Flux Representation for Effective $\mathbb{Z}(N)$ Theories for the Polyakov Loop

Marcio Woitek

Instituto de Física Teórica
IFT-UNESP

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Summary

Introduction

- It is not easy to investigate QCD in its non-perturbative regime by using analytical techniques.
- A fair amount of our understanding about *deconfinement phase transitions* (DPTs) in QCD and other gauge theories is based on numerical results of Monte Carlo (MC) simulations.
- An important problem that may be solved through simulations: constructing QCD's phase diagram.
- That requires we study QCD with *non-zero chemical potential*.
- MC methods for dealing with this kind of situation are in need of development.

Introduction

- This need exists because taking into account the effects of finite density is one of the ways to introduce a difficulty known as the **complex phase problem** (CPP).
- Often this hindrance is also called the **sign problem**.
- Theories involving fermions usually suffer from this problem too.
- As we shall see through the consideration of a model with non-zero chemical potential, the CPP essentially prevents us from using well-established MC methods.
- There is a large number of theories with fermions and/or non-vanishing chemical potential that *simply cannot be simulated with the aid of the existing methods*.
- Alternative ways of formulating these models so as to circumvent the CPP have received considerable attention in the last years.

Introduction

- Just to give you some examples:

1. Y. D. Mercado, H. G. Evertz and C. Gattringer, "*QCD Phase Diagram According to the Center Group*", Phys. Rev. Lett. **106**, 222001 (2011).
2. S. Chandrasekharan, "*Solutions to sign problems in lattice Yukawa models*", Phys. Rev. D **86**, 021701 (2012).
3. Y. D. Mercado, C. Gattringer and A. Schmidt, "*Dual Lattice Simulation of the Abelian Gauge-Higgs Model at Finite Density: An Exploratory Proof of Concept Study*", Phys. Rev. Lett. **111**, 141601 (2013).
4. E. F. Huffman and S. Chandrasekharan, "*Solution to sign problems in half-filled spin-polarized electronic systems*", Phys. Rev. B **89**, 111101 (2014).

- Our work represents a generalization of what has been achieved in Ref. 1.
- We have even kept the terminology which has been introduced by these authors.

Introduction

- Due to the computational cost, one usually does not simulate full QCD for gaining information about its phase diagram.
- The analysis of DPTs in gauge theories is often facilitated by considering *effective theories*.
- The *order parameter* for such transitions is the so-called *Polyakov loop* (PL).
- Following Ref. 1, we have analyzed an effective theory for the PL with non-zero chemical potential that suffers from the CPP.
- We will discuss here a strategy for circumventing this difficulty so that this theory can be approached by using computer methods.

Polyakov Loop Models

Effective Theories for the PL

- In principle, it is possible to start from the functional integral describing full QCD and integrate out all the degrees of freedom except for those related to the PL.
- The result of this procedure would be an effective theory for the PL.
- This has been done in the strong-coupling limit of many pure gauge theories: *every one of them reduces exactly to an equivalent spin system with first-neighbor ferromagnetic interactions*.
  [B. Svetitsky, Phys. Rep. **132**, 1–53 (1986).]
- In these cases, the DPT can be seen as a symmetry-breaking phase transition.
- These theories have a global invariance under transformations that are periodic in Euclidean time up to a factor belonging to the center of the gauge group.
- For DPTs in $SU(N)$ gauge theories, this means that the $\mathbb{Z}(N)$ symmetry plays an important role.

Vector Potts Model (PM)

- We consider the d-dimensional vector PM with external field κ and non-zero chemical potential μ.
- This theory corresponds to an entire class of effective PL models.

