Dual Simulations of Lattice Gauge Theories

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Motivation: Complex action problem

- In general lattice field theories with finite chemical potential μ have actions S with an imaginary part.

- The Boltzmann factor

$$e^{-S} \in \mathbb{C}$$

thus has a complex phase and cannot be used as a probability weight.

- Standard Monte Carlo simulation techniques are not available for a non-perturbative analysis.

"Complex action problem" or "Sign problem"

- Generic feature of finite density field theories both, on the lattice and in the continuum, for bosonic and fermionic theories.

The toolbox of the lattice QCD community

- Reweighting / phase quenching
- Analytic continuation from imaginary μ
- Expansions around the $\mu = 0$ ensemble: Taylor series.
- Expansions around the $\mu = 0$ ensemble: Fugacity series.
- Simulations with stochastic methods (complex Langevin etc)
- Canonical simulations
- Density of state / histogram methods
- Exploring symmetries - subset method
- Rewriting a system to new degrees of freedom - dual variables

Our dream: Map out the QCD phase diagram in the μ-T plane.

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Getting the idea across .....

Dual variables for charged ϕ^4 fields with chemical potential

Formal definition in the continuum:

- Action:

$$S = \int d^4x \Big[- \phi^* \triangle \phi + (m^2 - \mu^2)\, |\phi|^2 \; + \lambda \, |\phi|^4 \; + i \, \mu \, 2 \, \mathcal{I}m \, \phi^* \partial_4 \phi \Big]$$

- VEVs of observables:

$$\langle O \rangle \; = \; \frac{1}{Z} \int \mathcal{D}[\phi] \, e^{-S[\phi]} \, O[\phi] \qquad , \qquad Z \; = \; \int \mathcal{D}[\phi] \, e^{-S[\phi]}$$

- The path integral is well defined on the lattice: Discretize the action on a 4-d lattice and for $\mathcal{D}[\phi]$ use the product of the measures at all sites.

Lattice path integral for the charged scalar field

- Lattice action: $\quad (\, \phi_x \in \mathbb{C} \, , \quad M^2 = 8 + m^2 \,)$

$$S = \sum_x \Big[\, M^2 \, |\phi_x|^2 \; + \lambda \, |\phi_x|^4 \, \Big] - \sum_{x,\nu} \Big[e^{\,-\mu \, \delta_{\nu 4}} \, \phi_x^\star \, \phi_{x+\widehat{\nu}} \; + \; e^{\,\mu \, \delta_{\nu 4}} \, \phi_x \, \phi_{x+\widehat{\nu}}^\star \Big]$$

- Discretized partition sum $Z = \int \mathcal{D}[\phi] \, e^{-S[\phi]}$:

$$Z = \prod_x \int_{\mathbb{C}} d\phi_x \, \prod_x e^{\,-M^2 \, |\phi_x|^2 \, - \, \lambda |\phi_x|^4} \prod_{x,\nu} e^{\, e^{-\mu \, \delta_{\nu 4}} \, \phi_x^\star \, \phi_{x+\widehat{\nu}}} \prod_{x,\nu} e^{\, e^{\mu \, \delta_{\nu 4}} \, \phi_x \, \phi_{x+\widehat{\nu}}^\star}$$

Dual representation for the charged scalar field

- Expand the nearest neighbor terms of e^{-S}:

$$\prod_{x,\nu} \exp\left(e^{-\mu\,\delta_{\nu 4}}\,\phi_x^\star\,\phi_{x+\widehat{\nu}}\right) \;=\; \prod_{x,\nu} \sum_{j_{x,\nu}=0}^{\infty} \frac{\left(e^{-\mu\,\delta_{\nu 4}}\right)^{j_{x,\nu}}}{j_{x,\nu}\,!} \;\left(\phi_x^\star\right)^{j_{x,\nu}}\;\left(\phi_{x+\widehat{\nu}}\right)^{j_{x,\nu}}$$

$$\prod_{x,\nu} \exp\left(e^{\mu\,\delta_{\nu 4}}\,\phi_x\,\phi_{x+\widehat{\nu}}^\star\right) \;=\; \prod_{x,\nu} \sum_{\overline{j}_{x,\nu}=0}^{\infty} \frac{\left(e^{\mu\,\delta_{\nu 4}}\right)^{\overline{j}_{x,\nu}}}{\overline{j}_{x,\nu}\,!} \;\left(\phi_x\right)^{\overline{j}_{x,\nu}}\;\left(\phi_{x+\widehat{\nu}}^\star\right)^{\overline{j}_{x,\nu}}$$

- The $j_{x,\nu}$ and $\overline{j}_{x,\nu}$ are the new, "dual" degrees of freedom.

