up to $1/V^3$:

$$\begin{aligned} Z_{Q,V} \quad &= \\ = \quad & \frac{1}{\sqrt{2\pi\mathcal{E}_2 V}}\bigg(\exp\bigg(-E_0(0,V_s)T - \frac{1}{\mathcal{E}_2 V}\frac{1}{2}Q^2 - \frac{1}{(\mathcal{E}_2 V)^3}\frac{\mathcal{E}_4}{24\mathcal{E}_2}Q^4\bigg) \\ & \bigg(1 - \frac{1}{(\mathcal{E}_2 V)^2}\frac{\mathcal{E}_4}{2\mathcal{E}_2}Q^2\bigg)^{-1/2} \\ & \bigg(1 - \frac{1}{\mathcal{E}_2 V}\frac{\mathcal{E}_4}{8\mathcal{E}_2} + \frac{1}{(\mathcal{E}_2 V)^2}\bigg(-\frac{\mathcal{E}_6}{48\mathcal{E}_2} + \frac{35{\mathcal{E}_4}^2}{384{\mathcal{E}_2}^2}\bigg) \\ & + \frac{1}{(\mathcal{E}_2 V)^3}\bigg(-\frac{\mathcal{E}_8}{384\mathcal{E}_2} + \frac{7\mathcal{E}_4\mathcal{E}_6}{256{\mathcal{E}_2}^2} - \frac{385{\mathcal{E}_4}^3}{3072{\mathcal{E}_2}^3} + \bigg(\frac{\mathcal{E}_6}{16\mathcal{E}_2} - \frac{{\mathcal{E}_4}^2}{3{\mathcal{E}_2}^2}\bigg)Q^2\bigg) \\ & + \mathcal{O}\bigg(\frac{1}{{\mathcal{E}_2}^4 V^4}\,,\,\frac{1}{{\mathcal{E}_2}^4 V^4}Q^2\,,\,\frac{1}{{\mathcal{E}_2}^4 V^4}Q^4\bigg)\bigg). \end{aligned}$$

  - Parameters also present at unfixed topology: $E_0(0,V_s)$.
  - New "fixed topology parameters": $\mathcal{E}_2 = \chi_t$, $\mathcal{E}_4$, $\mathcal{E}_6$.

# $C_{Q,V}(t)$ ($C(t)$ at fixed $Q$ and finite $V$) (1)

- In the following: expansion of

$$C_{Q,V}(t) \equiv \frac{1}{Z_{Q,V}} \int DA\, D\psi\, D\bar{\psi}\, \delta_{Q,Q[A]} O^\dagger(t) O(0) e^{-S_E[A,\bar{\psi},\psi]},$$

the two-point correlation function at fixed topological charge $Q$ and spacetime volume $V$, in powers of $1/V$.

- $O$ is a suitably normalized hadron creation operator,

$$O \equiv \frac{1}{\sqrt{V_s}} \int d^3r\, O'(\mathbf{r}) \quad \Big(\text{e.g. } O \equiv \frac{1}{\sqrt{V_s}} \int d^3r\, \bar{d}(\mathbf{r})\gamma_5 u(\mathbf{r}) \text{ for the pion}\Big),$$

where $O'(\mathrm{r})$ is a local operator (parity $P$ is not a symmetry at $\theta \neq 0$).

- Then

$$\alpha(\theta) \equiv \Big|\langle H;\theta|O|0;\theta\rangle\Big|^2 = \sum_{k=0}^{\infty} \frac{\alpha^{(2k)}(0)\theta^{2k}}{(2k)!} = \alpha(0) \exp\Big(\sum_{k=1}^{\infty} \frac{\beta^{(2k)}(0)\theta^{2k}}{(2k)!}\Big).$$

# $C_{Q,V}(t)$ ($C(t)$ at fixed $Q$ and finite $V$) (2)

- Result for $C_{Q,V}(t)$ up to $1/V^3$:

