Lattice field theory with dual variables

Christof Gattringer

Karl-Franzens-Universität Graz, Austria

Ydalia Delgado Mercado, Thomas Kloiber, Alexander Schmidt

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Euclidean path integral, complex action problem and dual representation

- Vacuum expectation values with Feynman's path integral:

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

- In a Monte Carlo simulation observables are computed as averages over field configurations ψ distributed according to

$$P[\psi] \;=\; \frac{1}{Z}\, e^{-S[\psi]}$$

- For finite chemical potential μ the action $S[\psi]$ is complex and the Boltzmann factor cannot be used as probability weight in a stochastic process.

Rewriting a system in terms of new variables where only real and positive terms appear in the partition sum could overcome the complex action problem.

Charged scalar field

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- Continuum action:

$$S = \int d^4x \Big[-\phi(x)^* \triangle \phi(x) + [m^2 - \mu^2]\, |\phi(x)|^2 + \lambda\, |\phi(x)|^4 \Big] + i\mu N$$

- Action on the lattice:

$$S = \sum_x \Big[\kappa\, |\phi_x|^2 + \lambda\, |\phi_x|^4 - \sum_{j=1}^{3} \Big(\phi_x^\star \phi_{x+\hat{j}} + \phi_x^\star \phi_{x-\hat{j}} \Big) - \phi_x^\star e^{-\mu} \phi_{x+\hat{4}} - \phi_x^\star e^{\mu} \phi_{x-\hat{4}} \Big]$$

$\kappa = 8 + m^2$

Dual representation – I

- Expand the individual nearest neighbor terms:

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

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

- Idea: Use the $j_{x,\nu}$ and $\overline{j}_{x,\nu}$ as the new degrees of freedom.

- Remaining ϕ-integrals at a site x :

$$\int_{\mathbb{C}} d\,\phi_x\ \ e^{-\kappa|\phi_x|^2 - \lambda|\phi_x|^4}\ \left(\phi_x\right)^{F(j,\overline{j})}\left(\phi_x^\star\right)^{\overline{F}(j,\overline{j})}$$

$F_x(j,\overline{j})$, $\overline{F}_x(j,\overline{j}) \in \mathbb{N}_0$ are linear combinations of the j and $\overline{j}$ variables attached to the site x. They correspond to the total j, $\overline{j}$-flux at x.

Dual representation – II

- Using $\phi_x = r\, e^{i\theta}$ the integrals at a site x read:

$$\int_{\mathbb{C}} d\,\phi_x \;\; e^{-\kappa|\phi_x|^2 - \lambda|\phi_x|^4} \; (\phi_x)^{F(j,\bar{j})} \, (\phi_x^\star)^{\overline{F}(j,\bar{j})} \; =$$

$$\int_0^\infty dr \; r^{\,F_x + \overline{F}_x + 1} \; e^{-\kappa r^2 - \lambda r^4} \int_{-\pi}^{\pi} d\theta \; e^{\,i\theta\,[F_x - \overline{F}_x]} \; = \; \mathcal{I}(F_x + \overline{F}_x)\; \delta(F_x - \overline{F}_x)$$

- At every site there is a weight factor $\mathcal{I}(F_x + \overline{F}_x)$ and a constraint.

- The constraint $\delta(F_x - \overline{F}_x)$ forces the total flux $F_x - \overline{F}_x$ at x to vanish.

- The structure can be simplified by using linear combinations $k_{x,\nu} \in \mathbb{Z}$ and $l_{x,\nu} \in \mathbb{N}_0$ of the original variables $j_{x,\nu}$ and $\bar{j}_{x,\nu}$.

- Only the $k_{x,\nu}$ are subject to constraints.

Dual representation – III (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 $l_{x,\nu} \in \mathbb{N}_0$:

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

- Weight factor (real and positive):

$$\mathcal{W}(k,l) \;=\; \prod_{x,\nu} \frac{1}{(|\,k_{x,\nu}\,| + l_{x,\nu})!\; l_{x,\nu}!} \times \prod_x e^{-\mu\, k_{x,4}}\, \mathcal{I}\Big(\sum_\nu [|\,k_{x,\nu}\,| + |\,k_{x-\widehat{\nu},\nu}\,| + 2(l_{x,\nu} + l_{x-\widehat{\nu},\nu})] \Big)$$

- Constraint (only for k-variables):