Dual representation - integrating out the fields

- Integral over ϕ_x at site x: ($\Sigma_j, \overline{\Sigma}_j$ are sums of $j_{y,\nu}$, $\overline{j}_{y,\nu}$ connected to x)

$$\int_{\mathbb{C}} d\,\phi_x \;\; e^{-M^2|\phi_x|^2 - \lambda|\phi_x|^4} \; (\phi_x)^{\Sigma_j} \; (\phi_x^\star)^{\overline{\Sigma}_j}$$

- Polar coordinates $\phi_x = re^{i\theta}$ to separate radial and U(1) parts (symmetry):

$$\int_0^\infty dr \; r^{\,\Sigma_j + \overline{\Sigma}_j + 1} \; e^{-M^2r^2 - \lambda r^4} \int_{-\pi}^{\pi} d\theta \; e^{\,i\theta\,(\Sigma_j - \overline{\Sigma}_j)} \; = \; \mathcal{I}(\Sigma_j + \overline{\Sigma}_j) \; \delta(\Sigma_j - \overline{\Sigma}_j)$$

- At every site there is a weight factor $\mathcal{I}(\Sigma_j + \overline{\Sigma}_j)$ and a constraint.

- The constraint $\delta(\Sigma_j - \overline{\Sigma}_j)$ enforces vanishing flux of $\overline{j}_{x,\nu} - j_{x,\nu}$ at each x.

Dual representation – final form

- The original partition function is mapped exactly to a sum over configurations of the dual variables $k_{x,\nu} \in \mathbb{Z}$ and $l_{x,\nu} \in \mathbb{N}_0$. $k_{x,\nu}$ and $l_{x,\nu}$ are linear combinations of the original j and $\overline{j}$:

$$Z \;=\; \sum_{\{k,l\}} \mathcal{W}(k,l)\, \mathcal{C}(k)$$

- Real and positive weight factor from radial d.o.f. and combinatorics:

$$\mathcal{W}(k,l) = \prod_{x,\nu} \frac{e^{-\mu\, k_{x,4}\, \delta_{\nu,4}}}{(|k_{x,\nu}| + l_{x,\nu})!} \; \prod_x \mathcal{I}\Big(\sum_\nu \Big[|k_{x,\nu}| + |k_{x-\widehat{\nu},\nu}| + 2(l_{x,\nu} + l_{x-\widehat{\nu},\nu}) \Big] \Big)$$

- Constraint from integrating over the symmetry group:

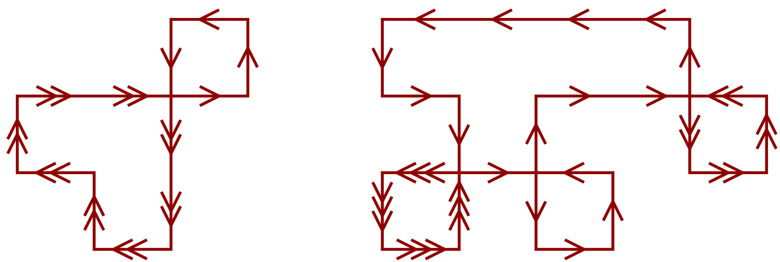
$$\mathcal{C}(k) \;=\; \prod_x \delta\Big(\sum_\nu \left[\, k_{x,\nu} - k_{x-\widehat{\nu},\nu} \, \right] \Big)$$

Admissible configurations are loops:

- Constraint from integrating over the symmetry group:

$$\forall\, x \;:\quad \sum_{\nu} \left[\, k_{x,\nu} - k_{x-\widehat{\nu},\nu} \,\right] \;=\; 0 \qquad\qquad (\,\vec{\nabla}\vec{k} \;=\; 0\,)$$

- Admissible configurations of dual variables are oriented loops of flux:



- Finite μ: Different weight for forward and backward temporal flux.
- We identify: Particle number = winding number of flux.

C. Gattringer, T. Kloiber, PLB 2013 & NPB 2013

Adding gauge fields $\Rightarrow$ U(1) gauge Higgs model

U(1) gauge Higgs model: Continuum

Continuum action:

$$
\begin{aligned}
S \;=\; & \int d^4x \Big\{ -\phi(x)^* \Big[\partial_\nu + iA_\nu(x)\Big]\Big[\partial_\nu + iA_\nu(x)\Big]\phi(x) \\
& \qquad + [m_\phi^2 - \mu_\phi^2]\;|\phi(x)|^2 \;+\lambda_\phi\;|\phi(x)|^4 \;\Big\} + i\mu_\phi N_\phi \\
+ \; & \int d^4x \Big\{ -\chi(x)^* \Big[\partial_\nu - iA_\nu(x)\Big]\Big[\partial_\nu - iA_\nu(x)\Big]\chi(x) \\
& \qquad + [m_\chi^2 - \mu_\chi^2]\;|\chi(x)|^2 \;+\lambda_\chi\;|\chi(x)|^4 \;\Big\} + i\mu_\chi N_\chi \\
+ \; & \frac{1}{4e^2}\int d^4x\, F_{\rho\sigma}(x)\, F_{\rho\sigma}(x)
\end{aligned}
$$

U(1) gauge Higgs model: Lattice

- Compact U(1)-valued gauge fields: $U_{x,\nu} = e^{iA_\nu(x)}$
- Lattice action for matter fields:

$$S_M = \sum_x \left[M^2 |\phi_x|^2 + \lambda |\phi_x|^4 \right] - \sum_{x,\nu} \left[e^{-\mu \delta_{\nu 4}} U_{x,\nu} \phi_x^\star \phi_{x+\widehat{\nu}} + e^{\mu \delta_{\nu 4}} U_{x,\nu}^\star \phi_x \phi_{x+\widehat{\nu}}^\star \right]$$

