

The constraint potential for fermionic order parameters

Gergely Markó*, with Gergely Endrődi*, Tamás G. Kovács^{†,*} and Laurin Pannullo*

*Fakultät für Physik, Universität Bielefeld, Bielefeld.

[†]Eötvös Loránd University, Budapest. *Institute for Nuclear Research, Debrecen.

29th of July, 2024, Liverpool, Lattice 2024

- Spontaneous symmetry breaking
- Bosonic order parameter
- Fermionic order parameter
- Summary

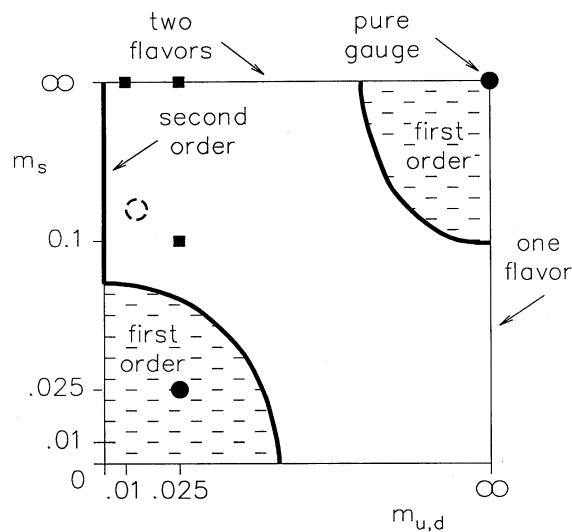


Motivation

- QCD in the chiral limit exhibits genuine phase transition.
- The order parameter is the quark condensate $\langle \bar{\psi}\psi \rangle$.

Motivation

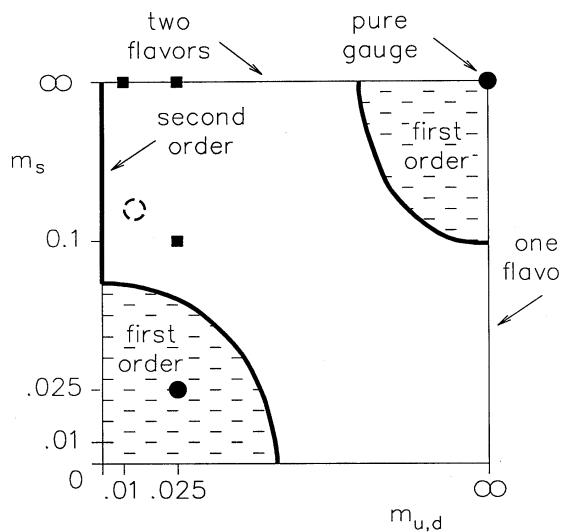
- QCD in the chiral limit exhibits genuine phase transition.
- The order parameter is the quark condensate $\langle \bar{\psi}\psi \rangle$.
- The study of this phase transition has a long history marked by the evolution of the Columbia-plot.



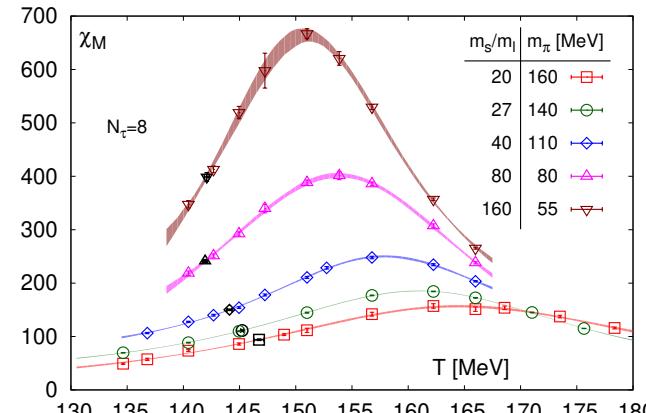
Brown et al., PRL 65 (1990)