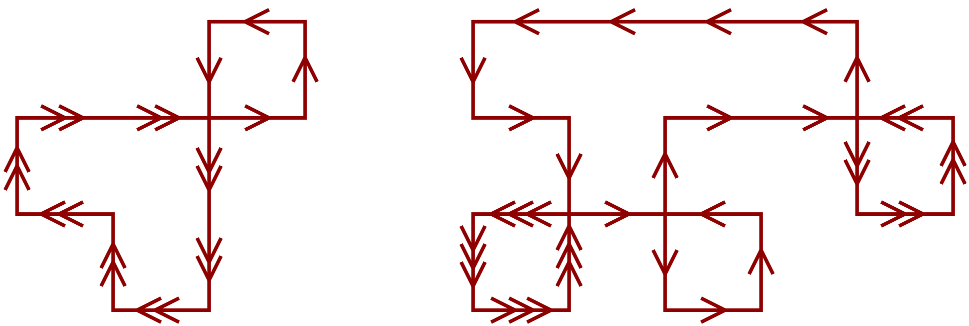
$$\mathcal{C}(k) \;=\; \prod_x \delta\Big(\sum_\nu \left[\, k_{x,\nu} - k_{x-\widehat{\nu},\nu} \,\right] \Big)$$

Admissible configurations are loops:

- Constraint from the integration over the U(1) phases:

$$\forall \; x \; : \qquad f_x \; = \; \sum_{\nu} \left[\, k_{x,\nu} - k_{x-\widehat{\nu},\nu} \, \right] \; = \; 0$$

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



- Chemical potential gives different weight to forward and backward temporal flux. Particle number $=$ net winding number of k-flux.

Coupling gauge fields

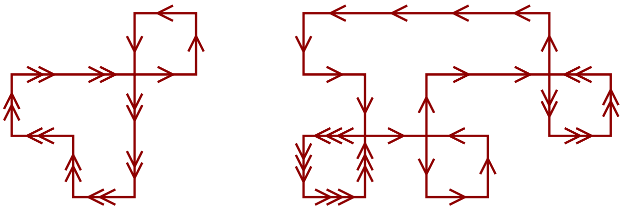
- The nearest neighbor terms can be gauged:

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

- Additional weight factor in the final form of the dual representation:

$$\prod_{x,\nu} (U_{x,\nu})^{k_{x,\nu}}$$

- Loops are dressed with gauge transporters.



Scalar QED / U(1) gauge Higgs model with 2 flavors

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Continuum action:

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

Adding dynamical gauge fields in the dual representation

- Two copies of the loop sum integrated over gauge fields:

$$Z = \sum_{\{k,l,\overline{k},\overline{l}\}} \mathcal{W}_\phi(k,l)\,\mathcal{W}_\chi(\overline{k},\overline{l})\,\mathcal{C}(k)\,\mathcal{C}(\overline{k})$$

$$\times \int D[U] \exp\left(\beta \sum_{x,\rho<\sigma} \text{Re}\, U_{x,\rho}\, U_{x+\hat{\rho},\sigma}\, U^\star_{x+\hat{\sigma},\rho}\, U^\star_{x,\sigma}\right) \prod_{x,\nu} (U_{x,\nu})^{k_{x,\nu}-\overline{k}_{x,\nu}}$$

- Expansion of the Boltzmann factor ....

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

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

- Integrating the gauge fields $dU_{x,\sigma}$ gives rise to new constraints that connect $p_{x,\rho\sigma}, k_{x,\nu}$ and $\overline{k}_{x,\nu}$ at each link.

Dual form of the partition function:

The original partition sum is mapped exactly to a sum over loop and surface configurations:

$$Z = \sum_{\{p,k,l,\overline{k},\overline{l}\}} \mathcal{W}_G(p)\, \mathcal{W}_\phi(k,l)\, \mathcal{W}_\chi(\overline{k},\overline{l})\, \mathcal{C}_L(p,k,\overline{k})\, \mathcal{C}_S(k)\, \mathcal{C}_S(\overline{k})$$

