Simulation of theories with a topological term

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Outline

- Motivation
- Difficulties
- Description of the methods
- Testing the methods
- The Schwinger model with a θ term
- Looking towards QCD
- Conclusions and outlook

Motivation

- To understand the behavior of QCD with a θ term
  - Does QCD break CP symmetry at $\theta = \pi$?
  - Reconstruct the θ-dependence of observables, such as the topological charge, or the vacuum energy.
- Strong CP problem: why is θ so small ($\theta < 10^{-9}$) in nature?
- Directly relevant for axion physics: Peccei-Quinn mechanism

$$\theta(x) = \frac{a(x)}{f_a}, \qquad \mathcal{L} = \cdots - \theta(x) q(x)$$

  Relation between the axion mass and the topological susceptibility in QCD:

$$m_a^2(T)\, f_a^2 = \chi(T) = \lim_{V\to\infty} \frac{\langle Q^2 \rangle |_{\theta=0}}{V}$$

- Possible extensions to other systems with a sign problem: finite density, condensed-matter models (Hubbard), etc.

Difficulties

- The notorious sign problem:

$$\mathcal{L}_{\theta}^{Eucl} = i\theta q(x)$$

- The Euclidean action is not real, and the partition function cannot be interpreted as a probability distribution.

- Standard simulation algorithms fail!

- We can calculate fairly accurately observables which can be obtained from $\theta = 0$ simulations.

$$\chi \sim \left\langle Q^2 \right\rangle, \left\langle Q^4 \right\rangle, \dots$$

Two methods

- Two methods to deal with/evade the sign problem in theories with a "topological" term.
- Both methods use the same input data: simulations at imaginary values of the field, $\theta = -ih$, where the sign problem is absent.
- **Method I**: reconstruction of the probability distribution function of the topological charge at $\theta = 0$.
- **Method II**: smooth analytic extrapolation.

Method I

Reconstruction of the probability distribution function of the topological charge at $\theta = 0$ (Azcoiti et al, Phys.Rev.Lett.89.141601 (2002)).

Defining the density of topological charge as $x_n = \frac{n}{V}$:

$$\frac{Z_V(\theta)}{Z_V(0)} = \sum_n p_V(n) e^{i\theta n} = \sum_{x_n} e^{-Vf_V(x_n)} e^{i\theta V x_n} = \sum_{x_n} e^{-V(f_V(x_n) - i\theta x_n)}$$

Let us suppose that in the infinite volume limit we can replace the sum by an integral:

$$\frac{Z_V(\theta)}{Z_V(0)} \approx \int e^{-Vf(x)} e^{i\theta x V} dx$$

where $f_V(x_n) \to f(x)$.

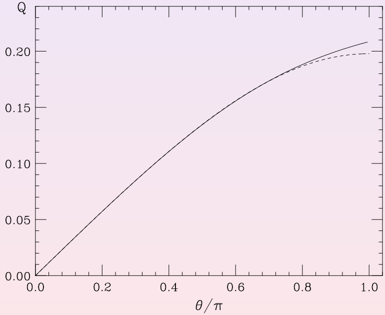
Method I

$$\frac{Z_V(\theta)}{Z_V(0)} \approx \int e^{-Vf(x)} e^{i\theta x V} dx = \int e^{-V(f(x)-i\theta x)} dx$$

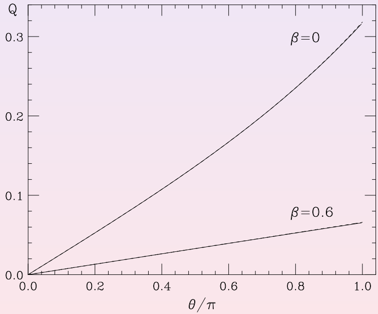
- Let us consider the expression above in the imaginary axis $\theta = -ih$, with h real. Then everything is positive definite, and the saddle point approximation gives $f'(x) = i\theta = h$
- Obtain x as a function of h to high precision from numerical simulations at $\theta = -ih$.
- Fit $f'(x)$ to a ratio of polinomials, and integrate the result analytically. This provides $f(x)$ to high precision.
- Use a multiprecision algorithm to compute the partition function and the order parameter for θ real using the $f(x)$ previously calculated.

Method I

1-d AF Ising model with an imaginary magnetic field: $i\theta T \frac{1}{2} \sum_i S_i$

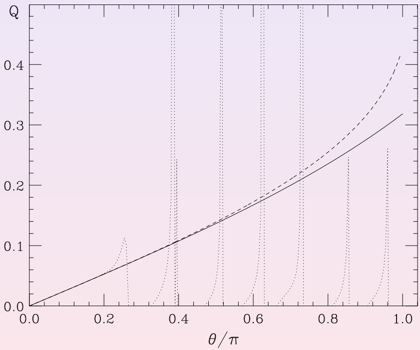


$U(1)$ model in $d = 2$.



