New developments for lattice field theory at non-zero density

Christof Gattringer

Karl-Franzens-Universität Graz, Austria

Complex action problem

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"

A bosonic and a fermionic example

- Charged scalar field:

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

- QCD (fermions integrated out):

$$S \; = \; S_{gauge} \; - \; \sum_{q=1}^{N_f} \ln \, \text{det} \, D(m_q, \mu_q)$$

$$\text{det} \, D(m, \mu) \; \in \; \mathbb{C} \qquad \text{for} \qquad \mu > 0$$

- Complex action problem is genuine for field theories with $\mu > 0$. It is not necessarily related to fermions or the lattice discretization.

Approaches to overcome the complex action problem

Lattice 2012: G. Aarts
Lattice 2011: L. Levkova
Lattice 2010: S. Gupta & U. Wolff
Lattice 2009: P. de Forcrand & A. Li
Lattice 2008: S. Ejiri & S. Chandrasekharan

- Reweighting / phase quenching
- Analytic continuation from imaginary μ
- Expansions around the $\mu = 0$ ensemble: Taylor, fugacity ...
- Simulations with stochastic methods
- Canonical simulations
- Density of state / histogram methods — K. Langfeld, Parallels 9A
- Exploring symmetries - subset method — J. Bloch, Parallels 9A
- Rewriting a system to new degrees of freedom - dual variables — This talk

See also J. Myers, plenary talk on Friday

Dual variables for bosonic systems

Dual representation for the charged scalar field

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

$$S = \sum_x \Big[M^2 \, |\phi_x|^2 \; + \lambda \, |\phi_x|^4 - \sum_{\nu=1}^{4} \Big(e^{-\mu \, \delta_{\nu 4}} \, \phi_x^\star \, \phi_{x+\widehat{\nu}} \; + \; e^{\mu \, \delta_{\nu 4}} \, \phi_x \, \phi_{x+\widehat{\nu}}^\star \Big) \Big]$$

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

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

- The $j_{x,\nu}$ 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 $j_{y,\nu}$ 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):

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

- 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 j-flux at each site.

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:

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

- 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:

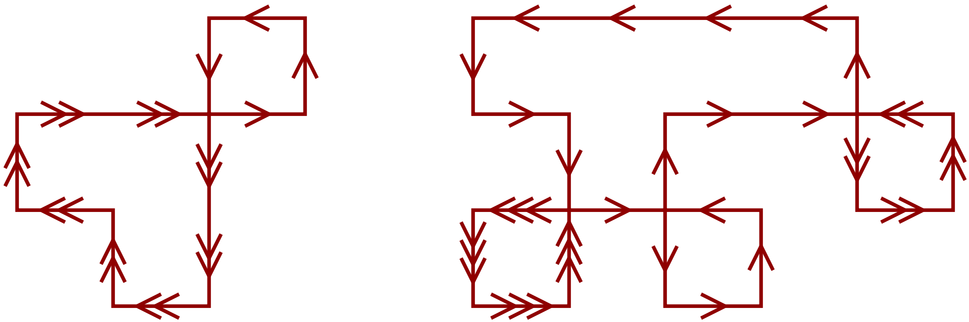
$$\mathcal{C}(k) \;=\; \prod_x \, \delta\Big(\sum_\nu \big[\, k_{x,\nu} - k_{x-\widehat{\nu},\nu} \,\big] \Big)$$

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.

Adding gauge fields: U(1) gauge Higgs model

- Nearest neighbor terms with link variables $U_{x,\nu} \in$ U(1):

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

$\Rightarrow$ Matter loops are dressed with gauge transporters.

- Expanding the plaquette terms ...

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

... new integer valued dual variables $p_{x,\rho\sigma}$ on the plaquettes.

- Integrating out the link variables gives rise to new constraints that connect matter flux and the dual plaquette variables.

