Structure of the Lefschetz thimbles decomposition of lattice fermion models

Maksim Ulybyshev,
Universität Würzburg, Germany
maksim.ulybyshev@physik.uni-wuerzburg.de

in collaboration with:
Fakher Assaad, Savvas Zafeiropoulos, Christofer Winterowd

PRD 101, 014508 (2020)

November 11th
XXXII International (ONLINE) Workshop on High Energy Physics "Hot problems of Strong Interactions"

Motivation (1)

Path integral is usually treated in Quantum Monte Carlo (QMC) in condensed matter physics as «black box»: once we have an algorithm for sampling, we are not looking into the details of the structure of path integral. Also, formulations with discrete fields in path integrals make such analysis more difficult (no theorems of calculus).

In Lattice Quantum Field theory, we have more knowledge on quasi-classical objects as special field configurations appearing in path integrals (monopoles, instantons, etc), but still some improvement is possible after several algorithmic developments.

The structure of path integrals (saddle points) is connected to the complexity of the sign problem through the Lefschetz thimbles decomposition.

Lefschetz thimbles decomposition (1)

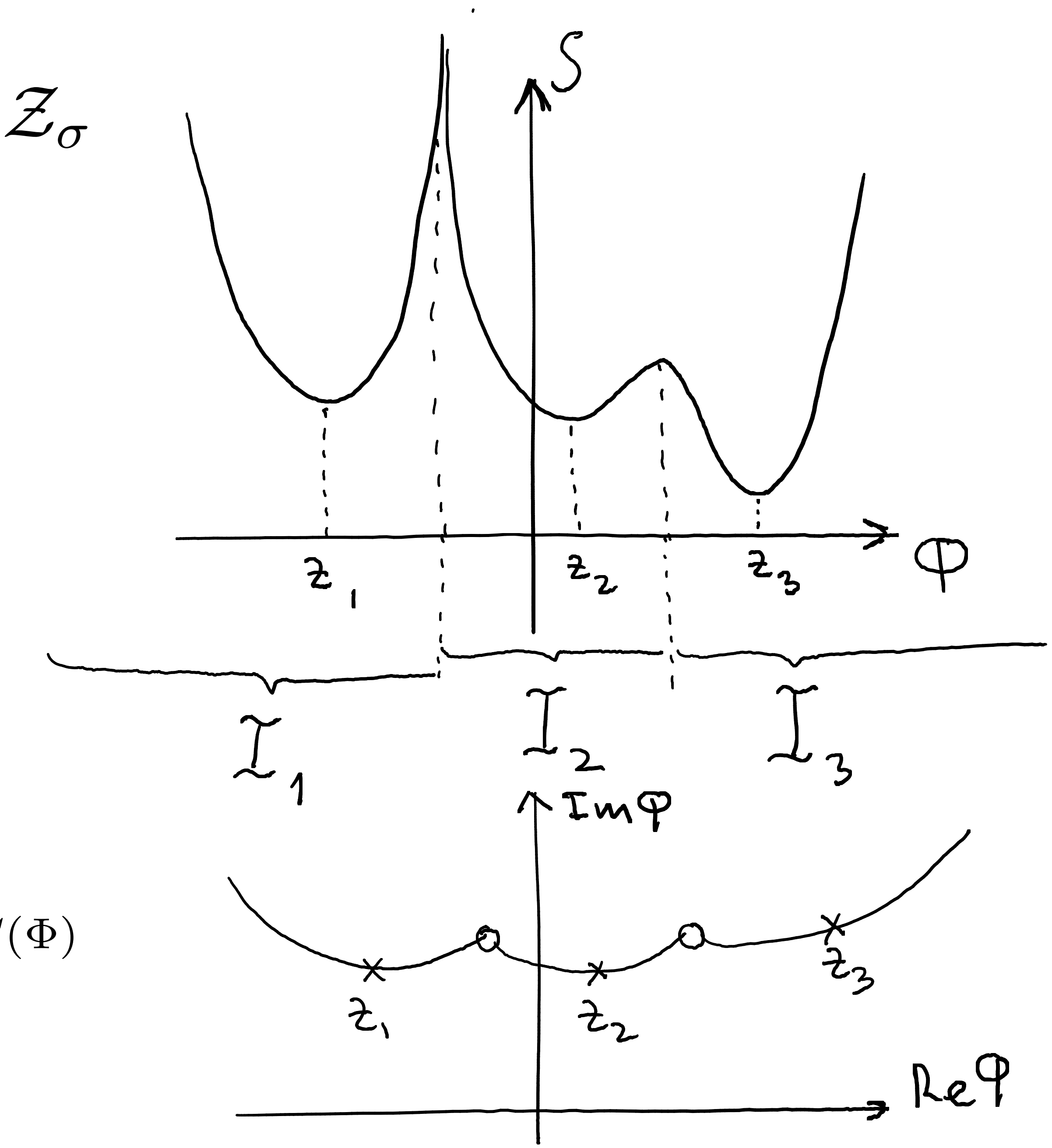
$$\mathcal{Z} = \int_{\mathbb{R}^N} \mathcal{D}\Phi\, e^{-S[\Phi]} = \sum_\sigma k_\sigma \mathcal{Z}_\sigma$$

$$\mathcal{Z}_\sigma = \int_{\mathcal{I}_\sigma} \mathcal{D}\Phi\, e^{-S[\Phi]}$$