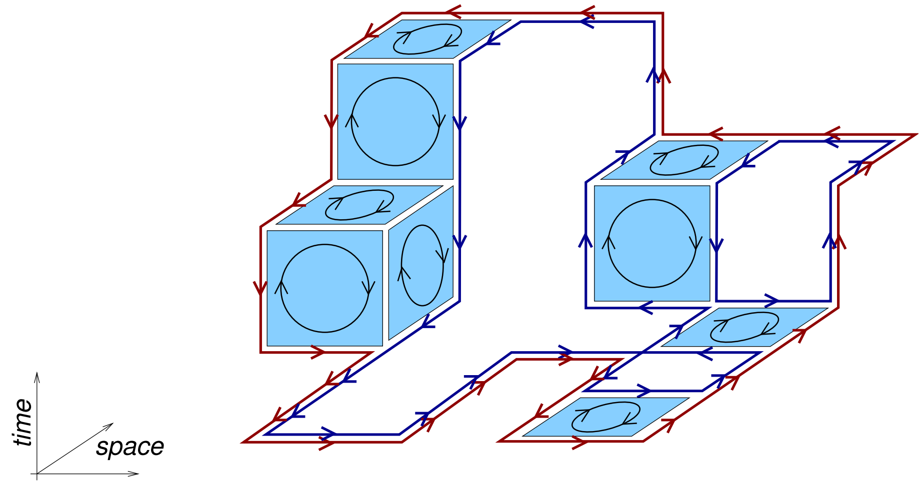
$\mathcal{W}_G(p)$: plaquette-based weight factor for gauge variables p
$\mathcal{W}_\chi(k,l), \mathcal{W}_\phi(\overline{k},\overline{l}),$: link-based weight factor for matter variables $k, l, \overline{k}, \overline{l}$
$\mathcal{C}_L(p,k,\overline{k})$: link-based constraint $\Rightarrow$ gauge surfaces
$\mathcal{C}_S(k), \mathcal{C}_S(\overline{k})$: site-based constraint $\Rightarrow$ matter loops

$$\mathcal{C}_L[p,k,\overline{k}] = \prod_{x,\nu} \delta\left(\sum_{\rho:\nu<\rho} [p_{x,\nu\rho} - p_{x-\hat{\rho},\nu\rho}] - \sum_{\rho:\nu>\rho} [p_{x,\rho\nu} - p_{x-\hat{\rho},\rho\nu}] + k_{x,\nu} - \overline{k}_{x,\nu} \right)$$

$$\mathcal{C}_S[k] = \prod_{x} \delta\left(\sum_{\nu=1}^{4} [k_{x-\hat{\nu},\nu} - k_{x,\nu}] \right)$$

Suitable worm algorithms

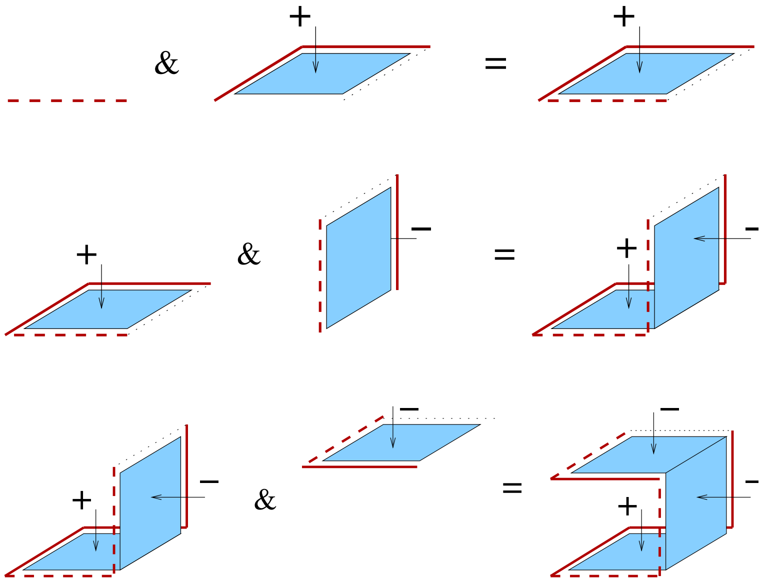
An admissible configuration:



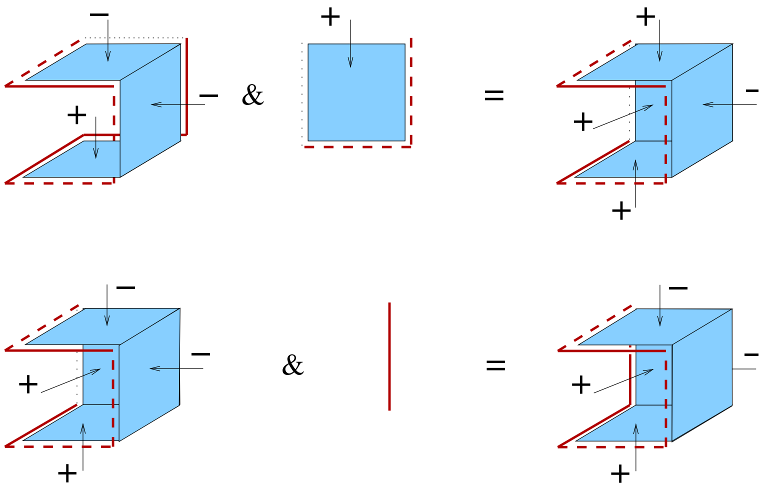
Chemical potential favors flux forward in time.

Generalized worm algorithm for gauge Higgs systems:

Worm starts by inserting a unit of matter flux. Adding segments transports both the site and link defects across the lattice ....



Generalized worm algorithm for gauge Higgs systems



Algorithm was tested in the 1-flavor U(1) model and in a $\mathbb{Z}_3$ gauge Higgs model at finite μ. Clearly outperforms local dual update.

Bulk observables

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

- They have the form of averages and fluctuations of the dual variables.

- Observables related to the particle number:

$$n \;=\; \frac{T}{V}\frac{\partial \,\ln Z}{\partial \mu} \;=\; \frac{1}{N_s^3\,N_t}\frac{\partial \,\ln Z}{\partial \mu} \quad , \quad \chi_n \;=\; \frac{\partial \, n}{\partial \mu}$$

- Observables related to field expectation values:

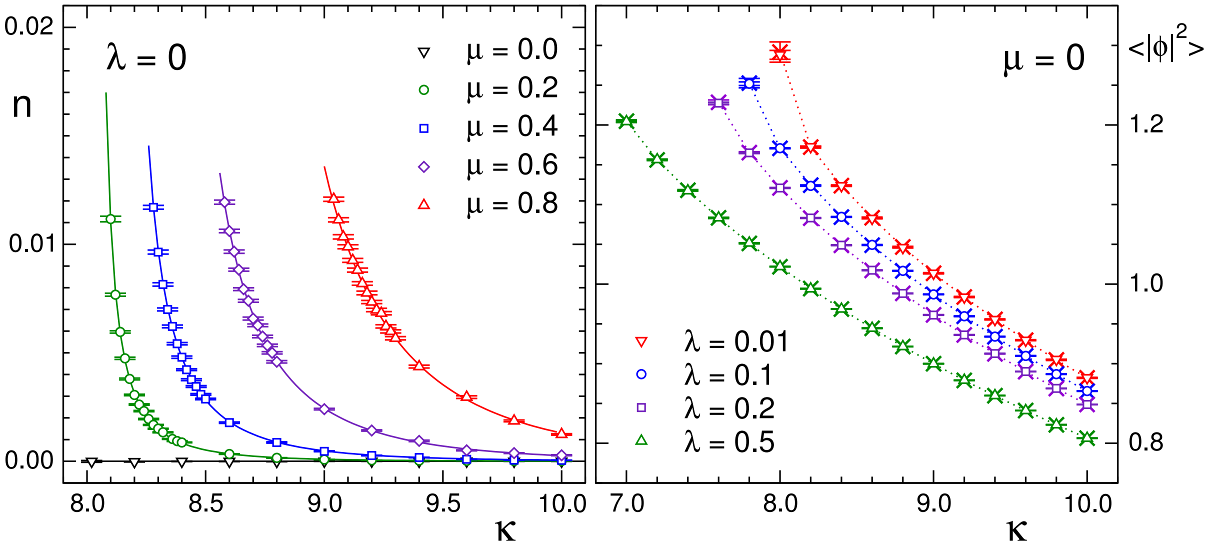
$$\langle |\,\phi\,|^2 \rangle \;=\; \frac{-T}{V}\frac{\partial \,\ln Z}{\partial \kappa} \;=\; \frac{-1}{N_s^3\,N_t}\frac{\partial \,\ln Z}{\partial \kappa} \quad , \quad \chi_\phi \;=\; \frac{-\partial\langle |\,\phi\,|^2 \rangle}{\partial \kappa}$$

- Dual forms:

$$n \;=\; \frac{1}{N_s^3\,N_t}\left\langle \sum_x k_{x,4} \right\rangle \quad , \quad \langle |\,\phi\,|^2 \rangle \;=\; \frac{1}{N_s^3\,N_t}\left\langle \sum_x \frac{\mathcal{I}(f_x+2)}{\mathcal{I}(f_x)} \right\rangle$$