- Lattice action for gauge fields: (Wilson plaquette action)

$$S_G = -\frac{\beta}{2} \sum_x \sum_{\rho<\sigma} \left[U_{x,\rho} U_{x+\hat{\rho},\sigma} U_{x+\hat{\sigma},\rho}^\star U_{x,\sigma}^\star + U_{x,\rho}^\star U_{x+\hat{\rho},\sigma}^\star U_{x+\hat{\sigma},\rho} U_{x,\sigma} \right]$$

- Gauge field measure:

$$\int \mathcal{D}[U] = \prod_{x,\nu} \int_{U(1)} dU_{x,\nu}$$

Mapping to dual variables

- Again we expand nearest neighbor terms, now with link variables $U_{x,\nu}$:

$$\exp\left(\phi_x^\star\, U_{x,\nu}\, \phi_{x+\widehat{\nu}}\right) \;=\; \sum_{j_{x,\nu}=0}^{\infty} \frac{\left(\,U_{x,\nu}\,\right)^{j_{x,\nu}}}{j_{x,\nu}\,!} \;\left(\phi_x\right)^{j_{x,\nu}} \left(\phi^\star_{x+\widehat{\nu}}\right)^{j_{x,\nu}}$$

$\Rightarrow$ Matter loops are dressed with gauge transporters $U_{x,\nu}$

- Inserting the dual representations for the matter fields:

$$Z \;=\; \int \mathcal{D}[U] e^{-S_G[U]}\, Z_\phi[U]\, Z_\chi[U] \;=\; \sum_{\{k,l,\overline{k},\overline{l}\}} \mathcal{W}_\phi(k,l)\, \mathcal{W}_\chi(\overline{k},\overline{l})\, \mathcal{C}(k)\, \mathcal{C}(\overline{k})$$

$$\times \int \mathcal{D}[U] \prod_{x,\rho<\sigma} e^{\,\frac{\beta}{2}\left[U_{x,\rho}\, U_{x+\hat{\rho},\sigma}\, U^\star_{x+\hat{\sigma},\rho}\, U^\star_{x,\sigma} \,+\, c.c.\right]} \prod_{x,\nu} \left(U_{x,\nu}\right)^{k_{x,\nu}-\overline{k}_{x,\nu}}$$

Integrating out the gauge fields ⇒ new constraints

- The remaining gauge field integral ...

$$\prod_{x,\nu} \int_{U(1)} dU_{x,\nu} \prod_{x,\rho<\sigma} e^{\frac{\beta}{2} U_{x,\rho} U_{x+\hat{\rho},\sigma} U^\star_{x+\hat{\sigma},\rho} U^\star_{x,\sigma}} \prod_{x,\rho<\sigma} e^{\frac{\beta}{2} U^\star_{x,\rho} U^\star_{x+\hat{\rho},\sigma} U_{x+\hat{\sigma},\rho} U^\star_{x,\sigma}} \prod_{x,\nu} (U_{x,\nu})^{k_{x,\nu}-\overline{k}_{x,\nu}}$$

- ... is again tackled by expanding the Boltzmann factor ....

$$e^{\frac{\beta}{2} U_{x,\rho} U_{x+\hat{\rho},\sigma} U^\star_{x+\hat{\sigma},\rho} U^\star_{x,\sigma}} = \sum_{p_{x,\rho\sigma}} \frac{(\beta/2)^{p_{x,\rho\sigma}}}{p_{x,\rho\sigma}!} \left[U_{x,\rho} U_{x+\hat{\rho},\sigma} U^\star_{x+\hat{\sigma},\rho} U^\star_{x,\sigma} \right]^{p_{x,\rho\sigma}}$$

  ... leading to new integer valued dual variables $p_{x,\rho\sigma}$, $\overline{p}_{x,\rho\sigma}$ living on plaquettes.

- The gauge field integrals give rise to constraints on each link (x,ν) of the lattice.

- The link constraints connect the matter flux $k_{x,\nu} - \overline{k}_{x,\nu}$ and the plaquette occupation numbers $p_{x,\rho\sigma}$, $\overline{p}_{x,\rho\sigma}$ touching that link.

- Admissible configurations are closed surfaces or surfaces bounded by matter flux.

Dual form of the partition function for the gauge Higgs model

The partition sum is mapped exactly to a sum over loops and surfaces:

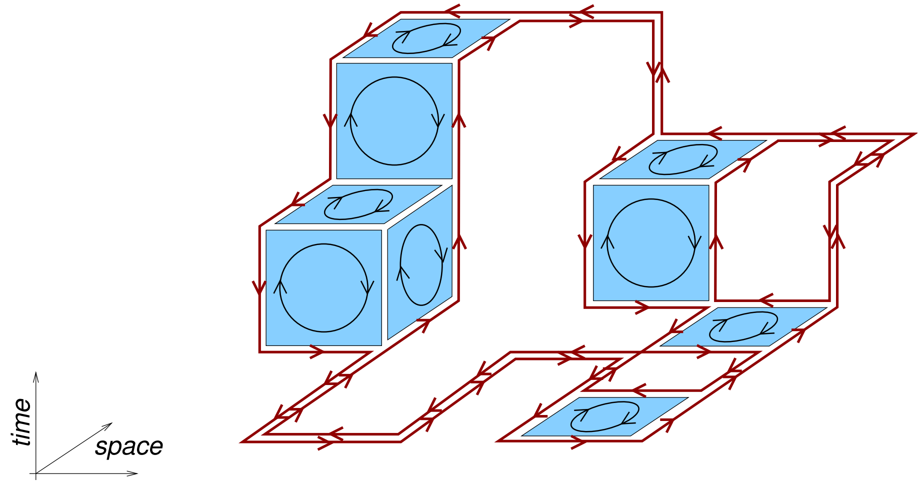
$$Z = \sum_{\{p,k,l\}} \mathcal{W}(p,k,l) \;\; \mathcal{C}(p,k)$$