Polyakov Loop Models

Vector Potts Model (PM)

- The vector PM is described by the following lattice action:

$$S[p] = -\sum_{x}\left[\tau\sum_{\nu=1}^{d}\left(p_x p^*_{x+\hat{\nu}} + \text{c.c.}\right) + \kappa e^{\mu} p_x + \kappa e^{-\mu} p^*_x\right]. \tag{1}$$

- In Eq. (1), the first summation runs over all sites x of a hypercubic lattice with periodic boundary conditions.
- The second sum is to be performed over all directions $\nu = 1, \ldots, d$.
- We use $\hat{\nu}$ to denote the unit vector in the direction ν.
- The PL variables p_x are complex numbers that can assume values from $\mathbb{Z}(N)$, the set of N-th roots of unity:

$$\mathbb{Z}(N) = \left\{\omega_m = \exp\left(\frac{2\pi\imath m}{N}\right)\middle|\, m = 1, \ldots, N\right\}. \tag{2}$$

- All the parameters τ, κ and μ involved in the definition (1) are *real and positive numbers*.

Polyakov Loop Models

Vector Potts Model (PM)

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Relation to the Gauge Theories

- τ is a monotonically increasing function of the temperature T which is associated with the underlying gauge theory.
- κ is proportional to the number of flavors and decreases as the mass of the theory's fermions ("quarks") increases.
- μ is the quark chemical potential in units of inverse temperature.
- The "Potts spins" p_x can be interpreted as sources of static quarks at the position x, i.e., they play the role of local PLs.
- In the above equation, the $\mathbb{Z}(N)$-symmetric first-neighbors term corresponds to the contribution from the gauge fields.
- The other terms, that explicitly break the $\mathbb{Z}(N)$ symmetry, are the contributions from the quarks.

Polyakov Loop Models

Vector Potts Model (PM)

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Relation to the Gauge Theories

- This theory's order parameter is defined in analogy with the magnetization:

$$P \equiv \sum_{x} p_x. \tag{3}$$

- When the expectation value of P is non-zero, there is no quark confinement.

Complex Phase Problem (CPP)

- Defining the quantities η and $\bar{\eta}$ in terms of κ and μ by

$$\eta \equiv \kappa e^{\mu} \tag{4}$$

and

$$\bar{\eta} \equiv \kappa e^{-\mu}, \tag{5}$$

one can rewrite the action $S[p]$ as

$$S[p] = -\sum_{x} \left[\tau \sum_{\nu=1}^{d} \left(p_x p^*_{x+\hat{\nu}} + \text{c.c.} \right) + \eta p_x + \bar{\eta} p^*_x \right]. \tag{6}$$

Complex Phase Problem (CPP)

- The corresponding *partition function* Z is given by

$$Z = \mathrm{Tr}\left\{e^{-S[p]}\right\} \equiv \sum_{\{p\}} e^{-S[p]}, \tag{7}$$

  where Tr represents the sum over all possible configurations $\{p\}$ of PL variables.
- Since $\mu \neq 0$, we have $\eta \neq \bar{\eta}$ and the lattice action $S\,[p]$ is a *complex quantity*.
- Therefore, $e^{-S[p]}$ is also a complex quantity.
- $\frac{e^{-S[p]}}{Z}$ cannot be given the probability interpretation it must have for the standard MC methods to be applicable.
- **This is what we call the CPP for the model under consideration**.
- The numerical study of the theory defined by Eq. (6) demands a new MC algorithm.
- An analogous statement can be made about full QCD.

Flux Representation

Solution to the CPP for the PM

- We are going to consider the theoretical solution to the CPP the action (6) has.
- We will change the PL variables to new ones, which we are going to call *dimer* and *monomer variables*.
- We will also call these new variables the *flux variables*, and say this change of variables corresponds to introducing a *flux representation* (FR) for the PM.
- The reason for these names will be made clear later, after we rewrite the partition function (7) as a sum over configurations of flux variables.
- Advantage of the new variables: *we are able to assign a well-defined probability to a given configuration of flux variables*.
- **In this sense, the FR solves the CPP for the PM**.
- MC methods for studying this model that are based on the FR can then be devised.