Saddle point: $$\left.\frac{\partial S}{\partial \Phi}\right|_{\Phi = z_\sigma} = 0$$

Gradient flow equations: $$\frac{d\Phi}{dt} = \overline{\frac{\partial S}{\partial \Phi}}$$

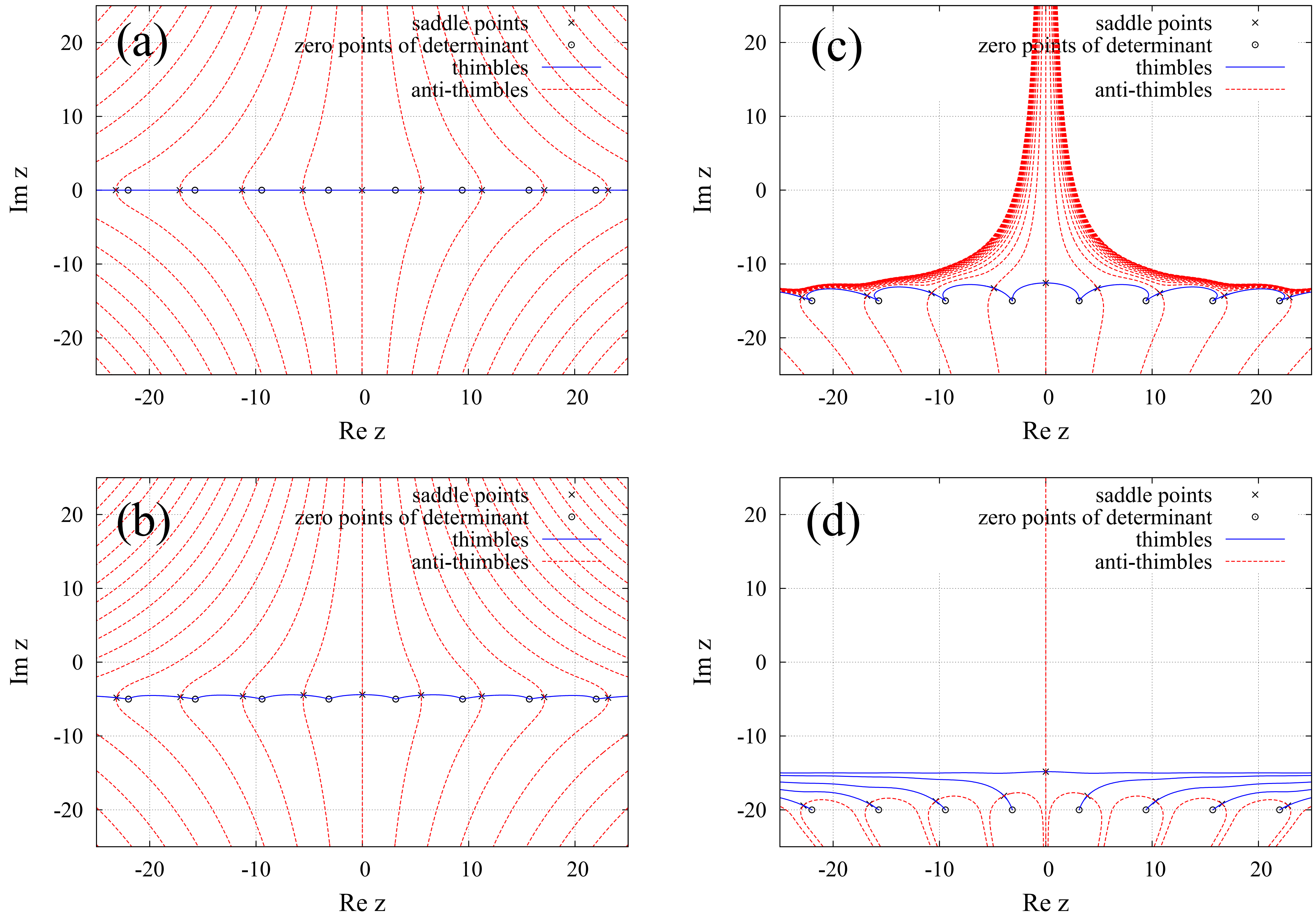
$$\mathcal{Z} = \sum_\sigma k_\sigma e^{-i\,\mathrm{Im}\,S(z_\sigma)} \int_{\mathcal{I}_\sigma} \mathcal{D}\Phi\, e^{-\mathrm{Re}\,S(\Phi)}$$



Questions to answer:

1) Scaling of the number of thimbles in the thermodynamic limit: one- or many-thimble regime?
2) Connection of the thimbles decomposition to the physics, in particular its reaction on the phase transition.