Dual form of the partition function for the gauge Higgs model

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

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

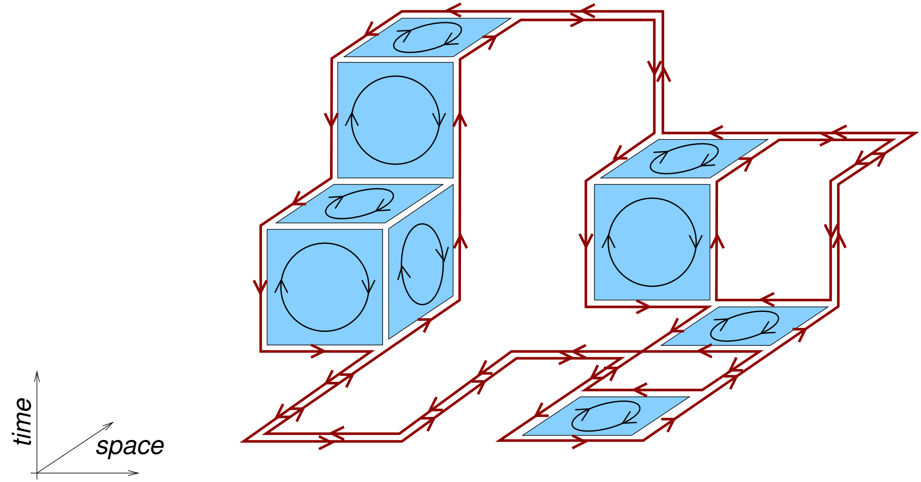
- $\mathcal{W}$ positive weight factors.
- $\mathcal{C}$ constraints that turn the sum over configurations of dual variables into summing over surfaces and loops.

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, arXiv:1307.6120

M. Ogilvie, Parallels 2B & Y. Delgado Mercado, Parallels 4A & A. Schmidt, Parallels 4A

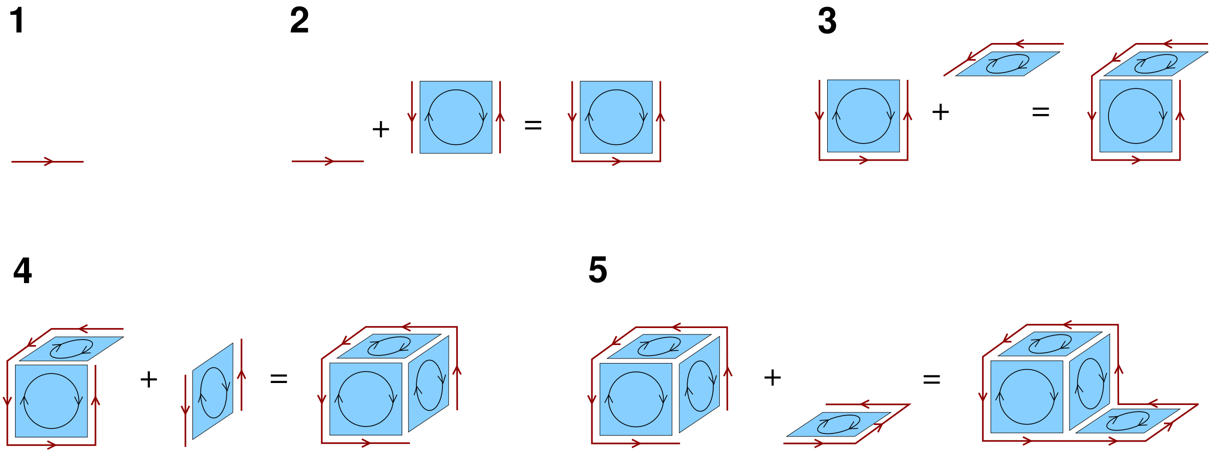
An admissible configuration for dual U(1) gauge Higgs theory:



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

Y. Delgado Mercado, Parallels 4A

Bulk observables

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

- Example: Observables related to the particle number:

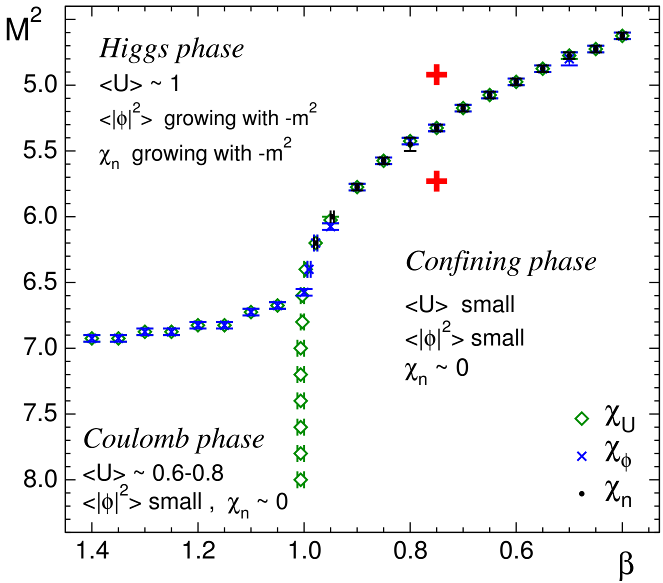
$$n = \frac{1}{N_s^3 \, N_t} \frac{\partial \, \ln Z}{\partial \mu}$$

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

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

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

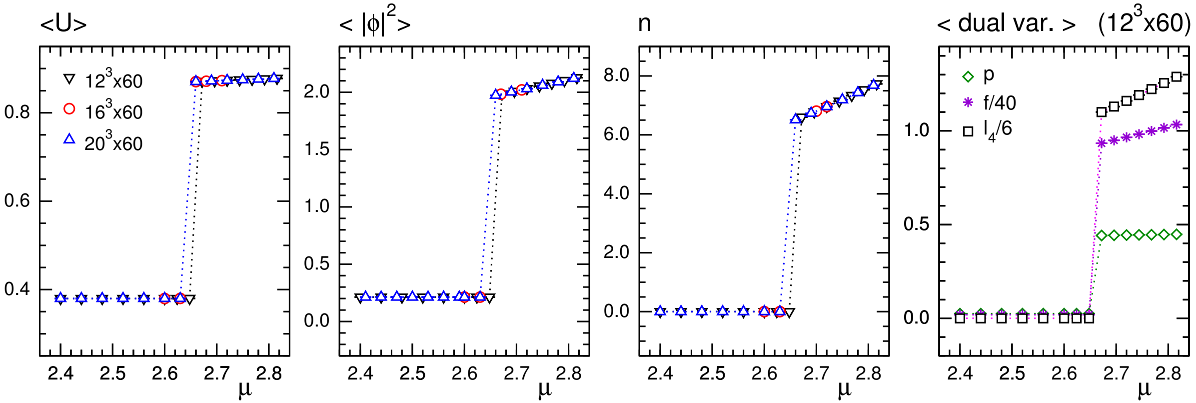
2-flavor gauge Higgs phase diagram at zero density



Y. Delgado Mercado, C. Gattringer, A. Schmidt, arXiv:1307.6120

Y. Delgado Mercado, Parallels 4A & A. Schmidt, Parallels 4A

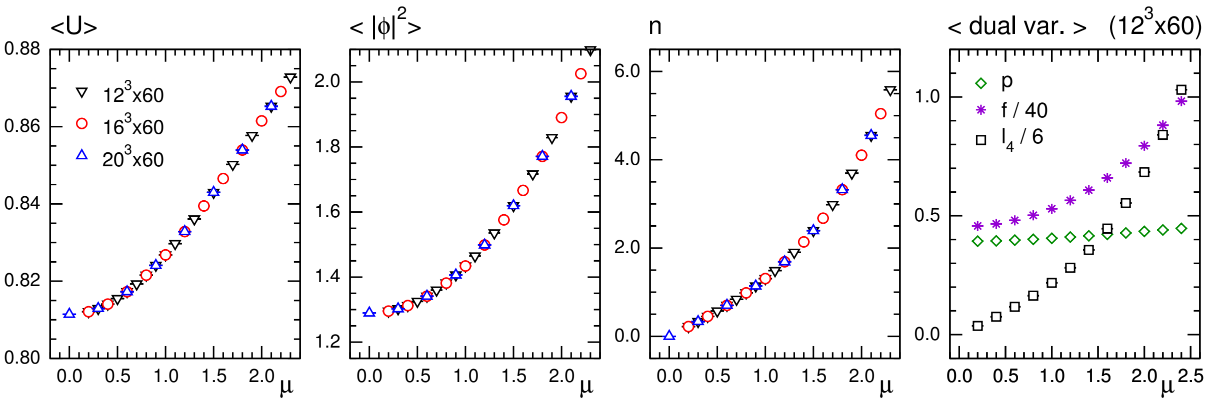
Observables in the confining phase at low T



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"

The corresponding BEC is accompanied by a condensation of dual variables.