Method I

How do numerical errors in the determination of $f(x)$ propagate?



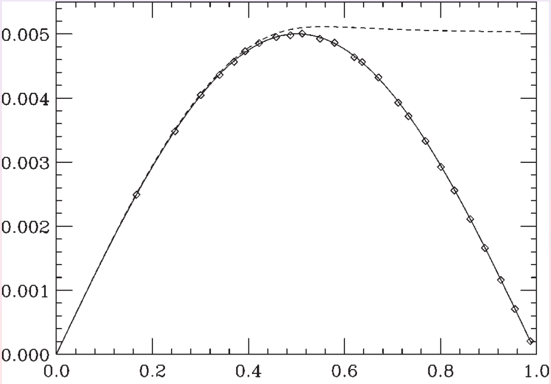
Small random error of 10^{-3} in $f(x)$.

Large correlated error:
$f(x) \to f(x)\left(1 + \frac{1}{2}\sin(x^2)\right)$.

Method I

Caveat: When the order parameter is not monotonous, the method fails: flattening.

$$Z_V(\theta) = (1 + A\cos\theta)^V$$



Method II

(Azcoiti et al, Phys.Lett.B 563 117 (2003))

$$Z_V(\theta) \approx \sum_{x_n} e^{-Vf_V(x_n)} e^{i\theta V x_n} = \sum_{y_n \geq 0} G_V(y_n) \left(\cos^2 \frac{\theta}{2}\right)^{Vy_n}$$

$G_V(y_n)$ is a functional of $f_V(x_n)$

$$z = \cos \frac{\theta}{2}; \quad y(z) = \frac{x(\theta)}{\tan \frac{\theta}{2}}$$

- Simulations at imaginary $\theta = -ih$ gives us access to the region $z = \cosh \frac{\theta}{2} >= 1$, whereas the physical region is $0 \leq z \leq 1$.

Method II

- Scaling of z: $y_\lambda(z) = y(e^{\lambda/2} z)$
- We study y_λ / y as $y \to 0$
- If $y(z)$ does not vanish at $z > 0$, and the quotient is smooth, we can hope to extrapolate to $y = 0$.

  At weak coupling we expect y to be small.

Caveat: If there is a phase transition in y we expect the method to fail.

Method II

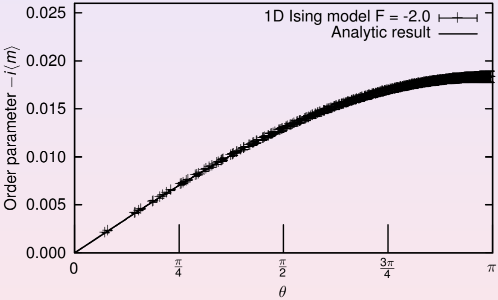
- We define

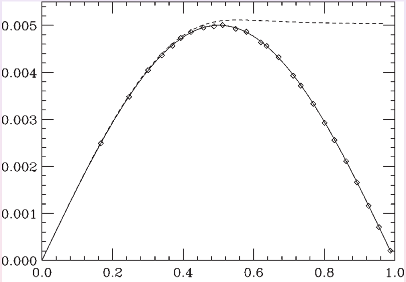
$$\gamma_\lambda = \frac{2}{\lambda} \log\left(\frac{y_\lambda}{y}\right) \ (y \to 0)$$

$$(\pi - \theta)^{\gamma_\lambda - 1} \ (\theta \to \pi)$$

- $\gamma_\lambda \to 1$: spontaneous symmetry breaking at $\theta = \pi$
- $\gamma_\lambda \in (1, 2)$: second order phase transition at $\theta = \pi$, with a divergent susceptibility.
- $\gamma_\lambda \to 2$: the symmetry is realized at $\theta = \pi$, and the free energy is analytic.
- In contrast with method I, this method has shown good results also for systems that do not break the symmetry at $\theta = \pi$.