Motivation

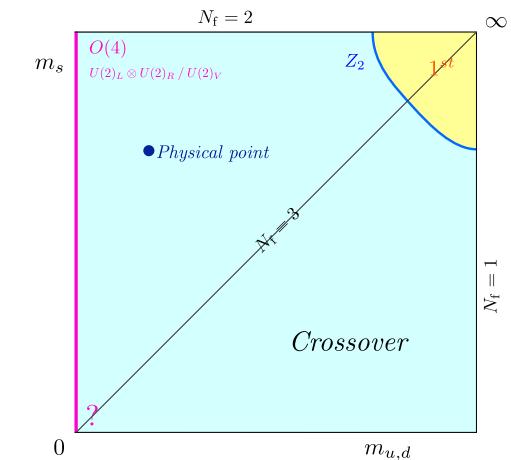
- QCD in the chiral limit exhibits genuine phase transition.
- The order parameter is the quark condensate $\langle \bar{\psi}\psi \rangle$.
- The study of this phase transition has a long history marked by the evolution of the Columbia-plot.
- Current Monte Carlo methods need $m \neq 0$, numerical extrapolation needed.
- Current successes (T_c , first order region discussion) rely on critical scaling around the transition.



Brown et al., PRL 65 (1990)



Ding et al., PRL 123 (2019)



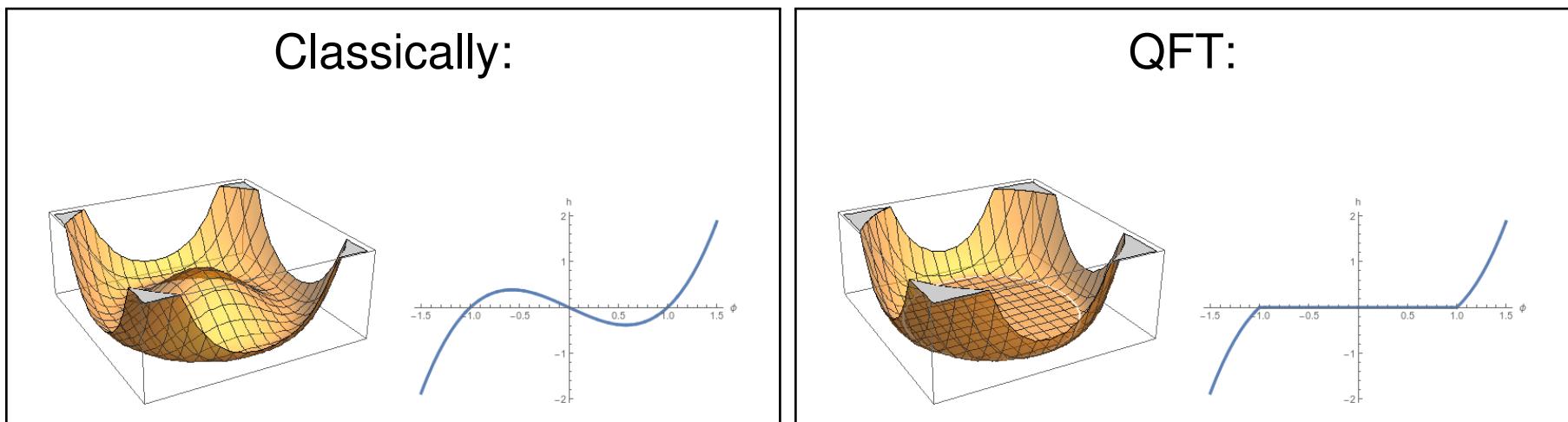
Cuteri et al., JHEP 11 (2021)

Spontaneous symmetry breaking

- Spontaneous breaking is defined as a **double-limit**: 1) volume, 2) explicit breaking

$$\langle \bar{\psi} \psi \rangle_{\min} = \lim_{m \rightarrow 0} \lim_{V \rightarrow \infty} \langle \bar{\psi} \psi \rangle_{V,m} .$$

- The **effective potential** between the different vacua is **flat** (Legendre-transformation), but cannot be accessed by usual simulations.
- Is there a way to evaluate the order parameter directly in the $m \rightarrow 0$ limit?
- And to access the flat region of the potential?