$$
\begin{aligned}
C_{Q,V}(t) &= \frac{\alpha(0)}{\sqrt{1+x_2/\mathcal{E}_2 V}} \exp\bigg(-M_H(0)t - \frac{1}{\mathcal{E}_2 V}\bigg(\frac{1}{1+x_2/\mathcal{E}_2 V}-1\bigg)\frac{1}{2}Q^2 - \frac{1}{(\mathcal{E}_2 V)^3}\frac{\mathcal{E}_4}{24\mathcal{E}_2}\bigg(\frac{1+x_4/\mathcal{E}_4 V}{(1+x_2/\mathcal{E}_2 V)^4}-1\bigg)Q^4\bigg) \\
&\quad \bigg(1-\frac{1}{(\mathcal{E}_2 V)^2}\frac{\mathcal{E}_4}{2\mathcal{E}_2}Q^2\bigg)^{+1/2}\bigg(1-\frac{1}{(\mathcal{E}_2 V)^2}\frac{\mathcal{E}_4(1+x_4/\mathcal{E}_4 V)}{2\mathcal{E}_2(1+x_2/\mathcal{E}_2 V)^3}Q^2\bigg)^{-1/2}\frac{G_{\mathcal{C}}}{G} + \mathcal{O}\bigg(\frac{1}{(\mathcal{E}_2 V)^4}Q^4\bigg) \\
G_{\mathcal{C}} &= 1 - \frac{1}{\mathcal{E}_2 V}\frac{\mathcal{E}_4(1+x_4/\mathcal{E}_4 V)}{8\mathcal{E}_2(1+x_2/\mathcal{E}_2 V)^2} + \frac{1}{(\mathcal{E}_2 V)^2}\bigg(-\frac{\mathcal{E}_6(1+x_6/\mathcal{E}_6 V)}{48\mathcal{E}_2(1+x_2/\mathcal{E}_2 V)^3} + \frac{35{\mathcal{E}_4}^2(1+x_4/\mathcal{E}_4 V)^2}{384{\mathcal{E}_2}^2(1+x_2/\mathcal{E}_2 V)^4}\bigg) \\
&\quad + \frac{1}{(\mathcal{E}_2 V)^3}\bigg(-\frac{\mathcal{E}_8(1+x_8/\mathcal{E}_8 V)}{384\mathcal{E}_2(1+x_2/\mathcal{E}_2 V)^4} + \frac{7\mathcal{E}_4(1+x_4/\mathcal{E}_4 V)\mathcal{E}_6(1+x_6/\mathcal{E}_6 V)}{256{\mathcal{E}_2}^2(1+x_2/\mathcal{E}_2 V)^5} - \frac{385{\mathcal{E}_4}^3(1+x_4/\mathcal{E}_4 V)^3}{3072{\mathcal{E}_2}^3(1+x_2/\mathcal{E}_2 V)^6} \\
&\qquad + \bigg(\frac{\mathcal{E}_6(1+x_6/\mathcal{E}_6 V)}{16\mathcal{E}_2(1+x_2/\mathcal{E}_2 V)^4} - \frac{{\mathcal{E}_4}^2(1+x_4/\mathcal{E}_4 V)^2}{3{\mathcal{E}_2}^2(1+x_2/\mathcal{E}_2 V)^5}\bigg)Q^2\bigg) + \mathcal{O}\bigg(\frac{1}{(\mathcal{E}_2 V)^4}\,,\,\frac{1}{(\mathcal{E}_2 V)^4}Q^2\bigg) \\
G &= 1 - \frac{1}{\mathcal{E}_2 V}\frac{\mathcal{E}_4}{8\mathcal{E}_2} + \frac{1}{(\mathcal{E}_2 V)^2}\bigg(-\frac{\mathcal{E}_6}{48\mathcal{E}_2} + \frac{35{\mathcal{E}_4}^2}{384{\mathcal{E}_2}^2}\bigg) \\
&\quad + \frac{1}{(\mathcal{E}_2 V)^3}\bigg(-\frac{\mathcal{E}_8}{384\mathcal{E}_2} + \frac{7\mathcal{E}_4\mathcal{E}_6}{256{\mathcal{E}_2}^2} - \frac{385{\mathcal{E}_4}^3}{3072{\mathcal{E}_2}^3} + \bigg(\frac{\mathcal{E}_6}{16\mathcal{E}_2} - \frac{{\mathcal{E}_4}^2}{3{\mathcal{E}_2}^2}\bigg)Q^2\bigg) + \mathcal{O}\bigg(\frac{1}{(\mathcal{E}_2 V)^4}\,,\,\frac{1}{(\mathcal{E}_2 V)^4}Q^2\bigg).
\end{aligned}
$$

  - Parameters also present at unfixed topology: $M_H(0)$, $\alpha(0)$.
  - New "fixed topology parameters": $\mathcal{E}_n$ ($\mathcal{E}_2 = \chi_t$), $x_n \equiv M_H^{(n)}(0)t + \beta^{(n)}(0)$, $n = 2, 4, 6, 8$ (i.e. 12 parameters).

# $C_{Q,V}(t)$ ($C(t)$ at fixed $Q$ and finite $V$) (3)

- For some applications it might be of interest to have $C_{Q,V}(t)$ up to $1/V^3$ in the form

$$C_{Q,V}(t) \quad = \quad \text{const} \times \exp\Big( - M_H(0)t + \text{fixed topology corrections as a power series in } 1/\mathcal{E}_2 V\Big),$$

which can be obtained by straightforward expansions in $1/V$:

$$\begin{aligned} C_{Q,V}(t) \quad = \quad & \alpha(0) \exp\Bigg( - M_H(0)t - \frac{1}{\mathcal{E}_2 V} \frac{x_2}{2} - \frac{1}{(\mathcal{E}_2 V)^2} \bigg( \frac{x_4 - 2(\mathcal{E}_4/\mathcal{E}_2)x_2 - 2{x_2}^2}{8} - \frac{x_2}{2} Q^2 \bigg) \\ & - \frac{1}{(\mathcal{E}_2 V)^3} \bigg( \frac{16(\mathcal{E}_4/\mathcal{E}_2)^2 x_2 + x_6 - 3(\mathcal{E}_6/\mathcal{E}_2)x_2 - 8(\mathcal{E}_4/\mathcal{E}_2)x_4 - 12 x_2 x_4 + 18(\mathcal{E}_4/\mathcal{E}_2){x_2}^2 + 8{x_2}^3}{48} \\ & - \frac{x_4 - 3(\mathcal{E}_4/\mathcal{E}_2)x_2 - 2{x_2}^2}{4} Q^2 \bigg) \\ & + \mathcal{O}\bigg( \frac{1}{(\mathcal{E}_2 V)^4} \, , \, \frac{1}{(\mathcal{E}_2 V)^4} Q^2 \, , \, \frac{1}{(\mathcal{E}_2 V)^4} Q^4 \bigg) \Bigg). \end{aligned}$$

  - Parameters also present at unfixed topology: $M_H(0)$, $\alpha(0)$.
  - New "fixed topology parameters": $\mathcal{E}_n$ ($\mathcal{E}_2 = \chi_t$), $x_n \equiv M_H^{(n)}(0)t + \beta^{(n)}(0)$, $n = 2, 4, 6$ (i.e. 9 parameters).