- $\mathcal{W}$ positive weight factors.
- $\mathcal{C}$ constraints that turn the sum over configurations of dual variables into summing over surfaces and loops in 4 dimensions.

T. Sterling, J. Greensite, A. Patel, T. DeGrand, C. DeTar, M. Panero,
V. Azcoiti, E. Follana, A. Vaquero, G. Di Carlo, T. Korzec, U. Wolff ...

M. Endres, PRD 75, 2007
C. Gattringer, A. Schmidt, PRD 86, 2012
T. Korzec and U. Wolff, NPB 871, 2013
Y. Delgado Mercado, C. Gattringer, A. Schmidt, Comp. Phys. Comm. 184, 2013
P.N. Meisinger, M. Ogilvie, arXiv:1306.1495
Y. Delgado Mercado, C. Gattringer, A. Schmidt, PRL 111, 2013

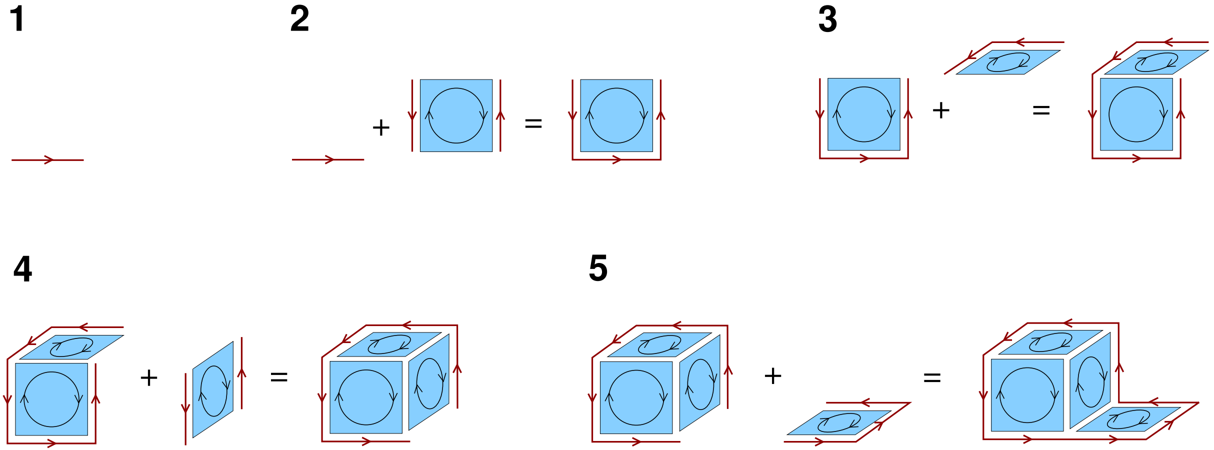
An admissible configuration for dual U(1) gauge Higgs theory:



Chemical potential favors flux forward in time. (2 flavors)

Generalized worm algorithm for gauge Higgs systems:

Worm starts by inserting a unit of matter flux. Adding segments transports the defect across the lattice until the defect is healed in a final step.



Y. Delgado Mercado, C. Gattringer, A. Schmidt, Comp. Phys. Comm. 184, 2013

Some results ...

Bulk observables

- Bulk observables are obtained as derivatives of the free energy with respect to the parameters.

- Example: Observables related to the particle number:

$$n = \frac{1}{N_s^3 \, N_t} \frac{\partial \, \ln Z}{\partial \mu}$$

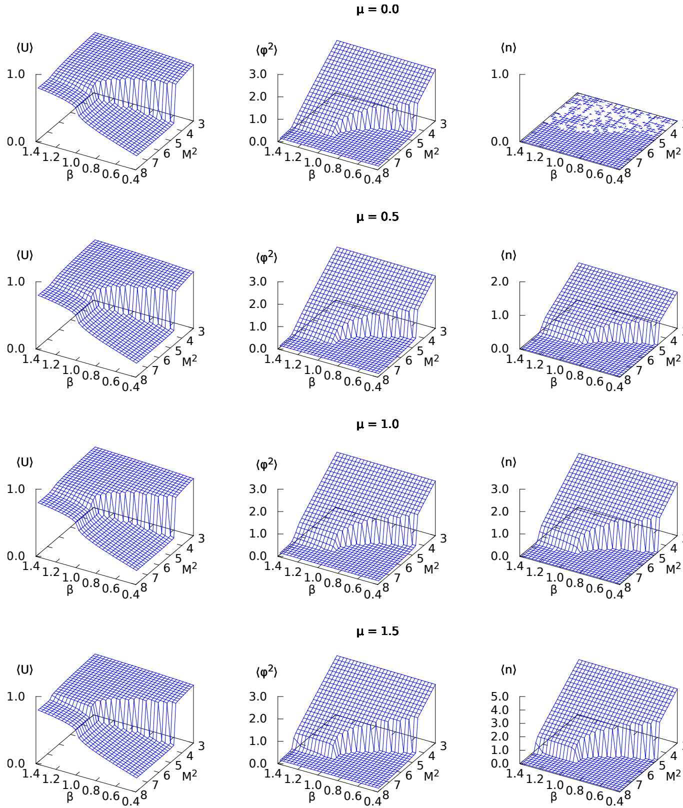
- Dual form: Particle number = temporal winding number of k-flux.