Constraint potential

Define the **constraint** effective potential

$$\exp(-V\Omega(\bar{\phi})) = \int \mathcal{D}\varphi \exp(-S[\varphi]) \delta\left(\int \varphi - V\phi\right) \equiv \mathcal{Z}_\phi.$$

- Full partition function recovered as

$$\mathcal{Z} = \int d\phi \mathcal{Z}_\phi.$$

Constraint potential

Define the **constraint** effective potential

$$\exp(-V\Omega(\bar{\phi})) = \int \mathcal{D}\varphi \exp(-S[\varphi]) \delta\left(\int \varphi - V\phi\right) \equiv \mathcal{Z}_\phi.$$

- Full partition function recovered as

$$\mathcal{Z} = \int d\phi \mathcal{Z}_\phi.$$

- In the **infinite volume** limit (and only there) agrees with the standard effective potential (Legendre-transform).

O'Raifeartaigh et al., NPB 271 (1986)

Constraint potential

Define the **constraint** effective potential

$$\exp(-V\Omega(\bar{\phi})) = \int \mathcal{D}\varphi \exp(-S[\varphi]) \delta\left(\int \varphi - V\phi\right) \equiv \mathcal{Z}_\phi.$$

- Full partition function recovered as

$$\mathcal{Z} = \int d\phi \mathcal{Z}_\phi.$$

- In the **infinite volume** limit (and only there) agrees with the standard effective potential (Legendre-transform).

O'Raifeartaigh et al., NPB 271 (1986)

- For scalar fields Markov chain Monte Carlo techniques can be constructed which **satisfy** the constraint.

Fodor et al., PoS LATTICE2007 056 (2007)

Constraint potential

Define the **constraint** effective potential

$$\exp(-V\Omega(\bar{\phi})) = \int \mathcal{D}\varphi \exp(-S[\varphi]) \delta\left(\int \varphi - V\phi\right) \equiv \mathcal{Z}_\phi.$$

- Full partition function recovered as

$$\mathcal{Z} = \int d\phi \mathcal{Z}_\phi.$$

- In the **infinite volume** limit (and only there) agrees with the standard effective potential (Legendre-transform).

O'Raifeartaigh et al., NPB 271 (1986)

- For scalar fields Markov chain Monte Carlo techniques can be constructed which **satisfy** the constraint.

Fodor et al., PoS LATTICE2007 056 (2007)

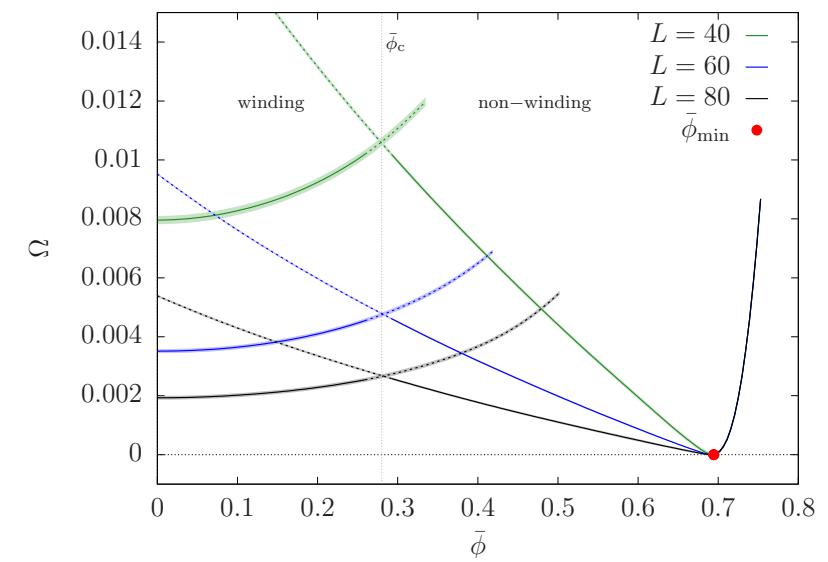
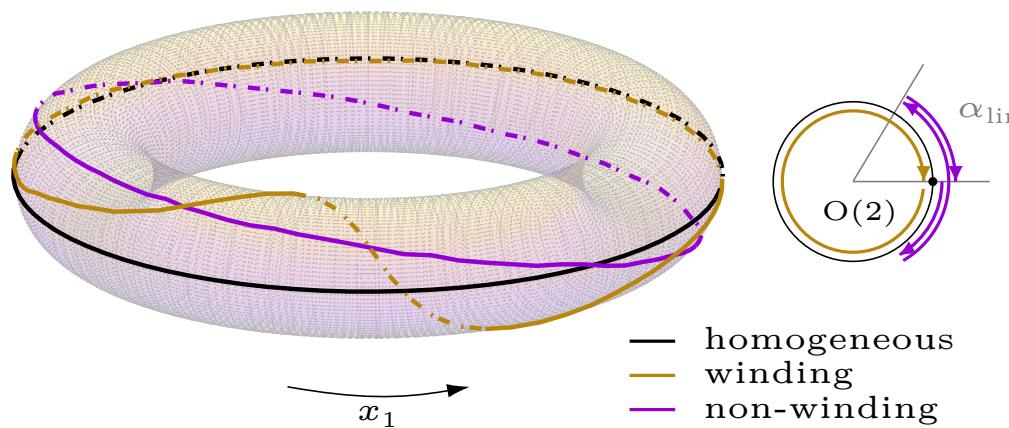
- Analogous to changing from **canonical** to **microcanonical** ensemble.