Flux Representation

Introducing the FR

- The first step is to conveniently rewrite the exponential $\exp\left(-S\left[p\right]\right)$.
- It is possible to show that this exponential can be factored in the following way:

$$\exp\left(-S\left[p\right]\right) = \left[\prod_{x,\nu} \exp\left(\tau P_{x,\nu} + \tau P^{*}_{x,\nu}\right)\right] \left[\prod_{x} \exp\left(\eta p_x + \overline{\eta} p^{*}_{x}\right)\right], \tag{8}$$

  where we defined $P_{x,\nu}$ through

$$P_{x,\nu} \equiv p_x p^{*}_{x+\hat{\nu}} \quad \left(\forall x,\, \nu = 1, \ldots, d\right). \tag{9}$$

- The first product in Eq. (8) is over all of the links (x, ν) of the lattice.
- The second one is to be performed over all lattice sites x.
- By using the group properties of $\mathbb{Z}\left(N\right)$, one can verify that $P_{x,\nu}$ is also an element of this group.

Some Mathematical Identities

- Let z be an element of $\mathbb{Z}(N)$.
- This group is formed by the N-th roots of unity, so that z must satisfy

$$z^N = 1. \tag{10}$$

- We can use the above property to prove that, if α is a real parameter, then the following identity must hold:

$$\exp(\alpha z) = \sum_{k=0}^{N-1} f_k(\alpha) z^k, \tag{11}$$

where the functions $f_k(\alpha)$ are given in terms of the elements ω_m of $\mathbb{Z}(N)$ by

$$f_k(\alpha) = \frac{1}{N} \sum_{m=1}^{N} \frac{1}{\omega_m^k} \exp(\alpha \omega_m), \quad k = 0, \ldots, N-1. \tag{12}$$

- Although this prescription involves complex numbers, the functions $f_k(\alpha)$ are real.

Flux Representation

Some Mathematical Identities

- The functions $f_k(\alpha)$ must be analytic functions of α.
- They have their Taylor series expansions given by

$$f_0(\alpha) = 1 + \frac{\alpha^N}{N!} + \frac{\alpha^{2N}}{(2N)!} + \cdots, \tag{13a}$$

$$f_1(\alpha) = \alpha + \frac{\alpha^{N+1}}{(N+1)!} + \frac{\alpha^{2N+1}}{(2N+1)!} + \cdots, \tag{13b}$$

$$\vdots$$

$$f_{N-1}(\alpha) = \frac{\alpha^{N-1}}{(N-1)!} + \frac{\alpha^{2N-1}}{(2N-1)!} + \frac{\alpha^{3N-1}}{(3N-1)!} + \cdots. \tag{13c}$$

- Clearly, if $\alpha > 0$, then the functions $f_k(\alpha)$ possess the following property:

$$f_k(\alpha) > 0, \forall k. \tag{14}$$

- *This remark is fundamental for solving the CPP.*

Flux Representation

Some Mathematical Identities

- It is possible to use the identity that allowed us to introduce the functions $f_k(\alpha)$, Eq. (11), to prove another identity.
- This second identity is the one we will need to introduce the FR for the PM.
- One can show that, if α and β are two real parameters and z is an element of $\mathbb{Z}(N)$, then the following equation is true:

$$\exp(\alpha z + \beta z^*) = \sum_{k=0}^{N-1} h_k(\alpha, \beta) z^k, \tag{15}$$

  where z^* denotes the complex conjugate of z.
- The functions $h_k(\alpha, \beta)$ are given in terms of the functions f_k.