# $C_{Q,V}(t)$ ($C(t)$ at fixed $Q$ and finite $V$) (4)

- To reduce the number of parameters, one can also consider lower orders in $1/V$, e.g. $C_{Q,V}(t)$ up to $1/V$,

$$C_{Q,V}(t) = \frac{\alpha(0)}{\sqrt{1 + x_2/\mathcal{E}_2 V}} \exp\bigg( - M_H(0)t - \frac{1}{\mathcal{E}_2 V}\bigg(\frac{1}{1 + x_2/\mathcal{E}_2 V} - 1\bigg)\frac{1}{2}Q^2\bigg)\frac{G_\mathcal{C}}{G}$$

$$G_\mathcal{C} = 1 - \frac{1}{\mathcal{E}_2 V}\frac{\mathcal{E}_4(1 + x_4/\mathcal{E}_4 V)}{8\mathcal{E}_2(1 + x_2/\mathcal{E}_2 V)^2} \quad , \quad G = 1 - \frac{1}{\mathcal{E}_2 V}\frac{\mathcal{E}_4}{8\mathcal{E}_2}.$$

  - Parameters: $M_H(0)$, $\alpha(0)$, $\mathcal{E}_n$ ($\mathcal{E}_2 = \chi_t$), $x_n \equiv M_H^{(n)}(0)t + \beta^{(n)}(0)$, $n = 2, 4$.

- Another strategy is to set certain parameters to zero (i.e. to just ignore the corresponding fixed topology corrections), e.g.

$$C_{Q,V}(t) = \frac{\alpha(0)}{\sqrt{1 + x_2/\mathcal{E}_2 V}} \exp\bigg( - M_H(0)t - \frac{1}{\mathcal{E}_2 V}\bigg(\frac{1}{1 + x_2/\mathcal{E}_2 V} - 1\bigg)\frac{1}{2}Q^2\bigg),$$

  which is the $1/V^3$ result with $x_2 \equiv M_H^{(2)}(0)t$ and $\mathcal{E}_n = 0$, $M_H^{(n)}(0) = 0$, $n = 4, 6, 8$, $\beta^{(n)}(0) = 0$, $n = 2, 4, 6, 8$.

  - Parameters: $M_H(0)$, $\alpha(0)$, $\mathcal{E}_2 = \chi_t$, $M_H^{(2)}(0)$.

# Validity of the expansion of $C_{Q,V}(t)$

- The presented expansions are good approximations, if the following four conditions are fulfilled:

**(C1)** $1/\mathcal{E}_2 V \ll 1 \quad , \quad |Q|/\mathcal{E}_2 V \ll 1.$
The volume $V$ must be large, the topological charge $Q$ may not be too large.

**(C2)** $|x_2| = |M_H^{(2)}(0)t + \beta^{(2)}(0)| \lesssim 1.$
The temporal separation may not be too large.

**(C3)** $m_\pi(\theta)L \gtrsim 3 \ldots 5 \gg 1$
No ordinary finite size effects.

**(C4)** $(M_H^*(\theta) - M_H(\theta))t \gg 1 \quad , \quad M_H(\theta)(T - 2t) \gg 1.$
No contamination from excited states or particles propagating backwards in time.

# Part 2

# Quantum mechanics on a circle, the Schwinger model and SU(2) Yang-Mills theory at fixed topology

# QM on a circle

- Lagrangian parameterized by the angle $\varphi$:

$$L \equiv \frac{mr^2}{2}\dot{\varphi}^2 - U(\varphi) = \frac{I}{2}\dot{\varphi}^2 - U(\varphi),$$

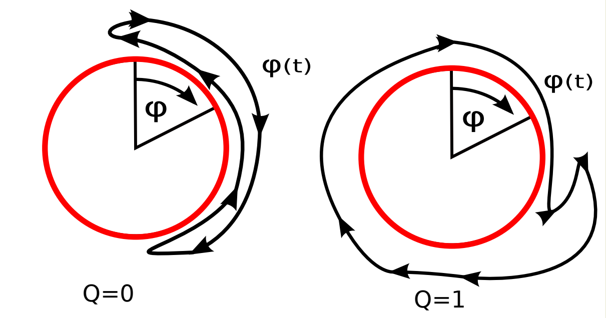
($m$: mass; $r$: radius; $I \equiv mr^2$: moment of inertia; $U(\varphi)$: potential).

- A periodic time with extension $T$ implies $\varphi(t+T) = \varphi(t) + 2\pi Q$, $Q \in \mathbb{Z}$, and gives rise to topological charge

$$\frac{1}{2\pi}\int_0^T dt\,\dot{\varphi} = \frac{1}{2\pi}(\varphi(T) - \varphi(0)) = Q.$$

- QM on a circle at fixed topology;

$$Z_{Q,T} \equiv \int D\varphi\,\delta_{Q,Q(\varphi)} e^{-S_E[\varphi]}.$$



# QM on a circle, free particle

- Can be solved analytically, also at fixed topology (hadron creation operator $O \equiv \sin(\varphi)$, hadron mass $M_H(\theta) \equiv E_1(\theta) - E_0(\theta)$).
- The expansions of $C_{Q,V}(t)$ from part 1 disagree with the analytical results.
- Reason: either assumption

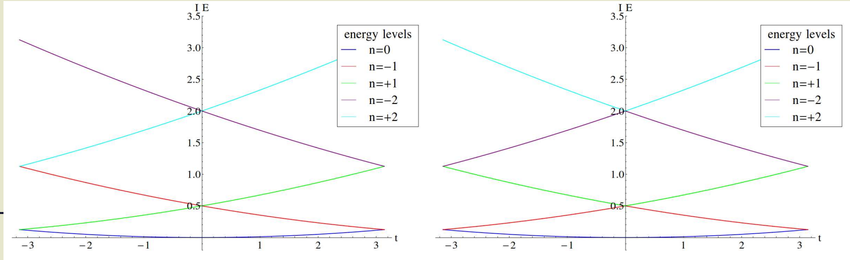
  $$E_n(+\theta) = E_n(-\theta)$$

  or condition

  **(C2)** $\quad |M_H^{(2)}(0)t + \beta^{(2)}(0)| \lesssim 1$

  not fulfilled (a particularity of the free case).
- One can derive the expansions of $C_{Q,V}(t)$ from part 1 for the more general case $E_n(+\theta) \neq E_n(-\theta)$; then there is perfect agreement.