Bosonic order parameter

- Toy model example: $D = 3$, $O(2)$ symmetric φ^4 model.
- Constrain: $\delta \left(\frac{1}{V} \int d^3x \varphi(x) - \bar{\phi} \right)$.

Bosonic order parameter

- Toy model example: $D = 3$, $O(2)$ symmetric φ^4 model.
- Constrain: $\delta \left(\frac{1}{V} \int d^3x \varphi(x) - \bar{\phi} \right)$.
- Inhomogeneous configurations dominate the path integral in the flat region.
- Two distinct topology of configurations.
- Constraint potential flattens towards infinite volume limit.



Endrődi, Kovács and GM, PRL 127 (2021)

Fermionic order parameter

- We turn to a general fermionic model with the action

$$\mathcal{Z} = \int \mathcal{D}\Phi \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp[\bar{\psi}Q\psi - S_b[\Phi]] = \int \mathcal{D}\Phi e^{-S_b[\Phi]} \det Q[\Phi].$$

- Q is the Dirac-operator,
- in QCD: $\Phi \rightarrow U \in SU(N_c)$

Fermionic order parameter

- We turn to a general fermionic model with the action

$$\mathcal{Z} = \int \mathcal{D}\Phi \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp[\bar{\psi} Q \psi - S_b[\Phi]] = \int \mathcal{D}\Phi e^{-S_b[\Phi]} \det Q[\Phi].$$

- Q is the Dirac-operator,
- in chiral-GN: $\Phi \rightarrow (\varphi_1, \varphi_2)$

see the next talk by
L. Pannullo

Fermionic order parameter

- We turn to a general fermionic model with the action

$$\mathcal{Z} = \int \mathcal{D}\Phi \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp[\bar{\psi}Q\psi - S_b[\Phi]] = \int \mathcal{D}\Phi e^{-S_b[\Phi]} \det Q[\Phi].$$

- Q is the Dirac-operator,
- in QCD: $\Phi \rightarrow U \in SU(N_c)$; in chiral-GN: $\Phi \rightarrow (\varphi_1, \varphi_2)$
- Fermionic order parameter

see the next talk by
L. Pannullo

$$\langle \bar{\psi}\psi \rangle = \mathcal{Z}^{-1} \underbrace{\int \mathcal{D}\Phi \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{\bar{\psi}Q\psi - S_b[\Phi]} \left(\frac{1}{V} \int d^Dx \bar{\psi}(x)\psi(x) \right)}_{\bar{\psi}\psi}.$$

Fermionic order parameter

- We turn to a general fermionic model with the action

$$\mathcal{Z} = \int \mathcal{D}\Phi \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp[\bar{\psi}Q\psi - S_b[\Phi]] = \int \mathcal{D}\Phi e^{-S_b[\Phi]} \det Q[\Phi].$$

- Q is the Dirac-operator,
- in QCD: $\Phi \rightarrow U \in SU(N_c)$; in chiral-GN: $\Phi \rightarrow (\varphi_1, \varphi_2)$
- Fermionic order parameter

see the next talk by
L. Pannullo

$$\langle \bar{\psi}\psi \rangle = \mathcal{Z}^{-1} \int \mathcal{D}\Phi \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{\bar{\psi}Q\psi - S_b[\Phi]} \underbrace{\left(\frac{1}{V} \int d^Dx \bar{\psi}(x)\psi(x) \right)}_{\bar{\psi}\psi}.$$

- Before we continue, let's fix the bosonic background for simplicity!