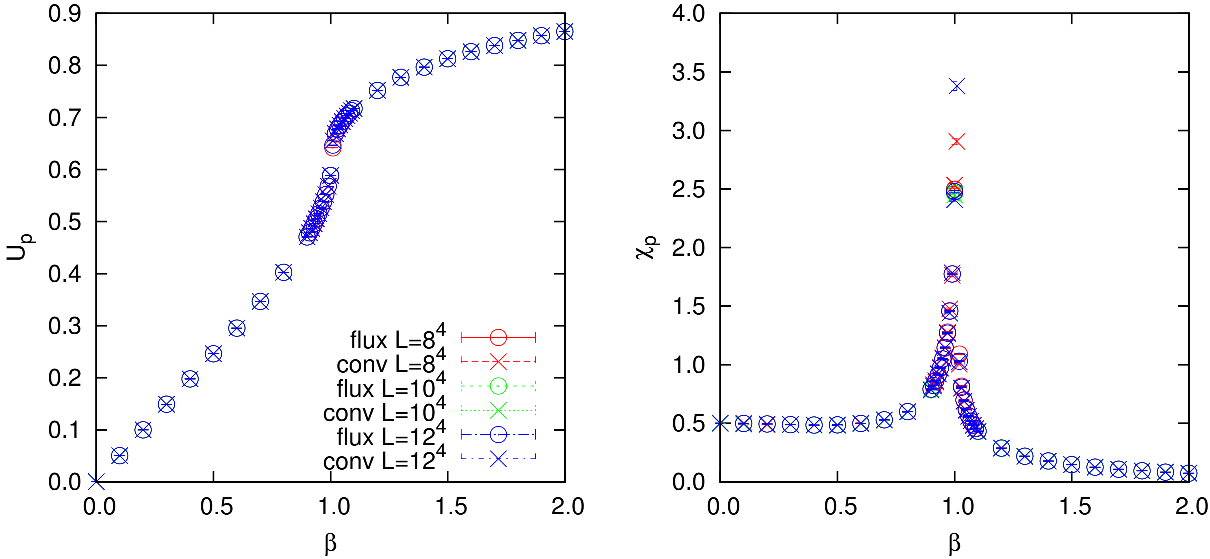
Checks - I

Simulation with dual variables can be checked with high precision:
(here for $\beta = \infty$)



Checks - II

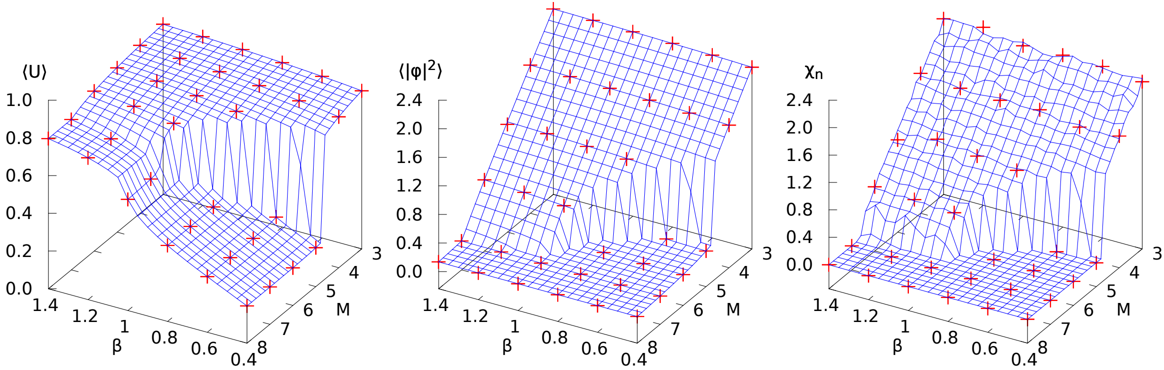
Comparison to conventional simulation:
$(\mu_\phi = \mu_\chi = 0, \kappa_\phi = \kappa_\chi = 9.0, \lambda_\phi = \lambda_\chi = 0.0)$