Lefschetz thimbles decomposition (2)



a) μ=0; b…d) increasing μ

Motivation (2)

Cond-mat algorithms:
Exact evaluation of fermionic forces and fermionic determinant (BSS-QMC)

Lattice field theory:
Gradient flow equations for continuous auxiliary fields

→ Better understanding of the structure of path integral

Ultimate goal is twofold:

1) Better understanding of the Lefschetz thimbles decomposition for large enough lattices, which factors influence its complexity, and if it's possible to weaken the residual sign problem.
2) to formulate some approximate theory which might be applicable to the regions of the phase diagram, where lattice simulations are not working (e.g. at non-zero chemical potential, lattice models with frustration, etc)

Exact calculation of fermonic forces (1)

$$S = S_b + \ln\det M$$

Staggered fermions:

$$M^{st}_{i,j} = 2am\delta_{i,j} + (\eta_{i,1} e^{\mu a} U_{i,1} \delta_{i+\hat{1},j} - \eta_{j,1} U^{\dagger}_{j,1} e^{-\mu a} \delta_{i-\hat{1},j}) + \sum_{\nu=2}^{4} (\eta_{i,\nu} U_{i,\nu} \delta_{i+\hat{\nu},j} - \eta_{j,\nu} U^{\dagger}_{j,\nu} \delta_{i-\hat{\nu},j})$$

$$\eta_{i,\nu} = (-1)^{i_1+\ldots+i_{\nu-1}}$$

$$M^{st}(U) = \begin{pmatrix} B_1 & e^{\mu a}[U_{(1,x),1}] & 0 & 0 & 0 & \ldots & e^{-\mu a}[U^{\dagger}_{(N_\tau,x),1}] \\ -e^{-\mu a}[U^{\dagger}_{(1,x),1}] & B_2 & e^{\mu a}[U_{(2,x),1}] & 0 & 0 & \ldots & 0 \\ 0 & -e^{-\mu a}[U^{\dagger}_{(2,x),1}] & B_3 & \ddots & 0 & \ldots & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & \ldots & 0 \\ \vdots & & & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \ldots & 0 & -e^{-\mu a}[U^{\dagger}_{(N_\tau-2,x),1}] & B_{N_\tau-1} & e^{\mu a}[U_{(N_\tau-1,x),1}] \\ -e^{\mu a}[U_{(N_\tau,x),1}] & 0 & \ldots & 0 & 0 & -e^{-\mu a}[U^{\dagger}_{(N_\tau-1,x),1}] & B_{N_\tau} \end{pmatrix}$$

(in terms of spatial $N_s \times N_s$ blocks)

Exact calculation of fermonic forces (2)

Following A. Hasenfratz and D. Toussaint, Nuclear Physics B 371, 539 (1992)

$$\overline{M}^{st}(U) = \begin{pmatrix} 1 & D_1 & 0 & 0 & 0 & \dots \\ 0 & 1 & D_2 & 0 & 0 & \dots \\ 0 & 0 & 1 & D_3 & 0 & \dots \\ 0 & 0 & 0 & 1 & D_4 & \dots \\ \vdots & & & & \ddots & \\ -D_{2N_\tau} & 0 & 0 & & \dots & 1 \end{pmatrix}$$

$$D_{2k} = \begin{pmatrix} e^{\mu a}[U_{(k,x),1}] & 0 \\ 0 & e^{\mu a}[U_{(k,x),1}] \end{pmatrix}$$

$$D_{2k-1} = \begin{pmatrix} B_k & I \\ I & 0 \end{pmatrix}, \; k = 1...N_\tau$$

$$\frac{\partial \ln \det M}{\partial \Phi} = \mathrm{Tr}\left(M^{-1} \frac{\partial M}{\partial \Phi} \right)$$

Inverse fermionic operator:

$$\overline{M}^{st^{-1}}(U) = \begin{pmatrix} g_1 & \dots & \dots & \dots & \dots & \bar{g}_{2N_\tau} \\ \bar{g}_1 & g_2 & \dots & \dots & \dots & \dots \\ \dots & \bar{g}_2 & g_3 & \dots & \dots & \dots \\ \dots & \dots & \bar{g}_3 & g_4 & \dots & \dots \\ \vdots & & & & \ddots & \\ \dots & \dots & \dots & & \dots & g_{2N_\tau} \end{pmatrix}$$