Fermionic order parameter

- We turn to a general fermionic model with the action

$$\mathcal{Z} = \int \mathcal{D}\Phi \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp[\bar{\psi}Q\psi - S_b[\Phi]] = \int \mathcal{D}\Phi e^{-S_b[\Phi]} \det Q[\Phi].$$

- Q is the Dirac-operator,

- Fermionic order parameter

$$\langle \bar{\psi}\psi \rangle = \mathcal{Z}^{-1} \int \mathcal{D}\Phi \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{\bar{\psi}Q\psi - S_b[\Phi]} \underbrace{\left(\frac{1}{V} \int d^Dx \bar{\psi}(x)\psi(x) \right)}_{\bar{\psi}\psi}.$$

- Before we continue, let's fix the bosonic background for simplicity!

Fermionic order parameter

- Constraining the fermionic order parameter

$$\mathcal{Z}_\phi = \int \mathcal{D}\bar{\psi} \mathcal{D}\psi \ e^{\bar{\psi} Q \psi} \delta(\phi - \bar{\psi}\psi) \equiv e^{-V\Omega(\phi)}.$$

Fermionic order parameter

- Constraining the fermionic order parameter

$$\mathcal{Z}_\phi = \int \mathcal{D}\bar{\psi} \mathcal{D}\psi \ e^{\bar{\psi} Q \psi} \delta(\phi - \bar{\psi}\psi) \equiv e^{-V\Omega(\phi)}.$$

- But what is a Dirac- δ of Grassmannian variables?
- $\bar{\psi}\psi$ commutes with anything. But $(\bar{\psi}\psi)^{N_{\text{lat}}+1} = 0$.

Fermionic order parameter

- Constraining the fermionic order parameter

$$\mathcal{Z}_\phi = \int \mathcal{D}\bar{\psi} \mathcal{D}\psi \ e^{\bar{\psi} Q \psi} \delta(\phi - \bar{\psi}\psi) \equiv e^{-V\Omega(\phi)}.$$

- But what is a Dirac- δ of Grassmannian variables?
- $\bar{\psi}\psi$ commutes with anything. But $(\bar{\psi}\psi)^{N_{\text{lat}}+1} = 0$.
- Finite many Grassmanns \rightarrow any function is a finite polynomial

$$\rightarrow \text{ e.g. } \delta(\phi - \bar{\psi}\psi) = \sum_k^{N_{\text{lat}}} \frac{(-1)^k}{k!} (\bar{\psi}\psi)^k \frac{\partial}{\partial \phi^k} \delta(\phi).$$

De Witt, *Supermanifolds*, Cambridge (1992)

Fermionic order parameter

- Constraining the fermionic order parameter

$$\mathcal{Z}_\phi = \int \mathcal{D}\bar{\psi} \mathcal{D}\psi \ e^{\bar{\psi} Q \psi} \delta(\phi - \bar{\psi}\psi) \equiv e^{-V\Omega(\phi)}.$$

- But what is a Dirac- δ of Grassmannian variables?
- $\bar{\psi}\psi$ commutes with anything. But $(\bar{\psi}\psi)^{N_{\text{lat}}+1} = 0$.
- Finite many Grassmanns \rightarrow any function is a finite polynomial

$$\rightarrow \text{ e.g. } \delta(\phi - \bar{\psi}\psi) = \sum_k^{N_{\text{lat}}} \frac{(-1)^k}{k!} (\bar{\psi}\psi)^k \frac{\partial}{\partial \phi^k} \delta(\phi).$$

De Witt, *Supermanifolds*, Cambridge (1992)

- Makes sense as a distribution

$$\int d\phi \mathcal{Z}_\phi \phi^m = \langle (\bar{\psi}\psi)^m \rangle,$$

- but impractical: each term in the \sum_k needs simulations with (strangely) modified fermion determinant.