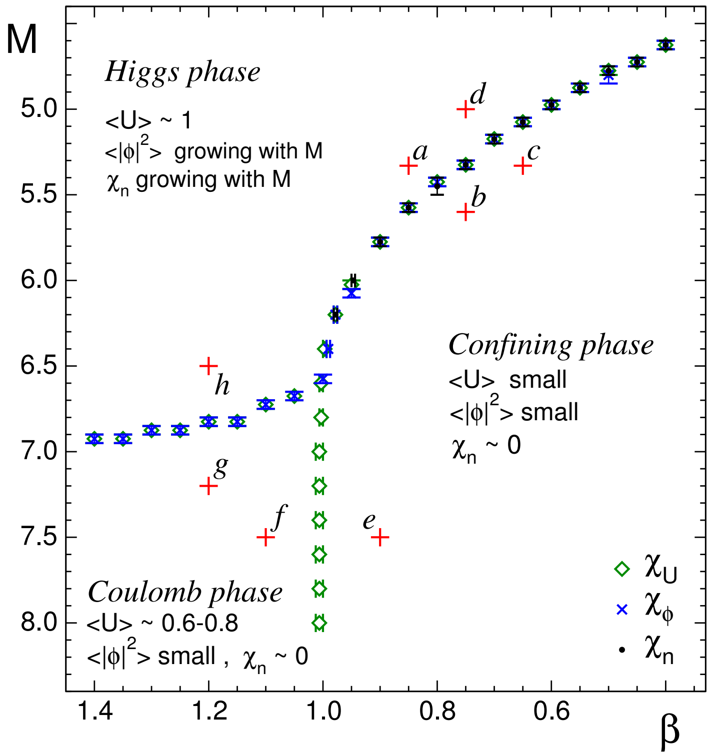
Phase diagram

Bulk observables at $\mu = 0$

Using: $\kappa_\phi = \kappa_\chi = M, \lambda_\phi = \lambda_\chi = 1.0$

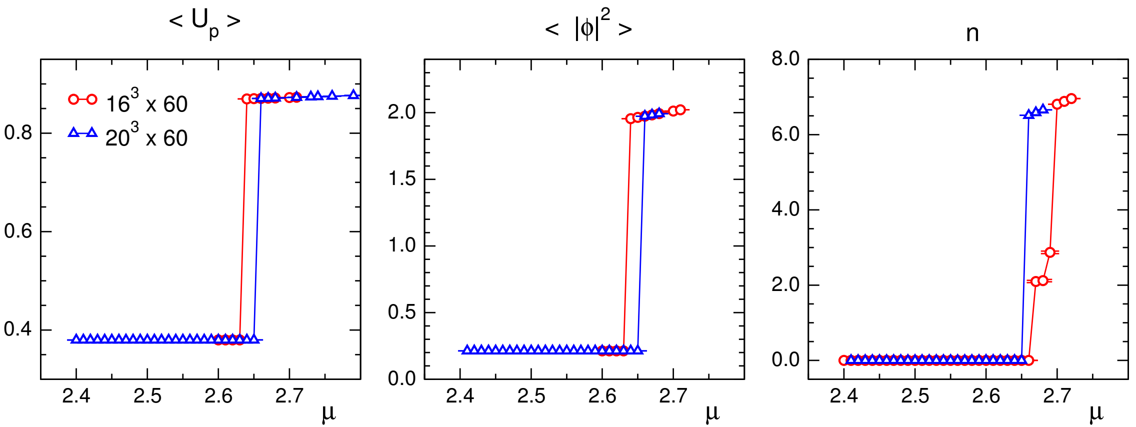


Phase diagram at $\mu = 0$



Turning on chemical potential

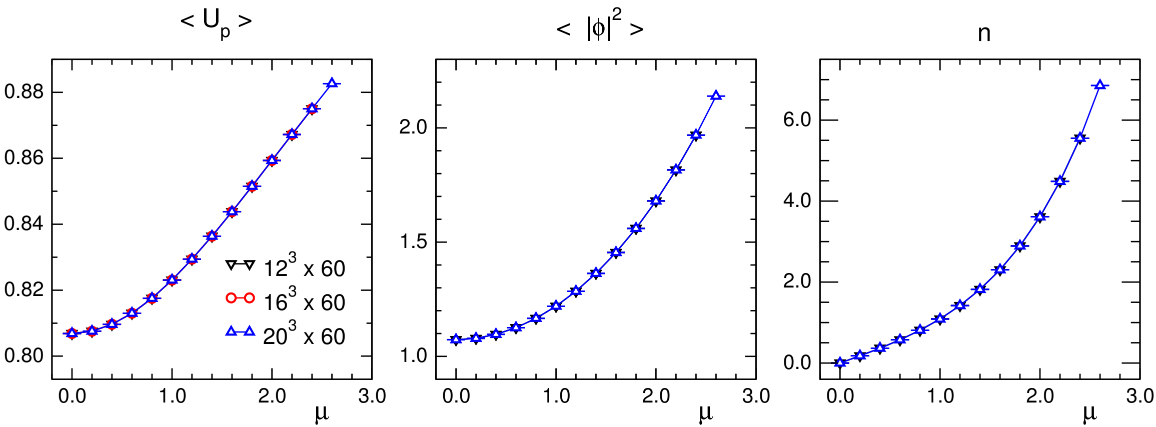
A point in the confining phase: $\kappa_\phi = \kappa_\chi = 5.73, \lambda_\phi = \lambda_\chi = 1.0, \beta = 0.75$



Silver blaze region that ends in a strong first order transition leading back into the Higgs phase.

Turning on chemical potential

A point in the Higgs phase: $\kappa_\phi = \kappa_\chi = 5.325, \lambda_\phi = \lambda_\chi = 1.0, \beta = 0.85$



Massless excitations in the Higgs phase $\rightarrow$ no Silver blaze behaviour.

Spectroscopy with dual variables

Spectroscopy for the charged scalar at finite density

- Zero momentum propagator

$$C(t) \;=\; \sum_{\vec{x}} \langle\, \phi_{\vec{x},t}\, \phi^*_{\vec{0},0}\, \rangle \;\;\propto\;\; e^{-E_0 t}$$

$$\langle\, \phi_y\, \phi^*_z\, \rangle \;=\; \frac{1}{Z} \int D[\phi]\, e^{-S}\, \phi_y\, \phi^*_z \;=\; \frac{Z_{y,z}}{Z}$$