$$n = \frac{1}{N_s^3 \, N_t} \left\langle \sum_x k_{x,4} \right\rangle = \frac{1}{N_s^3} \left\langle \, W[k] \, \right\rangle$$

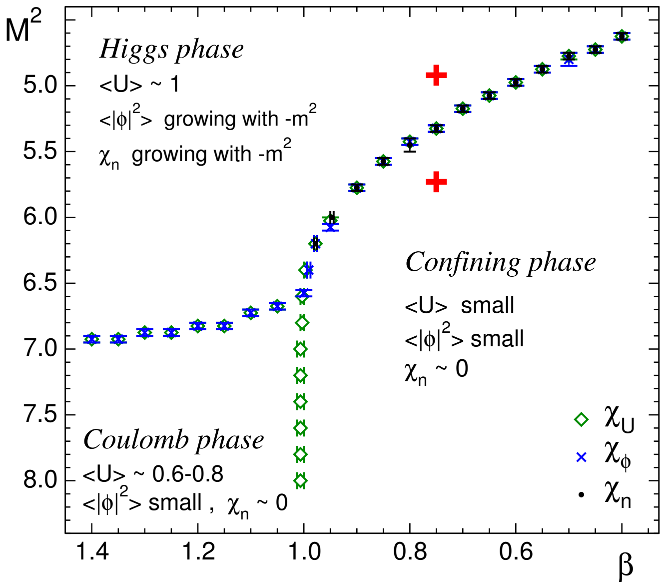
- Dual bulk observables are related to moments of the dual variables.

- 2-point functions via strings made gauge invariant with surfaces.