Some Mathematical Identities

- The function $h_0(\alpha, \beta)$ is given by

$$h_0(\alpha, \beta) = \sum_{k=0}^{N-1} f_k(\alpha) f_k(\beta) \tag{16}$$

and the other functions $h_k(\alpha, \beta)$ can be written as

$$h_k(\alpha, \beta) = \sum_{j=0}^{k-1} f_j(\alpha) f_{N+j-k}(\beta) + \sum_{j=k}^{N-1} f_j(\alpha) f_{j-k}(\beta), \quad k = 1, \ldots, N-1. \tag{17}$$

- We already know that, if $\alpha, \beta > 0$, then $f_j(\alpha) f_k(\beta) > 0$, $\forall j, k$.
- Eqs. (16) and (17) allow us to conclude that $h_k(\alpha, \beta)$ have the property

$$h_k(\alpha, \beta) > 0 \quad \text{if} \quad \alpha, \beta > 0 \qquad (k = 0, 1, \ldots, N-1). \tag{18}$$

- As we shall see, **the solution to the CPP through the introduction of the FR for the PM is a direct consequence of Eq. (18)**.

Flux Representation

Introducing the FR – Dimer Variables

- Recall Eq. (8) for $\exp\left(-S\left[p\right]\right)$:

$$\exp\left(-S\left[p\right]\right) = \left[\prod_{x,\nu} \exp\left(\tau P_{x,\nu} + \tau P^{*}_{x,\nu}\right)\right] \left[\prod_{x} \exp\left(\eta p_x + \overline{\eta} p^{*}_{x}\right)\right].$$

- Every factor is an exponential of the same kind we have on the LHS of Eq. (15).
- First consider the introduction of the **dimer variables**.
- It is possible to show that the product over links in Eq. (8) can be rewritten as

$$\prod_{x,\nu} \exp\left(\tau P_{x,\nu} + \tau P^{*}_{x,\nu}\right) = \prod_{x,\nu} \sum_{b_{x,\nu}=0}^{N-1} h_{b_{x,\nu}}\left(\tau,\tau\right) P_{x,\nu}^{b_{x,\nu}} \tag{19a}$$

$$= \sum_{\{b\}} \prod_{x,\nu} h_{b_{x,\nu}}\left(\tau,\tau\right) P_{x,\nu}^{b_{x,\nu}}, \tag{19b}$$

  where *we associated a dimer variable* $b_{x,\nu}$ *with every link* (x,ν) *of the lattice*.

- The summation symbol in Eq. (19b) represents the sum over all of the possible dimer configurations $\{b\}$.

Introducing the FR – Monomer Variables

- **Monomer variables** are introduced analogously.
- The identity involving $h_k(\alpha, \beta)$ allows us to *associate with every lattice site* x *a monomer variable* s_x by rewriting the second product in Eq. (8) as

$$\prod_x \exp\left(\eta p_x + \overline{\eta} p_x^*\right) = \prod_x \sum_{s_x=0}^{N-1} h_{s_x}(\eta, \overline{\eta})\, p_x^{s_x} \tag{20a}$$

$$= \sum_{\{s\}} \prod_x h_{s_x}(\eta, \overline{\eta})\, p_x^{s_x}\,. \tag{20b}$$

- The last summation sign denotes the sum over every possible configuration $\{s\}$ of monomer variables.

Flux Representation

Introducing the FR

- By substituting the last results into the expression for $\exp\left(-S\left[p\right]\right)$, one obtains

$$\exp\left(-S\left[p\right]\right)=\sum_{\{b,s\}}\left[\prod_{x,\nu}h_{b_{x,\nu}}\left(\tau,\tau\right)P_{x,\nu}^{b_{x,\nu}}\right]\left[\prod_{x}h_{s_{x}}\left(\eta,\overline{\eta}\right)p_{x}^{s_{x}}\right]. \tag{21}$$

- The sum on the RHS is over all of the configurations $\{b,s\}$ of flux variables.
- Define

$$w\left[b,s\right]\equiv\left[\prod_{x,\nu}h_{b_{x,\nu}}\left(\tau,\tau\right)\right]\left[\prod_{x}h_{s_{x}}\left(\eta,\overline{\eta}\right)\right] \tag{22}$$

and

$$\phi_{x}\equiv\sum_{\nu=1}^{d}\left(b_{x,\nu}-b_{x-\hat{\nu},\nu}\right)+s_{x},\,\forall x. \tag{23}$$