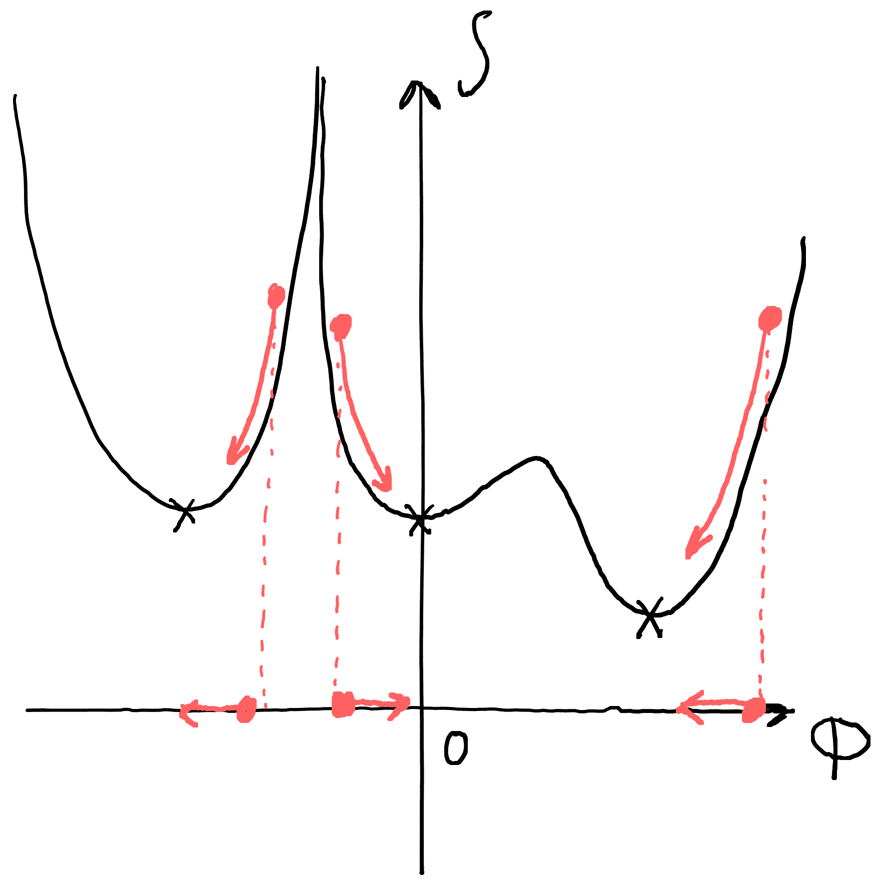
Iterations for blocks of fermonic propagator:

$$\bar{g}_{i+1} = D_{i+1}^{-1} \bar{g}_i D_i$$

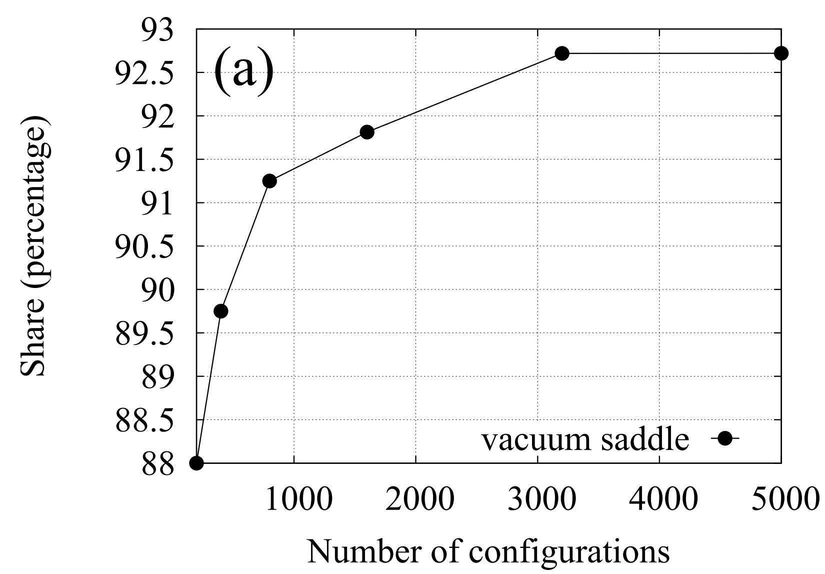
$N_s^3 N_\tau$ - scaling

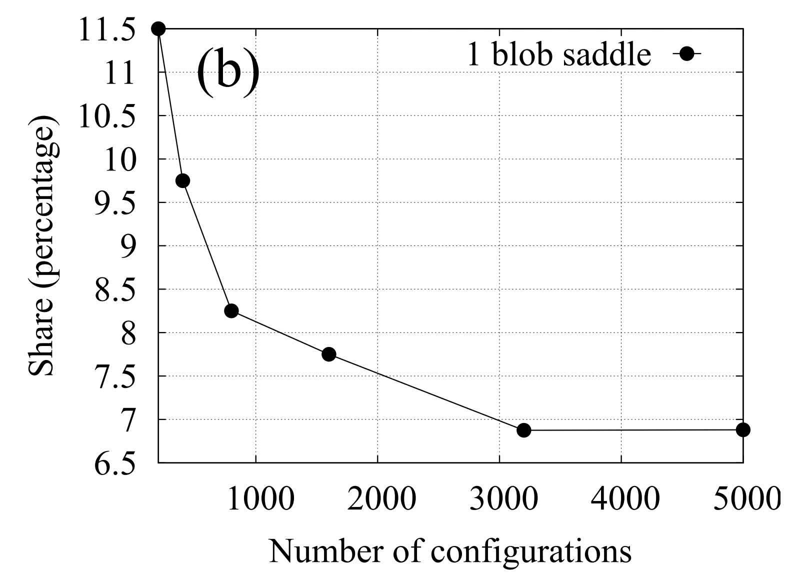
«seed» blocks for iterations - from Schur complement solver [arXiv 1803.05478]