- Dual representation of the partition sum $Z_{y,z}$ with two insertions:

$$Z_{y,z} = \sum_{\{k,l\}} \prod_{x,\nu} \frac{1}{(|\,k_{x,\nu}\,| + l_{x,\nu})!\, l_{x,\nu}!} \prod_x \delta\Big(\sum_\nu \left[\, k_{x,\nu} - k_{x-\widehat{\nu},\nu}\,\right] - \delta_{x,y} + \delta_{y,z} \Big)$$
$$\times \prod_x e^{-\mu\, k_{x,4}}\, \mathcal{I}\Big(\sum_\nu [\,|\,k_{x,\nu}\,| + |\,k_{x-\widehat{\nu},\nu}\,| + 2(l_{x,\nu} + l_{x-\widehat{\nu},\nu})] + \delta_{x,y} + \delta_{y,z} \Big)$$

- Admissible configurations in $Z_{y,z}$:

  Closed loops of flux plus an open string of flux connecting y and z.

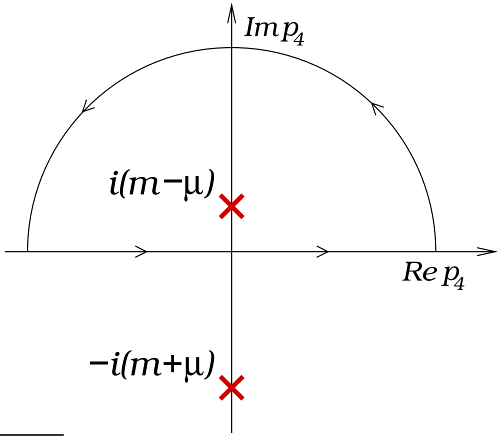
Worm strategy for correlators

- Since $Z_{y,z}$ consists of closed loop plus a single open string, every step of the worm corresponds to an admissible configuration for some $Z_{u,v}$.

- In our propagators we project to zero momentum, i.e., the spatial lattice indices are summed.

- To compute $C(t)$ one simply evaluates the temporal distance t of head and tail of the worm at every step and $C(t)$ is obtained as a histogram.

What do we expect? Analysis of the free case in the continuum.