Observables in the Higgs phase at low T



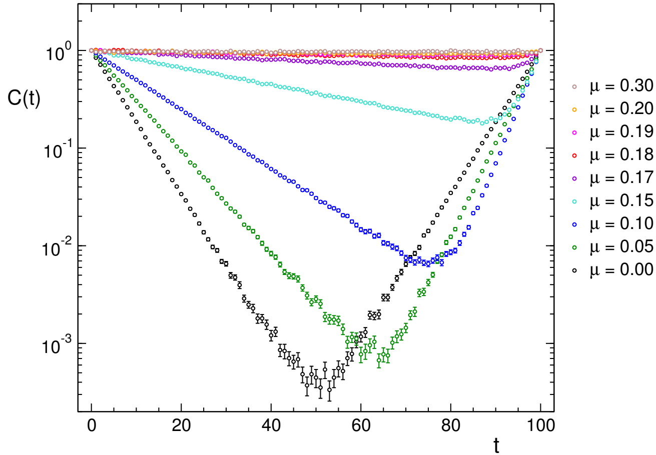
In the Higgs phase there is no mass gap and the non-trivial μ-dependence starts at $\mu = 0$.

No condensation of dual variables.

Spectroscopy at finite density ⇒ Dual spectroscopy

- Propagator: Use generalized ensemble with an additional open string.
- The 2-point function is obtained by sampling the positions of head and tail of the open string.

T. Korzec, I. Vierhaus, U. Wolff, Comp. Phys. Comm. 182, 2011



Asymmetric propagation for $\mu < \mu_c \simeq 0.17$.
Slopes understood quantitatively.

C. Gattringer, T. Kloiber, PLB 720, 2013

T. Kloiber, Parallels 4A

Applications and challenges

Reference systems for other approaches:

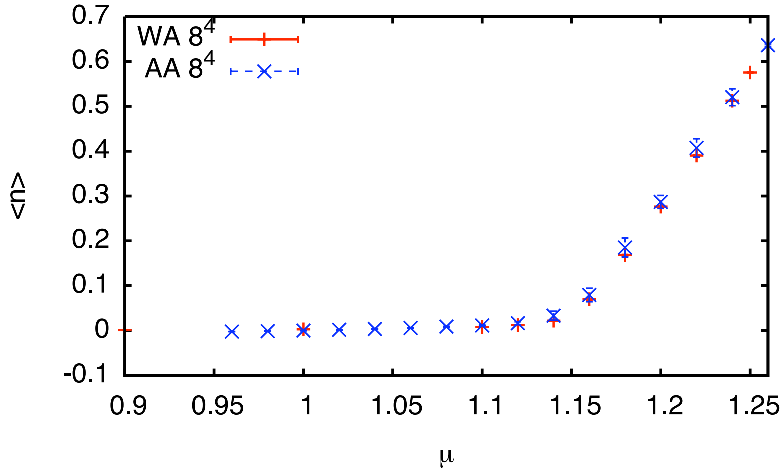
Finite density field theories which can be reliably analyzed with dual methods may be used to check and improve other approaches to finite density.

Two examples:

- Charged scalar field on a Lefschetz thimble.
- Comparison of series expansions for the Z_3 center model.

Charged scalar field on a Lefschetz thimble

QFT and Monte Carlo are formulated on a Lefschetz thimble (manifold that generalizes the notion of curves of steepest descent to higher dimensions).