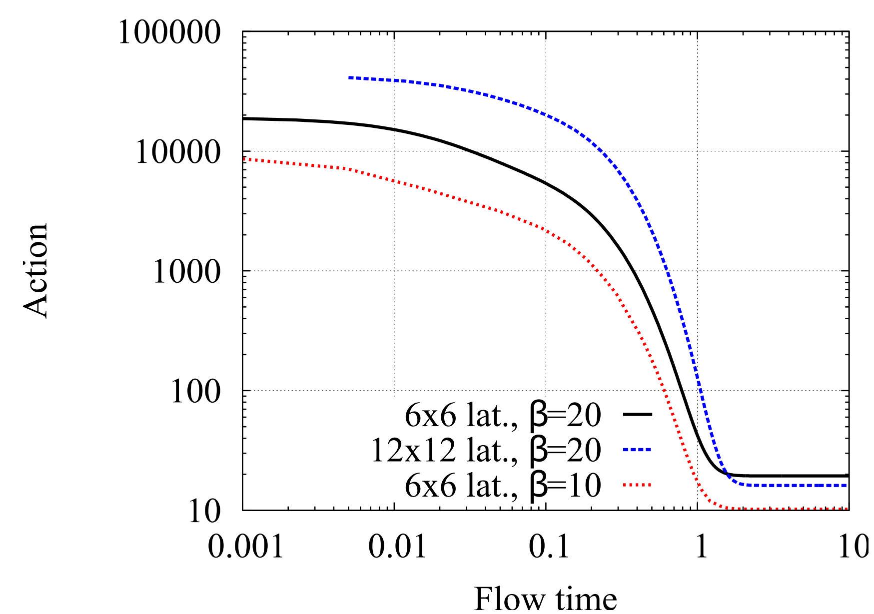
Recovering the saddle points from Hybrid Monte Carlo data