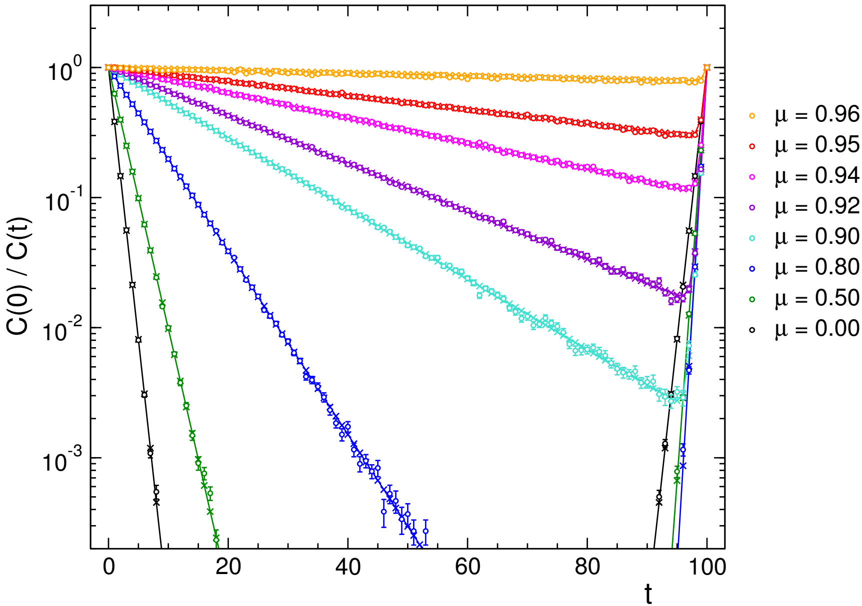
- Propagator in the continuum:

$$C(t) \;=\; \int \frac{dp_4}{2\pi}\,\frac{e^{ip_4 t}}{[p_4 - i(m-\mu)][p_4 + i(m+\mu)]}$$

- Asymmetry between forward and backward propagation:

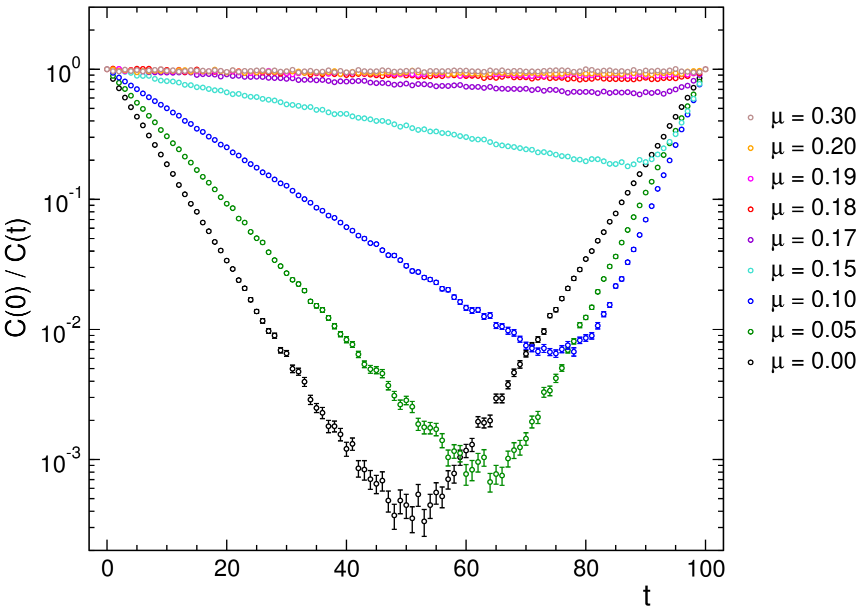
$$C(t) \;\propto\; \begin{cases} e^{-(m-\mu)t} & \text{for } t > 0 \\ e^{+(m+\mu)t} & \text{for } t < 0 \end{cases}$$

Test of free propagators against (lattice) Fourier transformation



Excellent agreement indicates that the finite density propagators computed from the dual representation are under control. $(16^3 \times 100,\ m = 1, \lambda = 0)$

Propagators at non zero coupling



Asymmetric propagation for $\mu < \mu_c \simeq 0.17$. Condensation (= constant propagator) for μ above μ_c. $(16^3 \times 100, \kappa = 7.44, \lambda = 1)$

Summary:

- Considerable progress was made towards rewriting several systems in representations where the partition sum has only real and positive terms.

- Dual degrees of freedom are surfaces for gauge fields and loops for matter.

- Constraints for dual variables can be handled with worm-type algorithms.

- Interesting new algorithmic options when surfaces have boundaries.

- Spectroscopy is under control.

- Systems may serve as solved test cases for other approaches.