Bulk observables for several $\mu > 0$

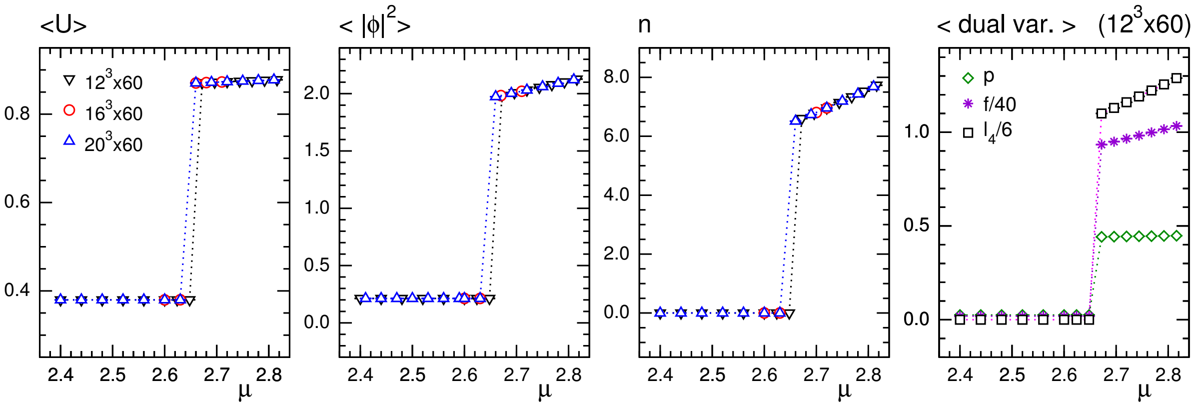


2-flavor gauge Higgs phase diagram at zero density



Y. Delgado Mercado, C. Gattringer, A. Schmidt, PRL 111, 2013

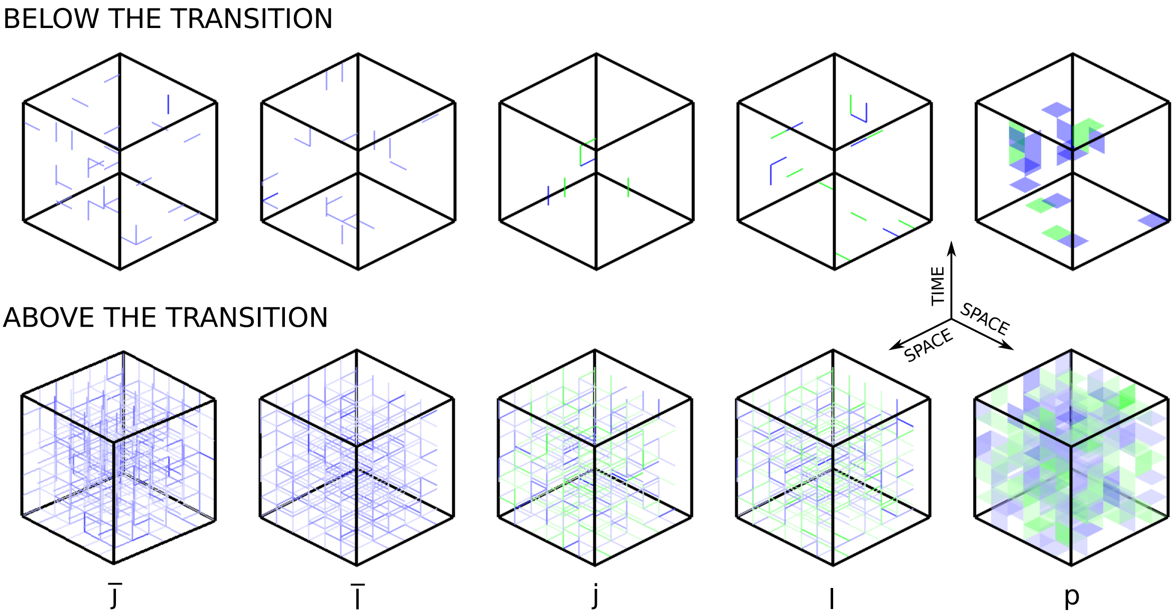
Observables in the confining phase at low T



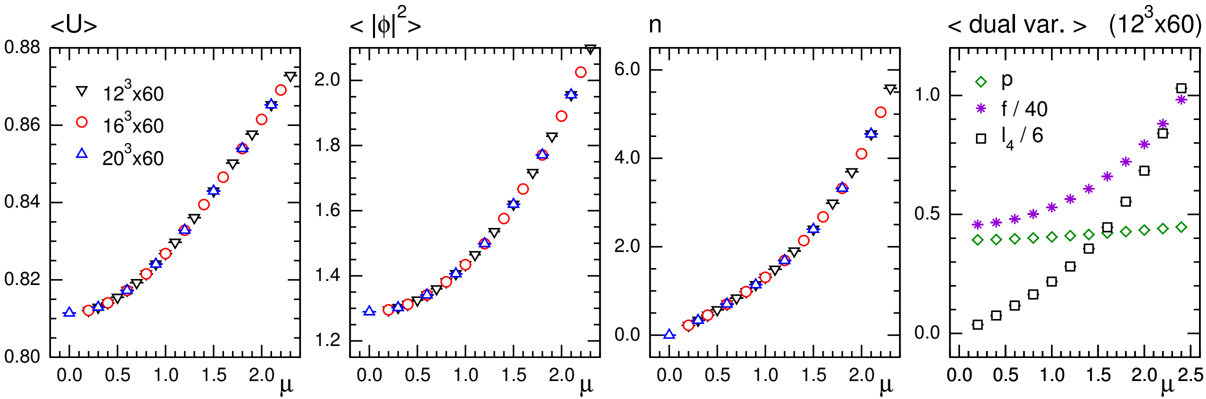
In the confining phase the dependence on the chemical potential μ sets in only when μ reaches the mass of the lowest excitation. "Silver Blaze behaviour"

Condensation of dual variables.

Condensation of dual variables



Observables in the Higgs phase at low T

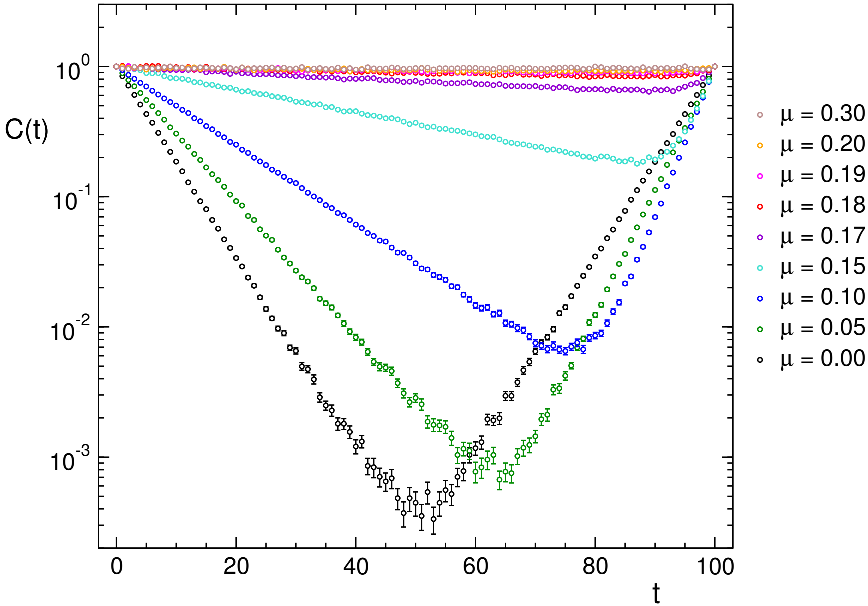


In the Higgs phase there is no mass gap and the non-trivial μ-dependence starts at $\mu = 0$.