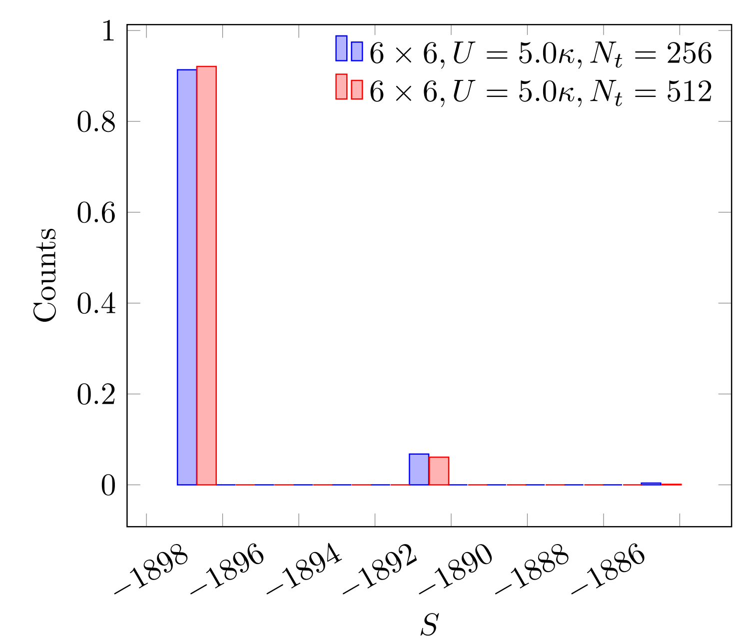


Final histogram shows $\frac{Z_6}{Z}$ shares



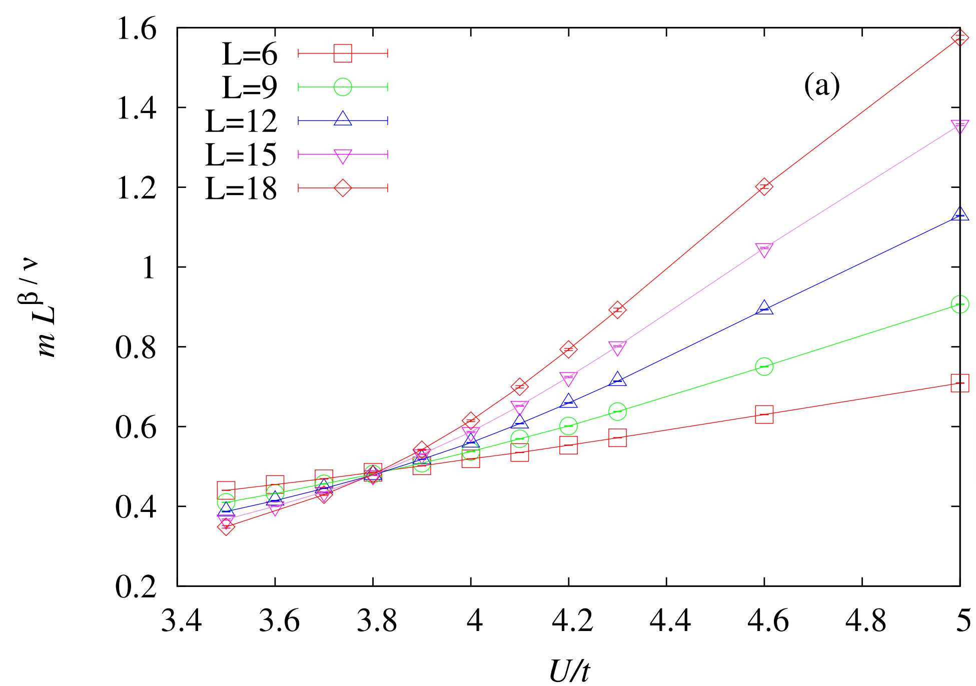






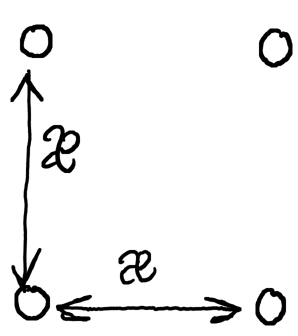
Hubbard model on bipartite lattice (1)

$$\hat{H} = -\kappa \sum_{\langle x,y\rangle,\sigma} (\hat{c}^{\dagger}_{x\sigma}\hat{c}_{y\sigma} + h.c.) + U \sum_{x} \hat{n}_{x\uparrow}\hat{n}_{x\downarrow} - \left(\frac{U}{2} - \mu\right) \sum_{x} (\hat{n}_{x\uparrow} + \hat{n}_{x\downarrow} - 1)$$

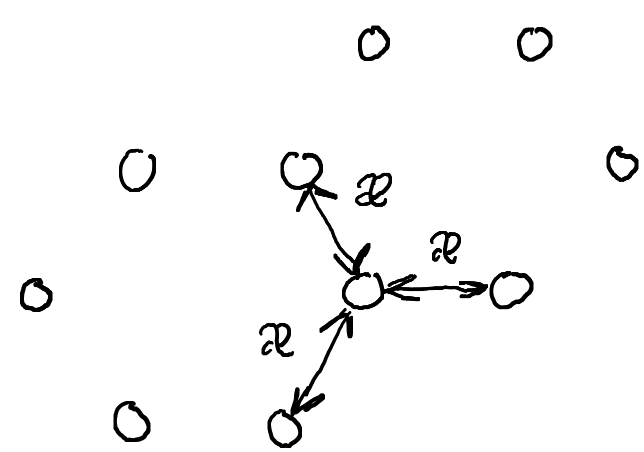


Semi-metal - AFM insulator transition at U=3.8 κ

F. Assaad, I. Herbut, PRX, 3, 031010 (2013)



Square lattice



Hexagonal lattice

Hubbard model on bipartite lattice (2)

$$\mathcal{Z} = \mathrm{Tr}\, e^{-\beta\hat{H}} \approx \mathrm{Tr}\left(e^{-\delta\hat{H}_{(2)}} e^{-\delta\hat{H}_{(4)}} e^{-\delta\hat{H}_{(2)}} e^{-\delta\hat{H}_{(4)}} \ldots\right)$$

Discrete auxiliary fields (BSS-QMC):

$$e^{-\delta U \hat{n}_\uparrow \hat{n}_\downarrow} = \frac{1}{2}\sum_{\nu=\pm 1} e^{2i\xi\nu(\hat{n}_\uparrow+\hat{n}_\downarrow-1)-\frac{1}{2}\delta U(\hat{n}_\uparrow+\hat{n}_\downarrow-1)}$$

$$\tan^2\xi = \tanh(\frac{\delta U}{4})$$

$$\mathcal{Z}_d = \sum_{\nu_{x,t}} \det D_{el.}(\nu_{x.t}) \det D_{h.}(\nu_{x,t})$$

$$D_{el.}(\nu_{x,t}) = I + \prod_{t=1}^{N_t}\left(e^{-\delta(h+\mu)} \mathrm{diag}\,\left(e^{2i\xi\nu_{x,t}}\right)\right)$$

$$D_{h.}(\nu_{x,t}) = I + \prod_{t=1}^{N_t}\left(e^{-\delta(h-\mu)} \mathrm{diag}\,\left(e^{-2i\xi\nu_{x,t}}\right)\right)$$