Fermionic order parameter

- Alternatively, use Fourier-representation: $\delta(x) = \int_{-\infty}^{\infty} \frac{d\eta}{2\pi} e^{i\eta x}$

$$\mathcal{Z}_\phi = \int \frac{d\eta}{2\pi} \tilde{\mathcal{Z}}_\eta e^{i\eta\phi}.$$

Fermionic order parameter

- Alternatively, use Fourier-representation: $\delta(x) = \int_{-\infty}^{\infty} \frac{d\eta}{2\pi} e^{i\eta x}$

$$\mathcal{Z}_\phi = \int \frac{d\eta}{2\pi} \tilde{\mathcal{Z}}_\eta e^{i\eta\phi}.$$

- The characteristic function, $\tilde{\mathcal{Z}}_\eta$ looks more familiar

$$\tilde{\mathcal{Z}}_\eta = \int \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp \left[\bar{\psi} \left(Q - \frac{i\eta}{V} \right) \psi \right] = \det \left[Q - \frac{i\eta}{V} \right].$$

Fermionic order parameter

- Alternatively, use Fourier-representation: $\delta(x) = \int_{-\infty}^{\infty} \frac{d\eta}{2\pi} e^{i\eta x}$

$$\mathcal{Z}_\phi = \int \frac{d\eta}{2\pi} \tilde{\mathcal{Z}}_\eta e^{i\eta\phi}.$$

- The characteristic function, $\tilde{\mathcal{Z}}_\eta$ looks more familiar

$$\tilde{\mathcal{Z}}_\eta = \int \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp \left[\bar{\psi} \left(Q - \frac{i\eta}{V} \right) \psi \right] = \det \left[Q - \frac{i\eta}{V} \right].$$

- If the spectrum of Q is directly known, physical information can be extracted from the η -dependence.
- This approach was used in the compact Schwinger model in [Azcoiti et al., PLB 354 \(1995\)](#).

Fermionic order parameter

- Alternatively, use Fourier-representation: $\delta(x) = \int_{-\infty}^{\infty} \frac{d\eta}{2\pi} e^{i\eta x}$

$$\mathcal{Z}_\phi = \int \frac{d\eta}{2\pi} \tilde{\mathcal{Z}}_\eta e^{i\eta\phi}.$$

- The characteristic function, $\tilde{\mathcal{Z}}_\eta$ looks more familiar

$$\tilde{\mathcal{Z}}_\eta = \int \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp \left[\bar{\psi} \left(Q - \frac{i\eta}{V} \right) \psi \right] = \det \left[Q - \frac{i\eta}{V} \right].$$

- If the spectrum of Q is directly known, physical information can be extracted from the η -dependence.
- This approach was used in the compact Schwinger model in [Azcoiti et al., PLB 354 \(1995\)](#).
- Larger lattices: approximate or partial spectrum lead to numerical instabilities (similar to Lee-Yang zeros).

Fermionic order parameter

- We follow a different route, use $\det X = e^{\text{Tr} \log X} \rightarrow \text{expand log in } V^{-1}$.

$$\tilde{\mathcal{Z}}_\eta = \det Q \times \exp \left[- \sum_k \left(\frac{i}{V} \right)^k \text{Tr} \left(Q^{-1} \eta \right)^k \right].$$

Fermionic order parameter

- We follow a different route, use $\det X = e^{\text{Tr} \log X} \rightarrow \text{expand log in } V^{-1}$.

$$\tilde{\mathcal{Z}}_\eta = \det Q \times \exp \left[- \sum_k \left(\frac{i}{V} \right)^k \text{Tr} (Q^{-1} \eta)^k \right].$$

- In the thermodynamic limit we can treat the η -integrals in a saddle-point approximation, keeping up to NLO in $1/V$

$$\begin{aligned} \mathcal{Z}_\phi &= \int \frac{d\eta}{2\pi} e^{i\eta\phi} \det Q \exp \left[- i\eta \underbrace{\frac{\text{Tr } Q^{-1}}{V}}_{\mathcal{M}} + \frac{\eta^2}{V} \underbrace{\frac{\text{Tr } Q^{-2}}{V}}_{-\chi} \right] \\ &= \det Q \exp \left[- \frac{V}{2} (\phi - \mathcal{M}) \chi^{-1} (\phi - \mathcal{M}) - \frac{1}{2} \log \det \chi \right]. \end{aligned}$$