No condensation of dual variables.

Y. Delgado Mercado, C. Gattringer, A. Schmidt, PRL 111, 2013

Propagators at finite density (charged ϕ^4, Method: Korzec, Vierhaus, Wolff 2011)



C. Gattringer, T. Kloiber, PLB 2013

Asymmetric propagation for $\mu < \mu_c \simeq 0.17$.
Condensation (= constant propagator) for μ above μ_c.

Challenges ....

... and some progress

Challenges for dual variables in lattice field theory

- Non-abelian gauge fields
- Relativistic fermions
- Complex action problem from a θ-term
- Physical interpretation of dual variables

.... progress in low-dimensional lattice field theories.

See also the talks by Falk Bruckmann and Tin Sulejmanpasic.

Massless Schwinger model on the lattice

- Partition sum and lattice action: ($\mu \neq 0 \;\Rightarrow$ 2 flavors)

$$Z \;=\; \int \mathcal{D}[U]\mathcal{D}[\,\overline{\psi},\psi\,]\; e^{-\,S_G[U]\,-\,i\,\theta\,Q[U]\,-\,S_F[U,\overline{\psi},\psi]}$$

$$S_F \;=\; \frac{1}{2}\sum_{x,\nu}\gamma_\nu(x)\Big[e^{\,+\mu\,\delta_{\nu,2}}\,U_\nu(x)\,\overline{\psi}(x)\,\psi(x+\hat{\nu}) \;-\; e^{\,-\mu\,\delta_{\nu,2}}\,U_\nu(x)^*\,\overline{\psi}(x+\hat{\nu})\,\psi(x)\Big]$$

staggered sign function: $\quad \gamma_1(x) \;=\; 1 \quad , \quad \gamma_2(x) \;=\; (-1)^{x_1}$

$$S_G[U] + i\,\theta\,Q[U] \;=\; -\,\frac{\beta}{2}\sum_n\left[\,U_p(x) \;+\; U_p(x)^*\,\right] + \frac{\theta}{4\pi}\sum_x\left[\,U_p(x) \;-\; U_p(x)^*\,\right]$$

$$=\; -\,\eta\,\sum_n U_p(x) \;-\; \overline{\eta}\sum_x U_p(x)^*$$

$$U_p(x) = U_1(x)U_2(x+\hat{1})U_1(x+\hat{2})^\star U_2(x)^\star \qquad\qquad \eta \;=\; \frac{\beta}{2} - \frac{\theta}{4\pi} \;\;,\;\; \overline{\eta} \;=\; \frac{\beta}{2} + \frac{\theta}{4\pi}$$

Expansion of the Boltzmann factor of the gauge fields:

- Factorization of the gauge action Boltzmann factor as product over plaquettes:

$$e^{-S_G[U]-i\theta Q[U]} \; = \; \prod_x \, e^{\eta \, U_p(x)} \, e^{\overline{\eta} \, U_p(x)^{-1}}$$

- Expansion of the individual exponentials:

$$e^{-\,\eta \, U_p(x)} \, e^{-\,\overline{\eta} \, U_p(x)^{-1}} \; = \; \sum_{p(x) \in \mathbb{Z}} (-1)^{p(x)} \, I_{|p(x)|}\left(\sqrt{\eta \overline{\eta}}\right) \left(\sqrt{\frac{\eta}{\overline{\eta}}}\right)^{p(x)} \; U_p(x)^{\,p(x)}$$

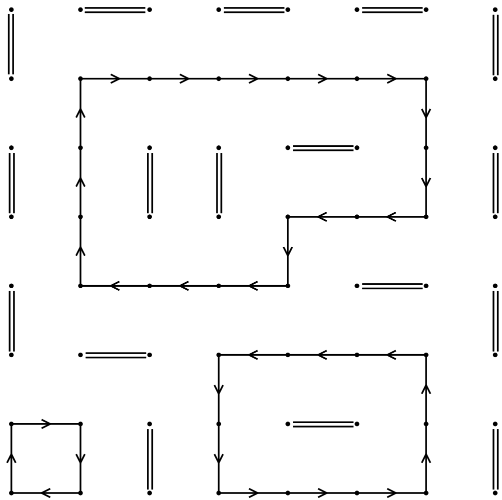
$p(x) \in \mathbb{Z}$ .... plaquette occupation numbers

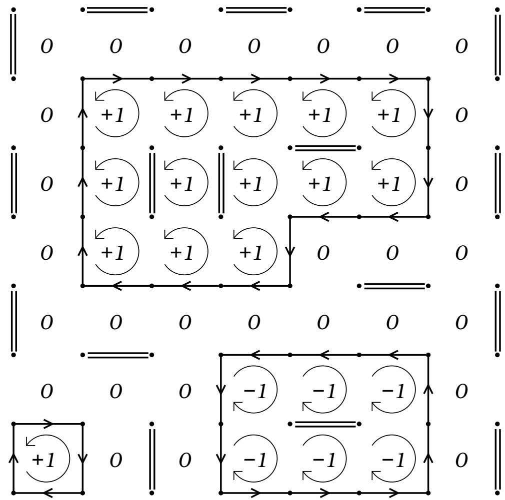
$I_{|p(x)|}(\sqrt{\eta\overline{\eta}}\,)$ .... modified Bessel functions

$$\eta \; = \; \frac{\beta}{2} - \frac{\theta}{4\pi} \quad , \qquad \overline{\eta} \; = \; \frac{\beta}{2} + \frac{\theta}{4\pi}$$

Fermion loops

- Saturating the Grassmann integral gives loops.
- Signs come from Grassmann ordering and from γ-matrices.
- The loops are dressed with gauge links that have to be saturated by plaquettes from the gauge field Boltzmann factor.