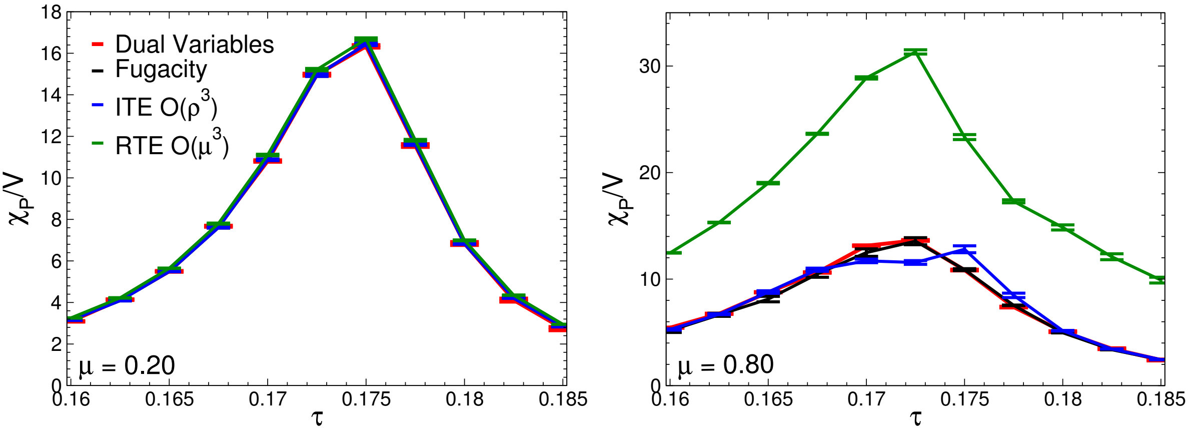


M. Cristoforetti, F. Di Renzo, A. Mukherjee, L. Scorzato, arXiv:1303.7204 (Lefschetz)
C. Gattringer, T. Kloiber, NPB 869, 2013 (dual variables)
G. Aarts, PRL 102, 2009 (complex Langevin)

L. Scorzato, Parallels 9A & M. Cristoferetti, Parallels 9A

Comparison of series expansions for the Z_3 center model

Z_3 spin model is an effective theory for the center degrees of freedom of QCD.



Y. Delgado Mercado, H.G. Evertz, C. Gattringer, PRL 106, 2011 (dual variables)

E. Grünwald & M. Wilfling, Poster

A major challenge: dual representation for non-abelian symmetries

- Previous attempts:

  N. Hari Dass, R. Anishetty, H. Sharatchandra, W. Cherington, H. Pfeiffer, R. Oeckl ...

  - Based on character expansion.
  - Gives negative weights already for pure SU(2) YM theory.

- Some progress with non-abelian spin systems:

  - O(N) spin systems: U. Wolff, NPB 824, 2010
  - CP(N-1) model: U. Wolff, NPB 832, 2010
  - SU(2)×SU(2) spin system: T. Kloiber, C. Gattringer, in preparation

- There is hope at least ...

Fermions

Loop representation for fermions

- In principle same structure as for bosons: Surfaces bounded by loops of matter flux.

- Loops have additional signs from Pauli principle / traces over γ-matrices.

- Certain limits alleviate the problem by restricting the contributing loops.

- Large amount of work in the strong coupling and heavy quark limits.

  F. Karsch, K.H. Mutter, R. De Pietri, A. Feo, E. Seiler, I.O. Stamatescu, P. de Forcrand, M. Fromm, O. Philipsen, J. Langelage, M. Neuman, W. Unger, K. Miura, C. Gattringer, Y. Delgado Mercado, T. Ichihara, A. Ohnishi, T. Nakano ...

- Some 2-D models mapped to positive dual representations.

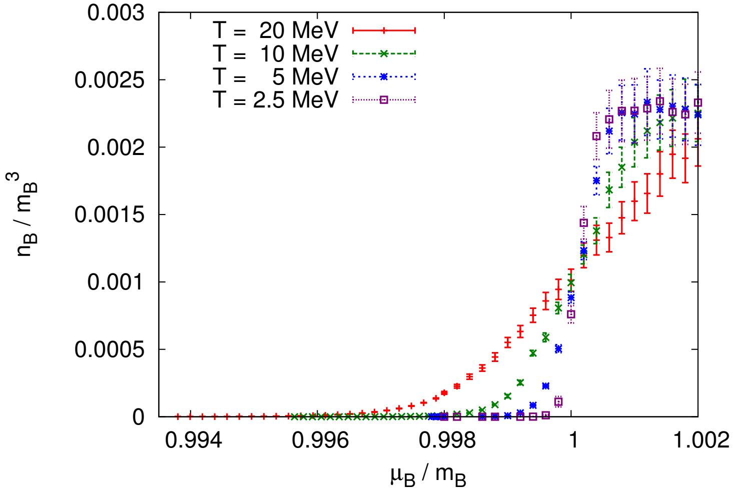
  H. Gausterer, C.B. Lang, M. Salmhofer, C. Gattringer, V. Hermann, M. Limmer, U. Wenger, B. Leder, F. Knechtli, T. Korzec, U. Wolff ...