Fermionic order parameter

- We follow a different route, use $\det X = e^{\text{Tr} \log X} \rightarrow \text{expand log in } V^{-1}$.

$$\tilde{\mathcal{Z}}_\eta = \det Q \times \exp \left[- \sum_k \left(\frac{i}{V} \right)^k \text{Tr} (Q^{-1} \eta)^k \right].$$

- In the thermodynamic limit we can treat the η -integrals in a saddle-point approximation, keeping up to NLO in $1/V$

$$\begin{aligned} \mathcal{Z}_\phi &= \int \frac{d\eta}{2\pi} e^{i\eta\phi} \det Q \exp \left[- i\eta \underbrace{\frac{\text{Tr } Q^{-1}}{V}}_{\mathcal{M}} + \frac{\eta^2}{V} \underbrace{\frac{\text{Tr } Q^{-2}}{V}}_{-\chi} \right] \\ &= \det Q \exp \left[- \frac{V}{2} (\phi - \mathcal{M}) \chi^{-1} (\phi - \mathcal{M}) - \frac{1}{2} \log \det \chi \right]. \end{aligned}$$

- Moments are correct up to V^{-2}

$$\begin{aligned} \int d\phi \mathcal{Z}_\phi \phi &= \mathcal{M} \equiv \langle \bar{\psi} \psi \rangle, \quad \int d\phi \mathcal{Z}_\phi \phi^2 = \mathcal{M}^2 + \frac{\chi}{V} \equiv \langle (\bar{\psi} \psi)^2 \rangle \\ \int d\phi \mathcal{Z}_\phi \phi^3 &= \langle (\bar{\psi} \psi)^3 \rangle + \mathcal{O}(V^{-2}). \end{aligned}$$

Fermionic order parameter

Putting the bosonic fields back

$$\mathcal{Z}_\phi = \int \mathcal{D}\Phi e^{-S_b[\Phi]} \frac{\det Q[\Phi]}{\sqrt{\det \chi[\Phi]}} \exp \left[-\frac{V}{2} (\phi - \mathcal{M}[\Phi]) \cdot \chi^{-1}[\Phi] \cdot (\phi - \mathcal{M}[\Phi]) \right]$$

- Simulations with a **modified action**.

Fermionic order parameter

Putting the bosonic fields back

$$\mathcal{Z}_\phi = \int \mathcal{D}\Phi e^{-S_b[\Phi]} \frac{\det Q[\Phi]}{\sqrt{\det \chi[\Phi]}} \exp \left[-\frac{V}{2} (\phi - \mathcal{M}[\Phi]) \cdot \chi^{-1}[\Phi] \cdot (\phi - \mathcal{M}[\Phi]) \right]$$

- Simulations with a **modified action**.
- Relies on **large volume expansion**, the constraint gets stronger towards the thermodynamic limit.
- Also relies on $\det \chi > 0$, which is ensured in the continuum limit.

Fermionic order parameter

Putting the bosonic fields back

$$\mathcal{Z}_\phi = \int \mathcal{D}\Phi e^{-S_b[\Phi]} \frac{\det Q[\Phi]}{\sqrt{\det \chi[\Phi]}} \exp \left[-\frac{V}{2} (\phi - \mathcal{M}[\Phi]) \cdot \chi^{-1}[\Phi] \cdot (\phi - \mathcal{M}[\Phi]) \right]$$

- Simulations with a **modified action**.
- Relies on **large volume expansion**, the constraint gets stronger towards the thermodynamic limit.
- Also relies on $\det \chi > 0$, which is ensured in the continuum limit.
- Similar to a **density of states** approach, but has a **natural width**, $\chi \rightarrow 0$ need for extra extrapolation!
- **Explicit results** in the chiral GN model:

see the next talk by
L. Pannullo

Summary and outlook

- The **constraint potential** is a tool to discuss **spontaneous symmetry breaking**.
- Directly at **vanishing** explicit breaking.
- Monte Carlo simulations for bosonic order parameters has been used.
- A generalization to fermionic order parameters is not straightforward.
- We gave a **generalization** which becomes **exact** in the **thermodynamic limit**.
- It is also feasible to simulate.
- **First results:**

see the next talk by
L. Pannullo
- More to follow!