  [A. Dromard and M. Wagner, arXiv:1404.0247 [hep-lat]]



# QM on a circle, square well potential (1)

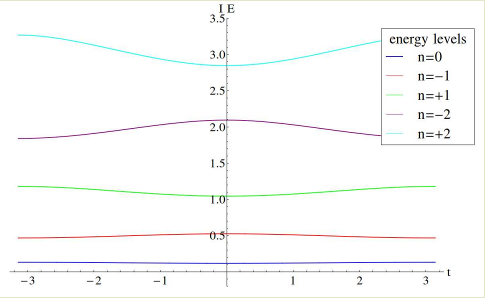
- Square well potential:

$$U(\varphi) \equiv \begin{cases} 0 & \text{if } -\rho/2 < \varphi < +\rho/2 \\ U_0 & \text{otherwise} \end{cases} .$$

- Can be solved numerically up to arbitrary precision (no simulations required), also at fixed topology
$\rightarrow$ ideal to test the expansions of $C_{Q,V}(t)$ from part 1.

- In the following: $\hat{U}_0 = U_0 I = 5.0$, $\rho = 0.9 \times 2\pi$.

| $n$ | $\hat{\mathcal{E}}_n$ | $\hat{M}_H^{(n)}(0)$ | $\alpha^{(n)}(0)$ | $\beta^{(n)}(0)$ |
|---|---|---|---|---|
| 0 | +0.11708 | +0.40714 | +0.50419 | |
| 2 | +0.00645 | −0.03838 | −0.00357 | +0.00709 |
| 4 | −0.00497 | +0.04983 | +0.00328 | −0.00636 |
| 6 | +0.00042 | −0.13191 | −0.04721 | +0.09308 |
| 8 | +0.00834 | +0.95631 | +0.91037 | −1.77931 |



# QM on a circle, square well potential (2)

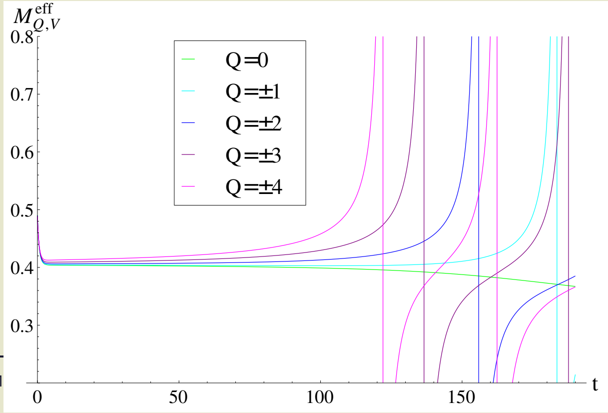
- Effective masses

$$\hat{M}^{\text{eff}}_{Q,\hat{T}}(\hat{t}) \equiv -\frac{d}{d\hat{t}} \ln\left(C_{Q,\hat{T}}(\hat{t})\right)$$

for different topological sectors $Q$ and $\hat{T} = T/I = 6.0/\hat{\mathcal{E}}_2 \approx 930.2$.

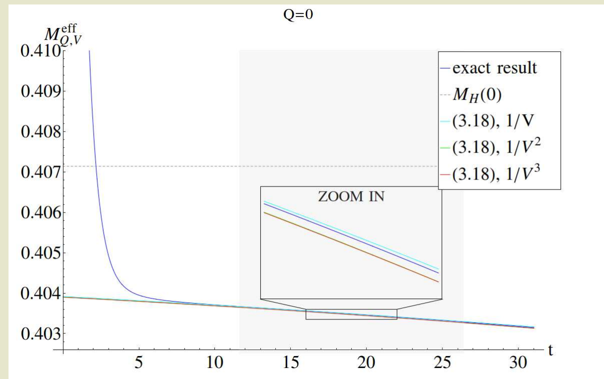
- At small temporal separations $\hat{M}^{\text{eff}}_{Q,\hat{T}}(\hat{t})$ quite large and strongly decreasing, due to the presence of excited states.

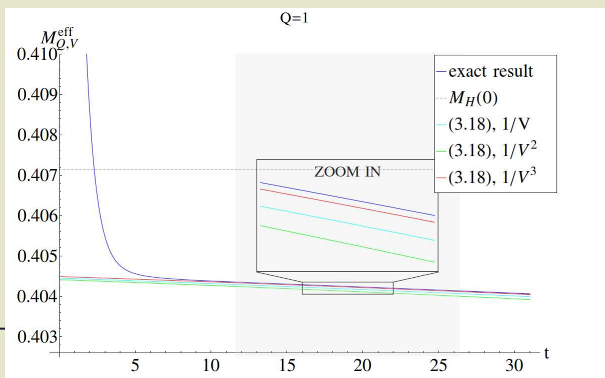
- At large temporal separations severe deviations from a constant behavior.