Introducing the FR – Partition Function

- By using the last definitions, it is possible to show the validity of the relation

$$\exp\left(-S\left[p\right]\right) = \sum_{\{b,s\}} w\left[b,s\right] \prod_{x} p_x^{\phi_x} . \tag{24}$$

- Now we can rewrite the partition function Z as a sum over configurations of flux variables.
- Recall that this quantity is given by

$$Z = \mathrm{Tr}\left\{ e^{-S[p]} \right\} .$$

- Tr corresponds to the sum over all of the configurations $\{p\}$ of "Potts spins", i.e.,

$$\mathrm{Tr} \equiv \prod_{x} \sum_{p_x \in \mathbb{Z}(N)} . \tag{25}$$

Introducing the FR – Partition Function

- By using this definition and the formula for $\exp\left(-S\left[p\right]\right)$, one shows that Z can be written as

$$Z = \sum_{\{b,s\}} w\left[b,s\right] \left(\prod_{x} \sum_{p_x \in \mathbb{Z}(N)} p_x^{\phi_x} \right). \tag{26}$$

- If we can determine the last sum in Eq. (26), Z will be specified in terms of flux variables only.
- The result we need is given by

$$\sum_{p_x \in \mathbb{Z}(N)} p_x^{\phi_x} = N\mathcal{N}\left(\phi_x\right), \tag{27}$$

where the function $\mathcal{N}\left(k\right)$ is defined through

$$\mathcal{N}\left(k\right) \equiv \delta_{k \bmod N,0}. \tag{28}$$

- The above definition shows us that $\mathcal{N}\left(\phi_x\right)$ equals 1 if ϕ_x is a multiple of N, and that $\mathcal{N}\left(\phi_x\right)$ vanishes in every other case.

Introducing the FR – Partition Function

- Substituting Eq. (27) into the expression for Z, one can verify that

$$Z = N^M \sum_{\{b,s\}} w\left[b,s\right] \prod_x \mathcal{N}\left(\phi_x\right), \tag{29}$$

  where M denotes the number of sites the lattice has.

- The factor N^M is irrelevant for *it does not alter the results for the observables*.
- Then we shall omit this factor and write Z simply as

$$Z = \sum_{\{b,s\}} w\left[b,s\right] \prod_x \mathcal{N}\left(\phi_x\right). \tag{30}$$

- This equation represents a reformulation of the problem so that the flux variables take the place of the model's original variables, the "Potts spins".

Flux Representation

Solution to the CPP

- Recall that the parameters in the definition of $S[p]$ are all real and positive: $\tau, \eta, \overline{\eta} > 0$.
- It was shown that the functions $h_k(\alpha, \beta)$ have the property $h_k(\alpha, \beta) > 0$, $\forall k$, if α and β are positive.
- Therefore, every factor in the definition of $w[b, s]$, Eq. (22), is a real and positive number, and the same is true for $w[b, s]$.
- Now notice that every configuration of flux variables gives a contribution to the partition function, and the weight of this contribution is

$$W[b, s] = w[b, s] \prod_x \mathcal{N}(\phi_x). \tag{31}$$

- The probability of finding the system in a given configuration $\{b, s\}$ must be

$$\mathrm{pr}[b, s] = \frac{W[b, s]}{Z}. \tag{32}$$

- The introduction of the flux variables $b_{x,\nu}$ and s_x leads to the solution of the CPP!
- **We are now able to assign a real and positive probability to every configuration of dimer and monomer variables**.