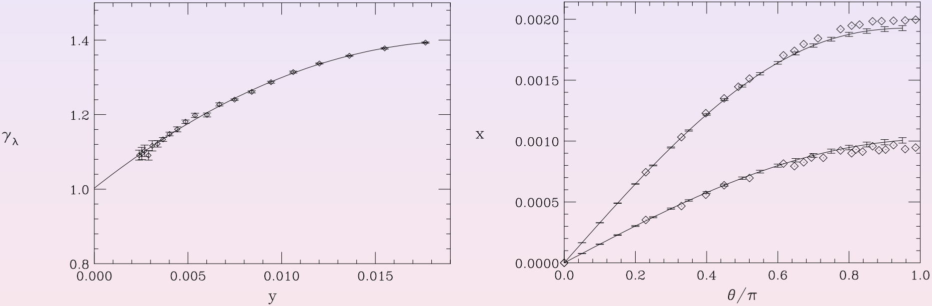
Method II





(Azcoiti et al., Nucl.Phys.B 851 (2011) 420)

CP^9



(Azcoiti et al., Phys.Rev.D 69 (2004) 056006)

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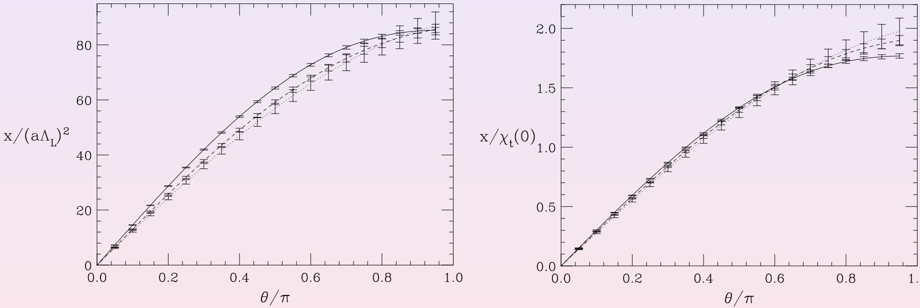


Schwinger model with a θ term

2d electrodynamics:

$$S = \int d^2x \{ \bar{\psi}\gamma_\mu \left(\partial_\mu + iA_\mu\right)\psi + m\bar{\psi}\psi + \frac{1}{4e^2}F_{\mu\nu}^2 + \frac{i\theta}{4\pi}\epsilon_{\mu\nu}F_{\mu\nu}\}$$

- Toy model for QCD
- A model with fermions.
- Confining
- Has non-trivial topology, axial anomaly, non-vanishing value of the chiral condensate in the 1-flavor case.

Schwinger model with a θ term

- At large fermion mass, it tends to pure gauge two-dimensional electrodynamics (exactly solvable) $\rightarrow$ spontaneous symmetry breaking.
- At small fermion mass no symmetry breaking:

$$\langle q \rangle = m\Sigma \sin\theta + O(m^2)$$

- We therefore expect a critical point separating large and small fermion masses.
  (Coleman, Ann. of Phys.101, (1976) 239; Hamer et al., Nucl.Phys.B208 (1982) 413; Byrnes et al., Phys.Rev.D 66 (2002) 013002; Shimizu et al., Phys.Rev.D 90 (2014) 014508).

Schwinger model with a θ term

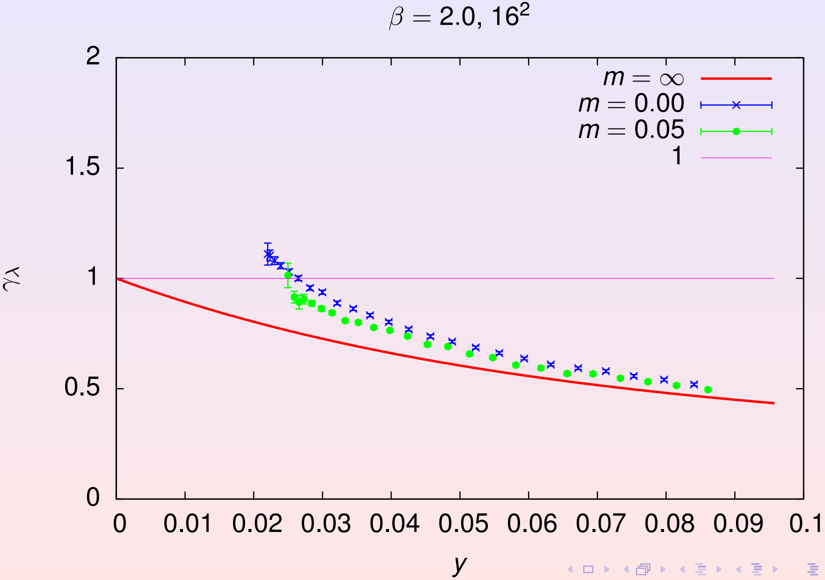
- Simulations with a standard Metropolis algorithm: wasteful, requires the calculation of the entire spectrum of the staggered Dirac operator for each change in the gauge field.