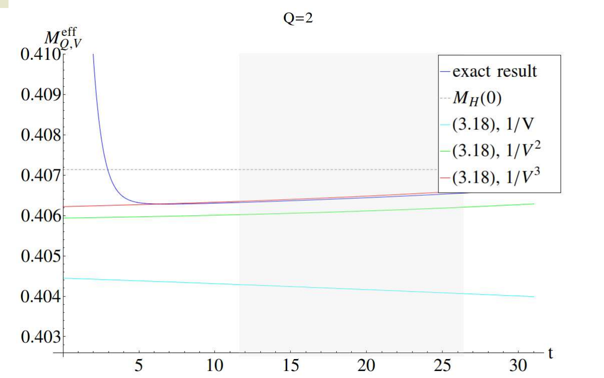


# QM on a circle, square well potential (3)

- Effective masses $\hat{M}^{\mathrm{eff}}_{Q,\hat{T}}$ derived from the $1/V$ expansions of two-point correlation functions for different topological sectors $Q$ and $\hat{T} = 6.0/\hat{\mathcal{E}}_2 \approx 930.2$.
  - $\mathcal{O}(1/V)$: 7 parameters.
  - $\mathcal{O}(1/V^2)$: 10 parameters.
  - $\mathcal{O}(1/V^3)$: 13 parameters.



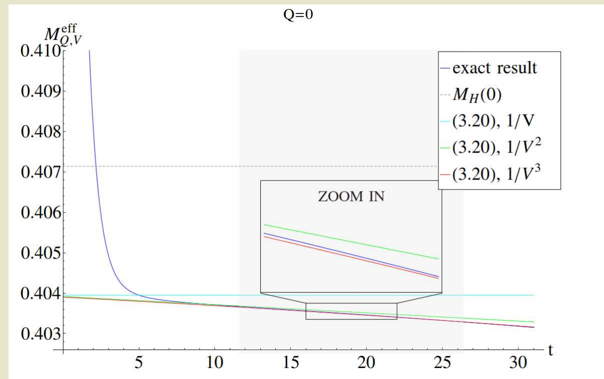



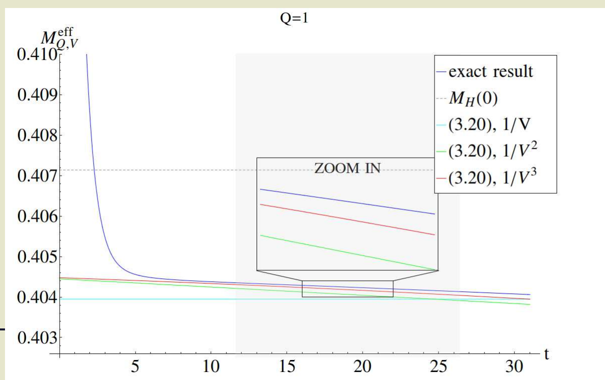
# QM on a circle, square well potential (4)

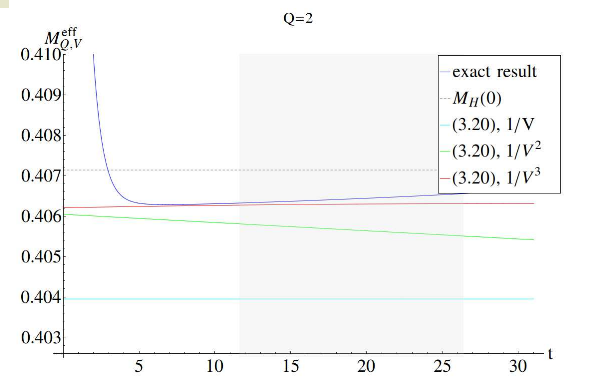
- Similar as before ... this time using expansions of the form

$$C_{Q,V}(t) \quad = \quad \text{const} \times \exp\big( - M_H(0)t + \text{fixed topology corrections}\big).$$

  - $\mathcal{O}(1/V)$: 4 parameters.
  - $\mathcal{O}(1/V^2)$: 7 parameters.
  - $\mathcal{O}(1/V^3)$: 10 parameters.