Flux Representation

Graphical Representation of the Configurations of Flux Variables

- The partition function was written as a sum over all of the configurations $\{b, s\}$ of flux variables.
- Notice that **not every configuration makes a non-zero contribution to this sum**.
- The product $\prod_x \mathcal{N}(\phi_x)$ will differ from zero only if the following condition is satisfied:

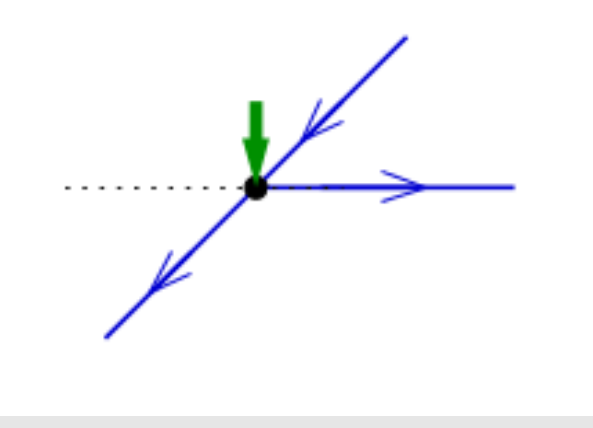
$$\phi_x = 0 \pmod{N}, \forall x. \tag{33}$$

- When this condition is satisfied, the product under consideration equals 1.
- By using the identities we proved, it is possible to conclude that the flux variables take integer values belonging to the interval from 0 to $N_M = N - 1$.
- With the understanding that the values which are outside this interval must be taken *modulo* N, we can consider that the dimer and monomer variables range from $-N_M$ to $+N_M$.

Flux Representation

Graphical Representation of the Configurations of Flux Variables

- This allows us to represent the flux variables by drawing arrows (with the direction of an arrow being determined by the sign of the corresponding variable).
- The dimer variables are represented by arrows between two lattice sites.
- Similarly, the monomer variables are represented by arrows on the lattice sites.
- Therefore, Eq. (33) can be interpreted as a zero flux condition for every site.
- This means that the number of arrows going into a given site minus the number of arrows coming out of it must equal zero (*modulo* N).



Conclusions

- We investigated the vector PM, that corresponds to an entire class of effective theories for the PL.
- To obtain a more realistic description, we have to take into account finite density effects, so that **the chemical potential μ must be non-zero**.
- Therefore, all of the effective theories we analyzed suffer from a CPP when they are formulated in terms of their original variables, the "Potts spins".
- We discussed the difficulty the CPP introduces for the simulation of theories suffering from it: **they simply cannot be simulated by using standard MC methods**.
- In the cases under investigation, this is due to the fact that we cannot assign a well defined probability to the configurations of "Potts spins".

Conclusions

- It is necessary to attempt a reformulation of the PM if we want to develop new algorithms for simulating the effective theories for the PL when μ is non-vanishing.
- The solution to the CPP for simpler theories like the PM is interesting, because it may offer some insight on how the analogous problem in QCD can be solved.
- For circumventing the CPP the vector PM suffers from, first we derived some identities that must be satisfied by the elements of the $\mathbb{Z}(N)$ group.
- Through these identities, the functions $f_k(\alpha)$ and $h_k(\alpha, \beta)$ were introduced.
- It was also shown that these functions take strictly positive values if their arguments are strictly positive.
- The identities we proved were then used for introducing

1. the **dimer variables** – which are related to the links of the lattice – and
2. the **monomer variables** – that are associated with the lattice sites.

Conclusions

- When the problem was reformulated in terms of these variables, the solution to the CPP presented itself naturally.
- We obtained a new expression for the partition function, proving it can be rewritten as a sum over every possible configuration of dimer and monomer variables.
- This allowed us to identify the weight associated with a given configuration of flux variables.
- Due to the property of $h_k(\alpha, \beta)$ we already mentioned, it was possible to conclude that this weight is a real and positive quantity.
- **We were then able to assign a well defined probability to the configurations of flux variables**.
- Hence MC methods can be devised for the vector PM if the problem is formulated by using the FR.
- We can say the CPP was solved for the effective theories for the PL we investigated.