- Three values of β: 2.0, 3.0, 4.0

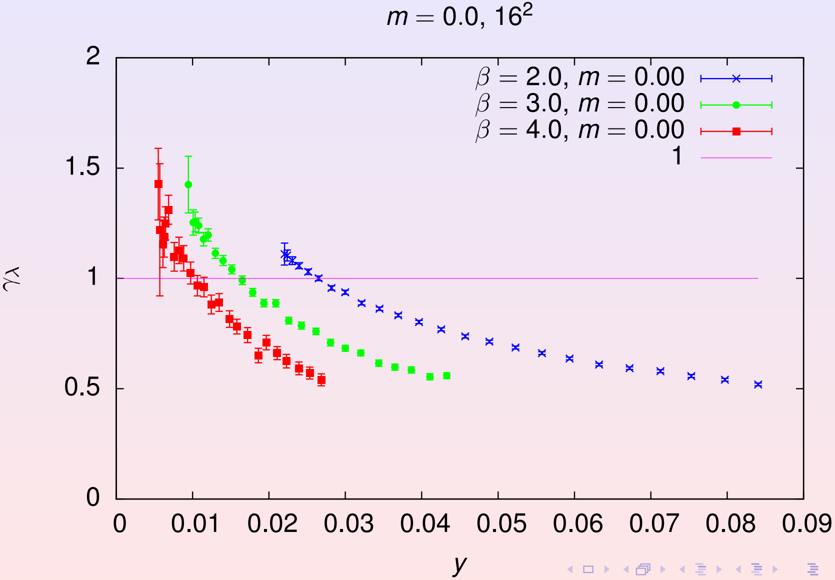
- Three values of m: 0, 0.05 and 0.5

- $\approx 10^5$ measurements per point.

Schwinger model with a θ term

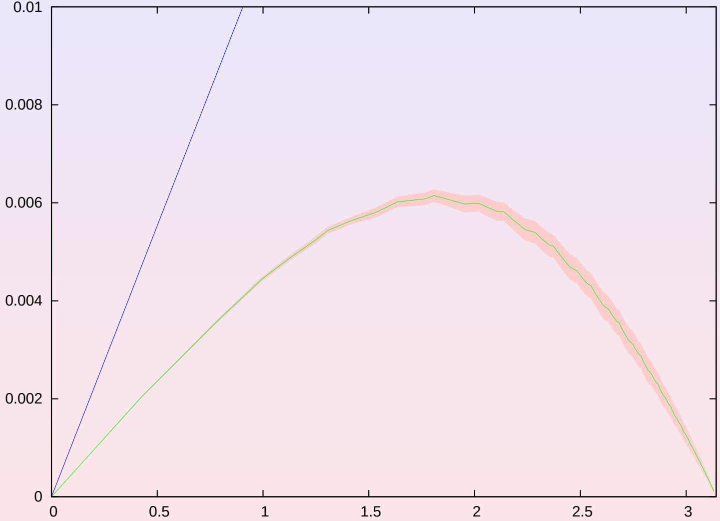


Schwinger model with a θ term



Schwinger model with a θ term

$\beta = 3.0$, $m = 0$ and $m = \infty$



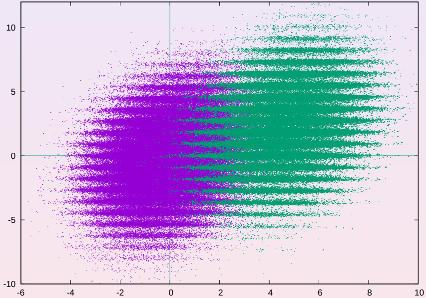
Looking towards QCD

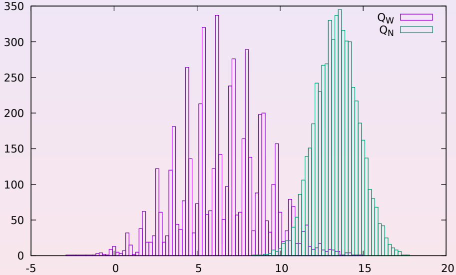
- In principle the methods described should work also for QCD with a θ term.
- Much more expensive numerically, especially with light quarks (which seem essential).
- Much more complicated implementation of the topological charge operator Q.

Looking towards QCD

- Geometrical Q: Either gluonic definition or through the eigenvectors of the overlap Dirac operator.
  - Integer
  - No renormalization
  - Numerically very expensive to calculate
- Definition through the Wilson flow
  - Quasi-integer
  - Numerically expensive
- Naive discretization
  - Numerically cheap
  - Non-integer
  - Requires a large renormalization

Looking towards QCD





Conclusions and outlook

- There are now methods that can treat systems with a θ-like term.
- They have been tested in a wide variety of models.
- The methods described here should be applicable to QCD with a θ term.
- We are starting simulations, first in quenched QCD, to test concrete implementations of both the dynamics and the topological charge operator.
- One likely problem is the topological freezing at small lattice spacings $a < .05$ fm.