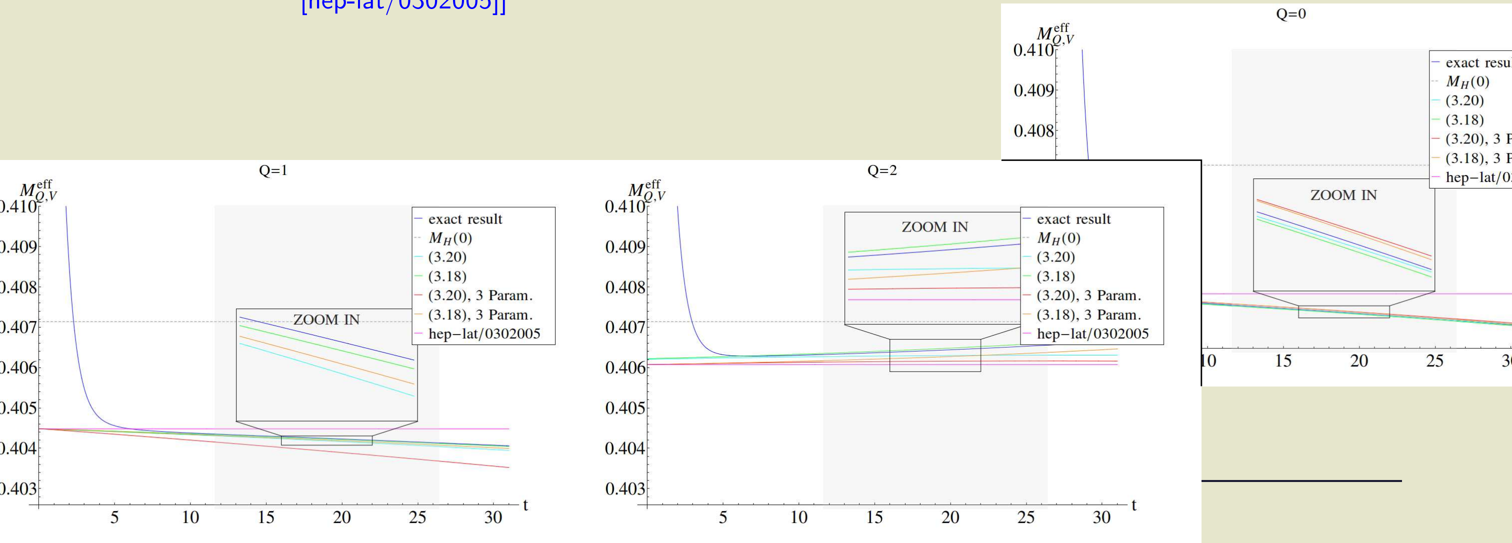



# QM on a circle, square well potential (5)

- Similar as before ... this time using only three parameters ($M_H(0)$, $\mathcal{E}_2 = \chi_t$, $M_H^{(2)}(0)$), all other parameters set to zero (seems to be a good compromise).
  - (3.18) $\rightarrow$ expansion as sketched in part 1.
  - (3.20) $\rightarrow$ $\text{const} \times \exp(-M_H(0)t + \text{fixed topology corrections})$.
  - hep-lat/0302005 $\rightarrow$

    [R. Brower, S. Chandrasekharan, J. W. Negele and U. J. Wiese, Phys. Lett. B **560**, 64 (2003) [hep-lat/0302005]]



# QM on a circle, square well potential (6)

- Determination of physical hadron masses (hadron masses at unfixed topology) from fixed topology simulations based on the $1/V$ expansions from part 1:

  1. Perform simulations at fixed topology for different topological charges $Q$ and spacetime volumes $V$. Determine "fixed topology hadron masses" defined e.g. via

     $$M_{Q,V} \quad \equiv \quad M^{\text{eff}}_{Q,V}(t_M) \quad = \quad -\frac{d}{dt} \ln\Big(C_{Q,V}(t)\Big)\Big|_{t=t_M}$$

     ($t_M$ should be chosen such that the expansions used in step 2 are good approximations).

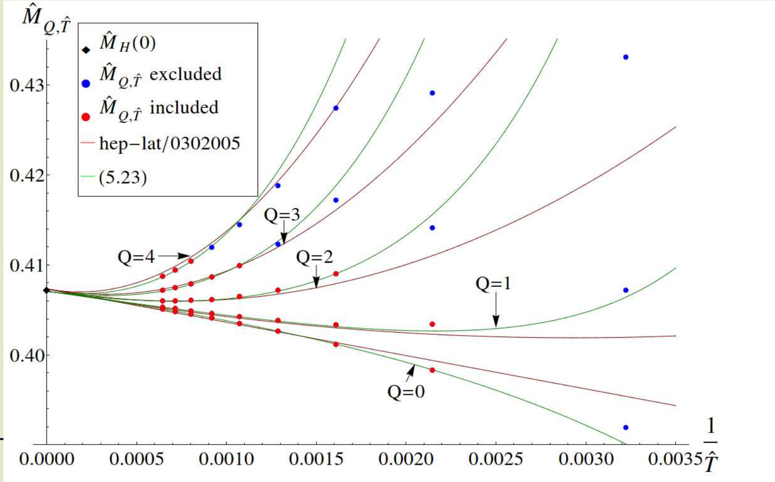
  2. Determine $M_H(0)$ (the hadron mass at unfixed topology), $\mathcal{E}_2 = \chi_t$, $M_H^{(2)}(0)$, ... by fitting an effective mass expression derived e.g. from

     $$C_{Q,V}(t_M) \quad = \quad \frac{\alpha(0)}{\sqrt{1 + x_2/\mathcal{E}_2 V}} \exp\bigg(-M_H(0) t_M - \frac{1}{\mathcal{E}_2 V}\bigg(\frac{1}{1 + x_2/\mathcal{E}_2 V} - 1\bigg)\frac{1}{2} Q^2\bigg),$$

     ($x_2 \equiv M_H^{(2)}(0) t_M$) to $M_{Q,V}$ obtained in step 1.

# QM on a circle, square well potential (7)

- Mimic the method to determine a physical hadron mass (at unfixed topology) from fixed topology computations:
  1. Use the exact result for the effective mass to generate $\hat{M}_{Q,\hat{T}}$ values (at $\hat{t}_M = 20.0$) for several topological charges $Q = 0, 1, 2, 3, 4$ and temporal extensions $\hat{T} = 2.0/\hat{\mathcal{E}}_2, 3.0/\hat{\mathcal{E}}_2, \ldots, 10.0/\hat{\mathcal{E}}_2$.
  2. Perform a single fit as explained on the previous slide (only those masses $\hat{M}_{Q,\hat{T}}$ enter the fit, for which the conditions **(C1)** and **(C2)** are fulfilled).



# QM on a circle, square well potential (8)

- Alternatively one could perform the fit directly on the "correlator level":
    1. Perform simulations at fixed topology for different topological charges $Q$ and spacetime volumes $V$. Determine $C_{Q,V}(t)$ for each simulation.
    2. Determine the physical hadron mass $M_H(0)$ by performing a single $\chi^2$ minimizing fit of one of the $1/V$ expansions of $C_{Q,V}(t)$ to the numerical results obtained in step 1. This input from step 1 is limited to those $Q$, $V$ and $t$ values, for which the conditions **(C1)**, **(C2)** and **(C4)** are fulfilled.