Continuous auxiliary fields:

$$\frac{U}{2}(\hat{n}_{el.}-\hat{n}_{h.})^2 = \frac{\alpha U}{2}(\hat{n}_{el.}-\hat{n}_{h.})^2 - \frac{(1-\alpha)U}{2}(\hat{n}_{el.}+\hat{n}_{h.})^2 + (1-\alpha)U(\hat{n}_{el.}+\hat{n}_{h.})$$

$$e^{-\frac{\delta}{2}\sum_{x,y} U_{x,y}\hat{n}_x\hat{n}_y} \cong \int D\phi_x e^{-\frac{1}{2\delta}\sum_{x,y}\phi_x U^{-1}_{xy}\phi_y} e^{i\sum_x \phi_x \hat{n}_x},$$

$$\boxed{\alpha = 0\ldots 1}$$

$$e^{\frac{\delta}{2}\sum_{x,y} U_{x,y}\hat{n}_x\hat{n}_y} \cong \int D\phi_x e^{-\frac{1}{2\delta}\sum_{x,y}\phi_x U^{-1}_{xy}\phi_y} e^{\sum_x \phi_x \hat{n}_x}$$

$$\mathcal{Z}_c = \int \mathcal{D}\phi_{x,\tau}\, \mathcal{D}\chi_{x,\tau}\, e^{-S_\alpha} \det M_{\mathrm{el.}} \det M_{\mathrm{h.}},$$

$$S_\alpha[\phi_{x,\tau},\chi_{x,\tau}] = \sum_{x,\tau}\left[\frac{\phi^2_{x,\tau}}{2\alpha\delta U} + \frac{(\chi_{x,\tau}-(1-\alpha)\delta U)^2}{2(1-\alpha)\delta U}\right]$$

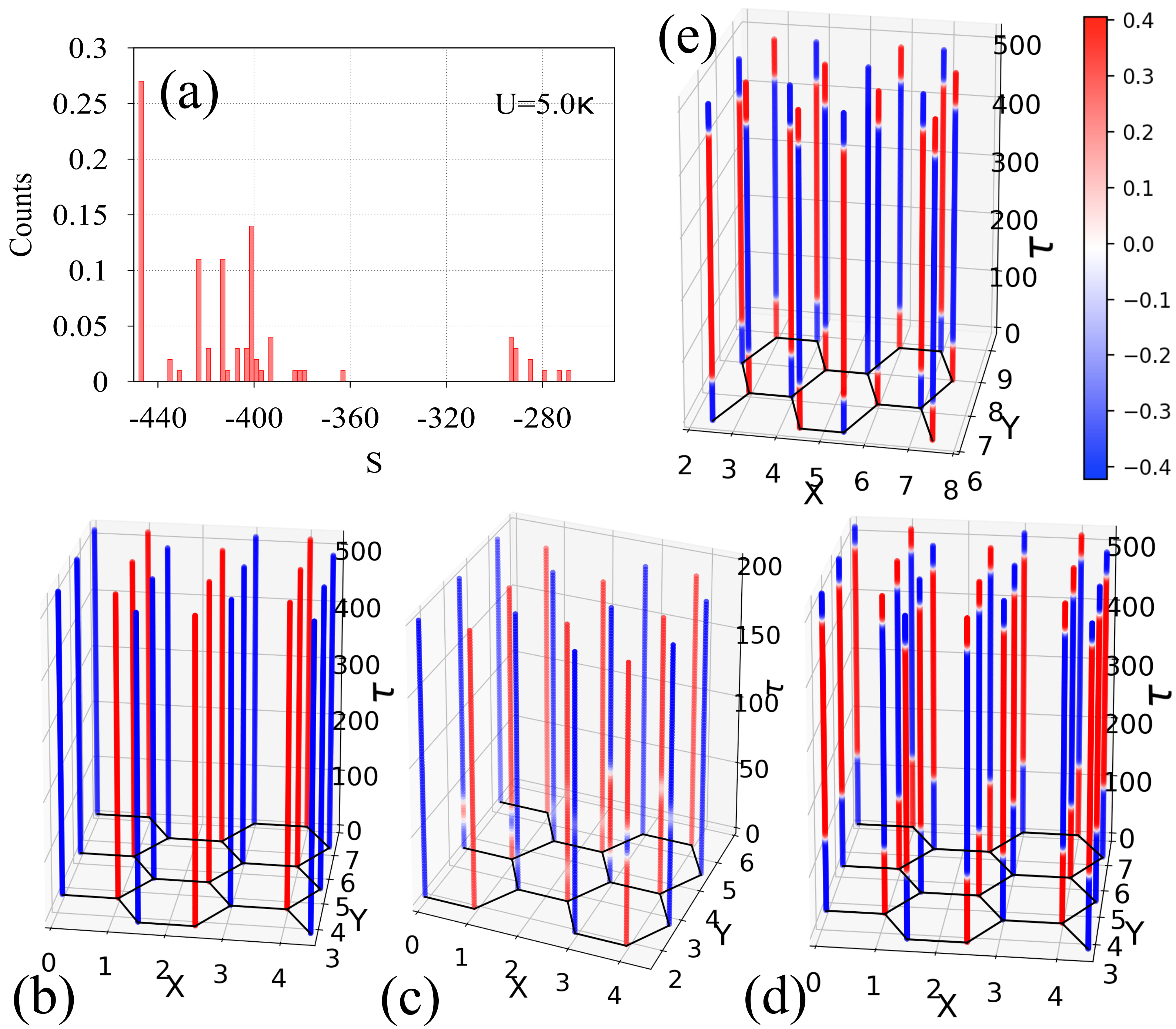
$$M_{\mathrm{el.,h.}} = I + \prod_{\tau=1}^{N_\tau}\left[e^{-\delta(h\pm\mu)} \mathrm{diag}\,\left(e^{\pm i\phi_{x,\tau}+\chi_{x,\tau}}\right)\right]$$