R. Lohmayer, R. Narayanan: Parallels 4A

Condensation phenomena for QCD at strong coupling and heavy quarks

M. Fromm, J. Langelage, S. Lottini, M. Neuman, O. Philipsen, PRL 110, 2013

- Combined strong coupling and heavy quark mass expansion.
- Various MC techniques compared.
- Scale setting.



J. Langelage & M. Neuman & W. Unger & T. Ichihara, Parallels 7A

Different strategy: Fermion bags

S. Chandrasekharan, A. Li

- Dual bosonic models: Expand nearest neighbor terms.
- Traditional loop representation for fermions:
  Expand the complete Grassmann integral.
- Fermion bags: Expand only interaction parts of the Boltzmann factor. Remaining terms correspond to a reduced system without sign problem.

S. Chandrasekharan, Parallels 5E

Fermion bags - I

Consider an action of the form:

$$S = \sum_{ij} \overline{\psi}_i M_{ij} \psi_j + \sum_i g_i^{(1)} \overline{\psi}_i \psi_i + \sum_{ij} g_{ij}^{(2)} \overline{\psi}_i \psi_i \overline{\psi}_j \psi_j + \sum_{ijk} g_{ijk}^{(3)} \overline{\psi}_i \psi_i \overline{\psi}_j \psi_j \overline{\psi}_k \psi_k \ldots$$

The couplings $g^{(\alpha)}$ are assumed to be positive and the matrix M has a form that gives rise to a theory without sign problem:

$$M = \begin{bmatrix} 0 & B \\ -B^\dagger & 0 \end{bmatrix}$$

Expansion of the Boltzmann factor for the first interaction terms:

$$e^{\sum_i g_i \overline{\psi}_i \psi_i} = \prod_i e^{g_i \overline{\psi}_i \psi_i} = \prod_i [\, 1 + g_i \overline{\psi}_i \psi_i \,] = \prod_i \sum_{n_i = 0,1} (g_i)^{n_i} \, (\overline{\psi}_i \psi_i)^{n_i}$$

The expansion indices n_i activate terms that locally saturate the Grassmann integral. The n_i are dual variables for the interaction terms.

Fermion bags - II

For a given configuration of the n_i the Grassmann integral reads:

$$\int \mathcal{D}[\,\overline{\psi}, \psi\,]\, e^{-\overline{\psi} M \psi} \prod_i (\,\overline{\psi}_i \psi_i\,)^{n_i} \;=\; \int \widetilde{\mathcal{D}}[\,\overline{\psi}, \psi\,]\, e^{-\overline{\psi}\,\widetilde{M}\,\psi}$$

The result is a reduced partition sum with the activated $\overline{\psi}_i \psi_i$ taken out. The reduced partition sum is without sign problem.

$$\widetilde{M} \;=\; \begin{bmatrix} 0 & \widetilde{B} \\ -\widetilde{B}^\dagger & 0 \end{bmatrix}$$

- Every problem that can be cast into the standard form can be reduced to a system without sign problem.
- Ideally the $n_i = 1$ are abundant (depends on couplings) such that the reduced problem factorizes into many small systems.

Fermion bags

- Several interesting systems were analyzed with fermion bags.
  - SU(2) Yukawa models with Wilson fermions.
  - Gauged Nambu-Jona-Lasinio model.
  - Gross-Neveu model.
  - Massless Thirring model.
  - Models to study metal-insulator phase transitions.

- Lattice gauge theories with fermions seem not to be tractable with the current formulation.

S. Chandrasekharan, Lectures at Schladming Winter School 2013

`http://physik.uni-graz.at/schladming2013/index.php?sf=18`

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 surfaces for gauge fields and loops for matter. Update with worm algorithms.

- Dual representations of non-abelian bosonic theories are a challenge.

- Traditional loop representations for fermions have additional minus signs from Pauli principle / traces over γ-matrices.

- Large mass and strong coupling alleviate the sign problem.

- Fermion bag approach completely solves the sign problem for a certain class of QFT with fermions.