# QM on a circle, square well potential (9)

- $\hat{M}_H(0)$ from fixed topology computations (exact result: $M_H = 0.40714$):

| | | fitting to $\hat{M}_{Q,\hat{T}}$ | | fitting to correlators | |
|---|---|---|---|---|---|
| | expansion | $\hat{M}_H(0)$ result | rel. error | $\hat{M}_H(0)$ result | rel. error |
| $\frac{1}{\chi_t V}, \frac{\|Q\|}{\chi_t V} \leq 0.5$ | hep-lat/0302005 | $0.40733$ | $0.047\%$ | $0.40702$ | $0.029\%$ |
| | $1/V^3$, 3 param. | $0.40708$ | $0.014\%$ | $0.40706$ | $0.019\%$ |
| $\frac{1}{\chi_t V}, \frac{\|Q\|}{\chi_t V} \leq 0.3$ | hep-lat/0302005 | $0.40739$ | $0.062\%$ | $0.40732$ | $0.044\%$ |
| | $1/V^3$, 3 param. | $0.40695$ | $0.046\%$ | $0.40713$ | $0.002\%$ |

- $\hat{\chi}_t$ from fixed topology computations (exact result: $\hat{\chi}_t = 0.00645$):

| | | fitting to $\hat{M}_{Q,\hat{T}}$ | | fitting to correlators | |
|---|---|---|---|---|---|
| | expansion | $\hat{\chi}_t$ result | rel. error | $\hat{\chi}_t$ result | rel. error |
| $\frac{1}{\chi_t V}, \frac{\|Q\|}{\chi_t V} \leq 0.5$ | hep-lat/0302005 | $0.00586$ | $9.1\%$ | $0.00629$ | $2.5\%$ |
| | $1/V^3$, 3 param. | $0.00631$ | $2.2\%$ | $0.00633$ | $1.9\%$ |
| $\frac{1}{\chi_t V}, \frac{\|Q\|}{\chi_t V} \leq 0.3$ | hep-lat/0302005 | $0.00590$ | $8.5\%$ | $0.00627$ | $2.8\%$ |
| | $1/V^3$, 3 param. | $0.00592$ | $8.2\%$ | $0.00630$ | $2.3\%$ |

- Expansions give rather accurate results for $\hat{M}_H(0)$ (relative errors are below $0.1\%$) and reasonable results for $\hat{\chi}_t$ (relative errors of a few percent).

- Smaller relative errors for both $\hat{M}_H(0)$ and $\hat{\chi}_t$, when using "$1/V^3$, 3 param.".

# Schwinger model (1)

- Schwinger model (2D Euclidean quantum electrodynamics):

$$\mathcal{L}(\psi, \bar{\psi}, A) \quad = \quad \sum_{f=1}^{N_f} \bar{\psi}^{(f)}(\gamma_\mu(\partial_\mu + igA_\mu) + m)\psi^{(f)} + \frac{1}{4}F_{\mu\nu}F_{\mu\nu}.$$

- Several similarities to QCD:
  - Topological charge:

    $$Q \quad = \quad \frac{1}{\pi}\int \mathrm{d}^2x \, \epsilon_{\mu\nu}F_{\mu\nu}.$$

  - For $N_f = 2$ there is a rather light iso-triplet (pions).
  - Fermion confinement.

- First determination of physical hadron masses (pion mass) from fixed topology simulations by Bietenholz et. al.

  [W. Bietenholz, I. Hip, S. Shcheredin and J. Volkholz, Eur. Phys. J. C **72**, 1938 (2012) [arXiv:1109.2649 [hep-lat]]]

# Schwinger model (2)

- Schwinger model on the lattice:
  - Periodic spacetime lattice with $N_L^2$ lattice sites (extension of $L = N_L a$, spacetime volume $V = L^2$).
  - $N_f = 2$ flavors of Wilson fermions and the Wilson plaquette gauge action.
  - Dimensionful quantities are expressed in units of $a$, e.g. $\hat{g} = ga$ and $\hat{m} = ma$ (it is common to also use the dimensionless inverse squared coupling constant $\beta = 1/\hat{g}^2$).
  - Approach the continuum limit by increasing $N_L$, while keeping the dimensionless ratios $gL = \hat{g}N_L$ and $M_\pi L = \hat{M}_\pi N_L$ fixed ($M_\pi$: pion mass); this requires to decrease both $\hat{g}$ and $\hat{M}_\pi$ proportional to $1/N_L$ (for the latter $\hat{m}$ has to be adjusted appropriately).

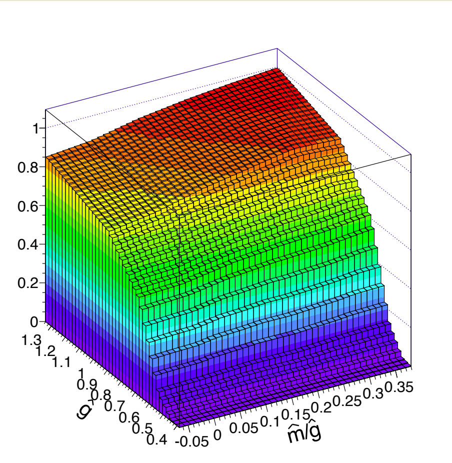
# Schwinger model (3)

- Schwinger model on the lattice:
  - Geometric definition of topological charge on the lattice,

$$Q \quad = \quad \frac{1}{2\pi} \sum_P \phi(P),$$

    where $\sum_P$ denotes the sum over all plaquettes $P = e^{i\phi(P)}$ with $-\pi < \phi(P) \leq +\pi$ (with this definition $Q \in \mathbb{Z}$).
  - Simulations at various values of $\beta$, $\hat{m}$ and $N_L$ using a Hybrid Monte Carlo (HMC) algorithm with multiple timescale integration and mass preconditioning.