Dual form of the partition sum:

- The partition function is a sum over all admissible configurations of loops l, dimers d and plaquette occupation numbers p:

$$Z \;=\; \left(\frac{1}{2}\right)^V \sum_{\{l,d,p\}} (-1)^{N_L \,+\, N_P \,+\, \frac{1}{2}\sum_l L(l)} \; \prod_x I_{|p(x)|}\!\left(\sqrt{\eta\overline{\eta}}\right) \left(\sqrt{\frac{\eta}{\overline{\eta}}}\right)^{p(x)}$$

Here we have introduced:

$$N_P \;=\; \sum_x p(x)$$

N_L number of loops

$L(l)$ length of the loop l

- Constructive proof:

$$(-1)^{N_L \,+\, N_P \,+\, \frac{1}{2}\sum_l L(l)} \;=\; 1$$ $\forall$ admissible configurations (wrong with mass or $d > 2$)

C. Gattringer, T. Kloiber, V. Sazonov, Nucl. Phys. B, 2015

Dual representation of the massless Schwinger model with θ-term:

- Partition function is a sum over admissible configurations of loops, dimers and plaquette occupation numbers:

$$Z = \left(\frac{1}{2}\right)^V \sum_{\{l,d,p\}} \prod_x I_{|p(x)|}\left(\sqrt{\eta\overline{\eta}}\right) \left(\sqrt{\frac{\eta}{\overline{\eta}}}\right)^{p(x)}$$

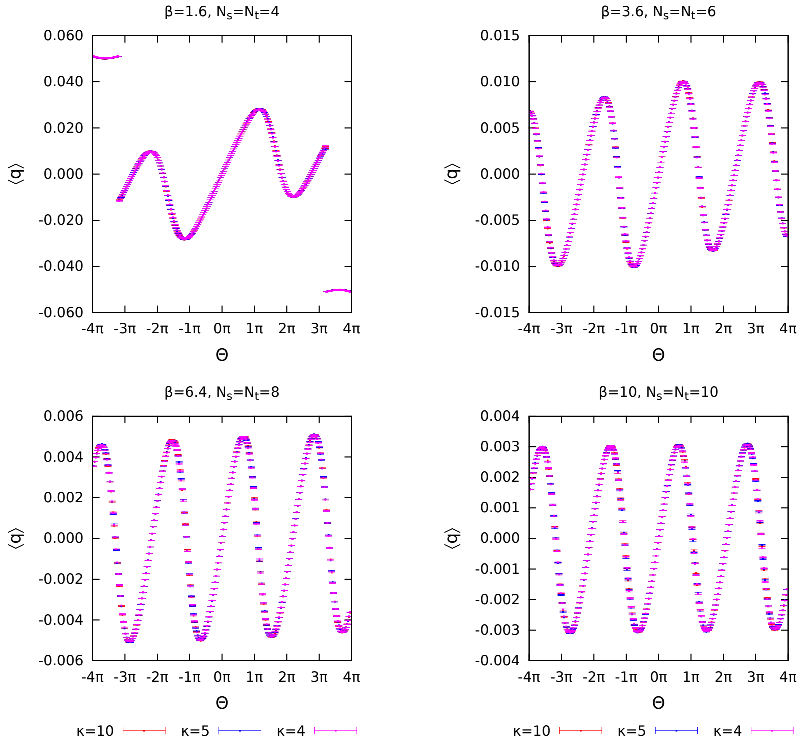
- Fermion loops that wind forward (backward) in time are weighted with $e^{+\mu N_2}$ ($e^{-\mu N_2}$)

- The partition sum has only real and positive terms for positive $\eta = \frac{\beta}{2} - \frac{\theta}{4\pi}$ and $\overline{\eta} = \frac{\beta}{2} + \frac{\theta}{4\pi}$.

- $\theta \neq 0$ introduces an imbalance between positive and negative $p(x)$.

C. Gattringer, T. Kloiber, V. Sazonov, Nucl. Phys. B, 2015

Emergence of 2π periodicity in θ in the continuum limit (scalar QED_2):



C. Gattringer, T. Kloiber, M. Müller-Preussker, arXiv:1508.00681

Summary

- Complex action problems for scalar field theories and abelian gauge-Higgs models are resolved by mapping them to positive dual representations.
- Dual degrees of freedom are loops for matter and surfaces for gauge fields.
- Bulk observables, phase diagram, 2-point functions ...
- Models with positive dual representation serve as test cases for other techniques.
- Main challenges: Relativistic fermions, non-abelian gauge fields, topology ...
- Progress in low-dimensional lattice field theories.
- Dual variables shed light on different aspects of the physics. We should try to understand these aspects better.