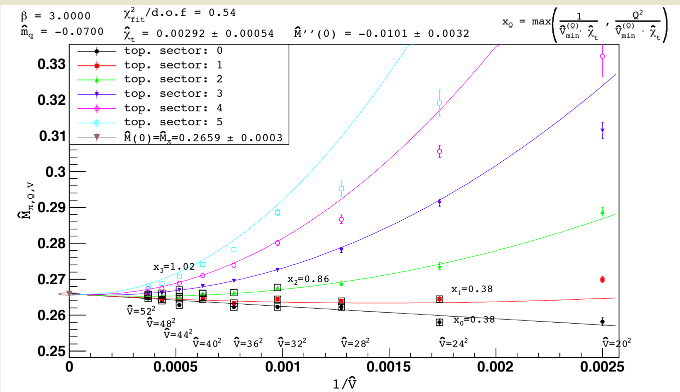
    [https://github.com/urbach/schwinger]
  - Figure: probability for a transition to another topological sector per HMC trajectory, plotted versus $\hat{g} = 1/\sqrt{\beta}$ (proportional to $a$) and $\hat{m}/\hat{g} = \hat{m}\sqrt{\beta}$ (proportional to $\hat{m}/a$), while $gL = \hat{g}N_L = N_L/\sqrt{\beta} = 24/\sqrt{5} =$ constant.

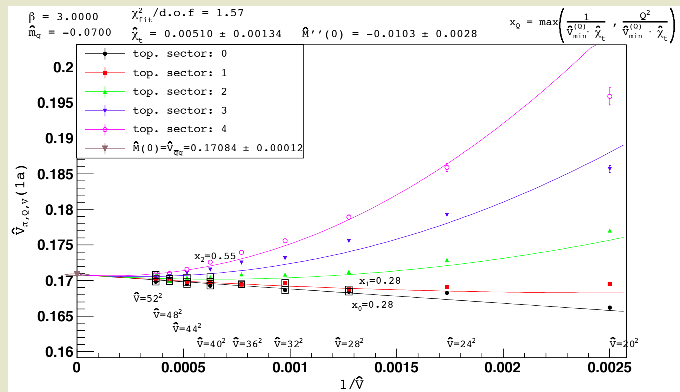


# Schwinger model (4)

- As for "QM on a circle" determine physical hadron masses from fixed topology computations.
  - Pion mass and static potential, hadron creation operators

$$O_\pi \;=\; \sum_x \bar{\psi}^{(u)}(x)\gamma_1\psi^{(d)}(x) \quad , \quad O_{\bar{q}q} \;=\; \bar{q}(x_1)U(x_1,x_2)q(x_2).$$



# Schwinger model (5)

- Hadron masses (the pion mass, the static potential) can be determined rather precisely (uncertainty $\ll 1\%$).
- There is a rather large error associated with the topological susceptibility (uncertainty up to $\approx 20\%$).

| observable | $\beta$ | $\hat{m}$ | $\hat{M}$ (fixed top.) | $\hat{M}$ (conv.) | $\hat{\chi}_t$ (fixed top.) | $\hat{\chi}_t$ ($\langle Q^2 \rangle / \hat{V}$) |
|---|---|---|---|---|---|---|
| $M_\pi$ | 3.0 | -0.07 | 0.2659(3) | 0.2663(3) | 0.00292(54) | 0.00454(6) |
| $V_{Q\bar{Q}}(1)$ | | | 0.1708(1) | 0.17108(5) | 0.0051(13) | |
| $V_{Q\bar{Q}}(2)$ | | | 0.2914(3) | 0.2927(2) | 0.00247(20) | |
| $M_\pi$ | 4.0 | -0.03 | 0.2743(6) | 0.2743(3) | 0.00228(39) | 0.00353(14) |
| $V_{Q\bar{Q}}(1)$ | | | 0.12552(7) | 0.12551(4) | 0.00313(26) | |
| $V_{Q\bar{Q}}(2)$ | | | 0.2250(2) | 0.2247(2) | 0.00329(15) | |

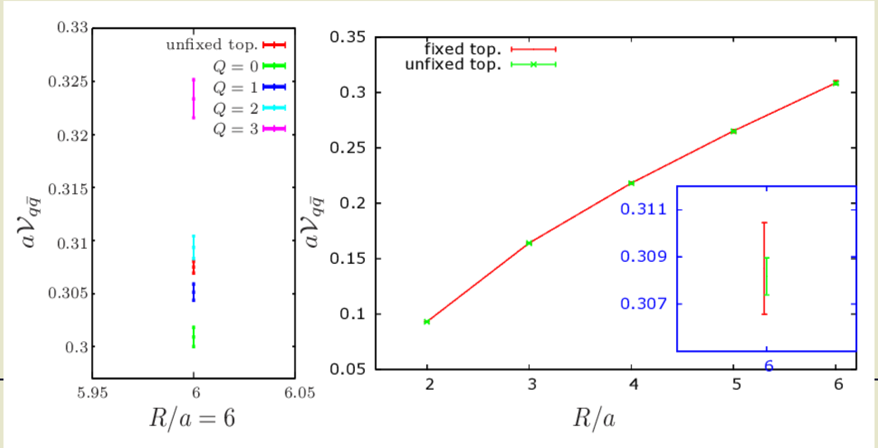
# SU(2) Yang-Mills theory

- SU(2) Yang-Mills theory:

$$\mathcal{L}(A_\mu) \equiv \frac{1}{4} F^a_{\mu\nu} F^a_{\mu\nu}.$$

- Left plot: there is a significant discrepancy between the static potential from computations restricted to a single topological sector and corresponding results obtained at unfixed topology.

- Right plot: comparison of the static potential obtained from Wilson loops at fixed topology and from standard lattice simulations.



# Conclusions, outlook

- The presented equations and techniques might be a starting point/might help to overcome the problem of topology freezing in QCD (present for overlap quarks and at small values of the lattice spacing).

  [A. Dromard and M. Wagner, PoS LATTICE **2013**, 339 (2013) [arXiv:1309.2483 [hep-lat]]]
  [C. Czaban and M. Wagner, PoS LATTICE **2013**, 465 (2013) [arXiv:1310.5258 [hep-lat]]]
  [A. Dromard and M. Wagner, arXiv:1404.0247 [hep-lat]]

- Future plans are mainly focused on first tests in QCD.