Fierz identities:

$$\delta^a_b\delta^c_d = \frac{1}{2}\delta^a_d\delta^c_b + \frac{1}{2}\sum_i \sigma^{(i)}{}^a_d \sigma^{(i)}{}^c_b$$

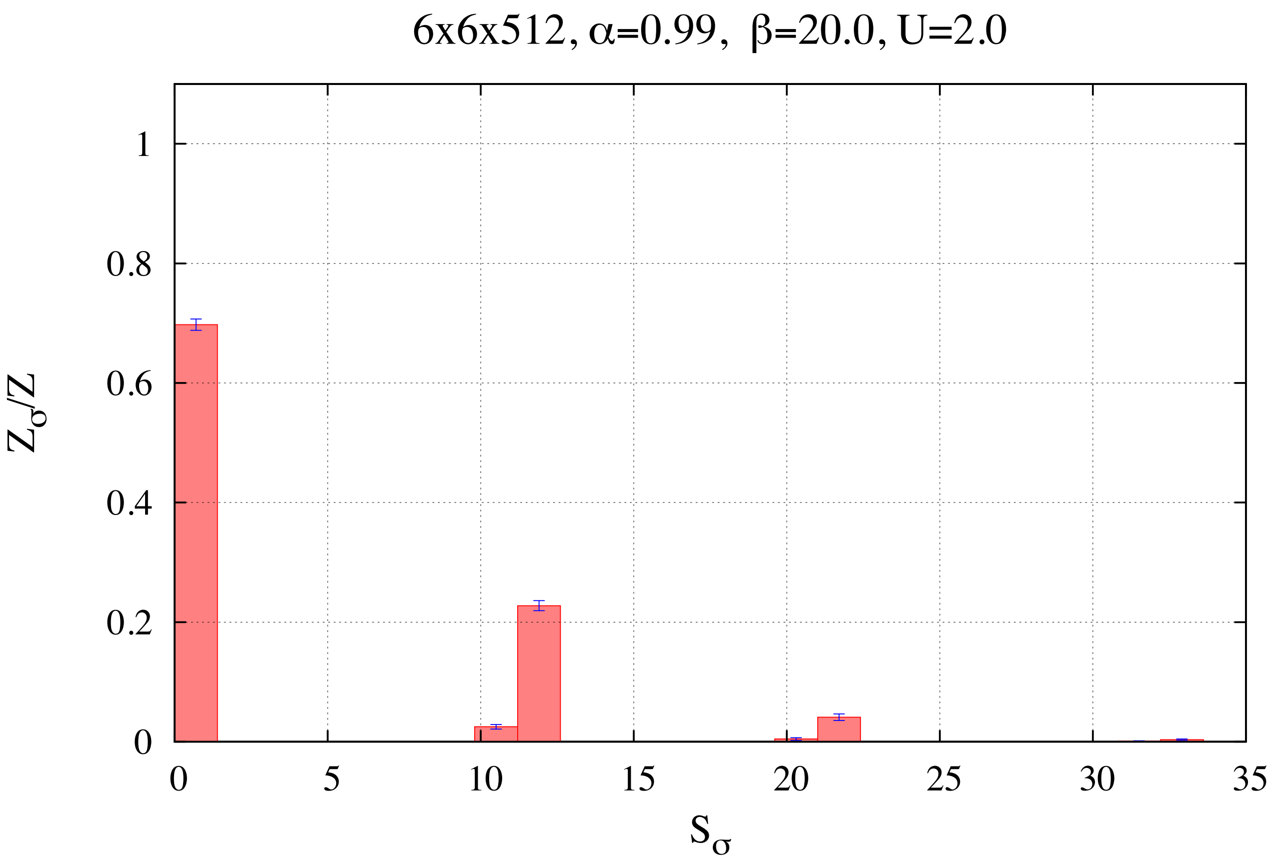
$$(\bar{a}O_i b)\left(\bar{c}O^i d\right) = \sum_k C_{ik}\left(\bar{a}O_k d\right)\left(\bar{c}O^k b\right)$$

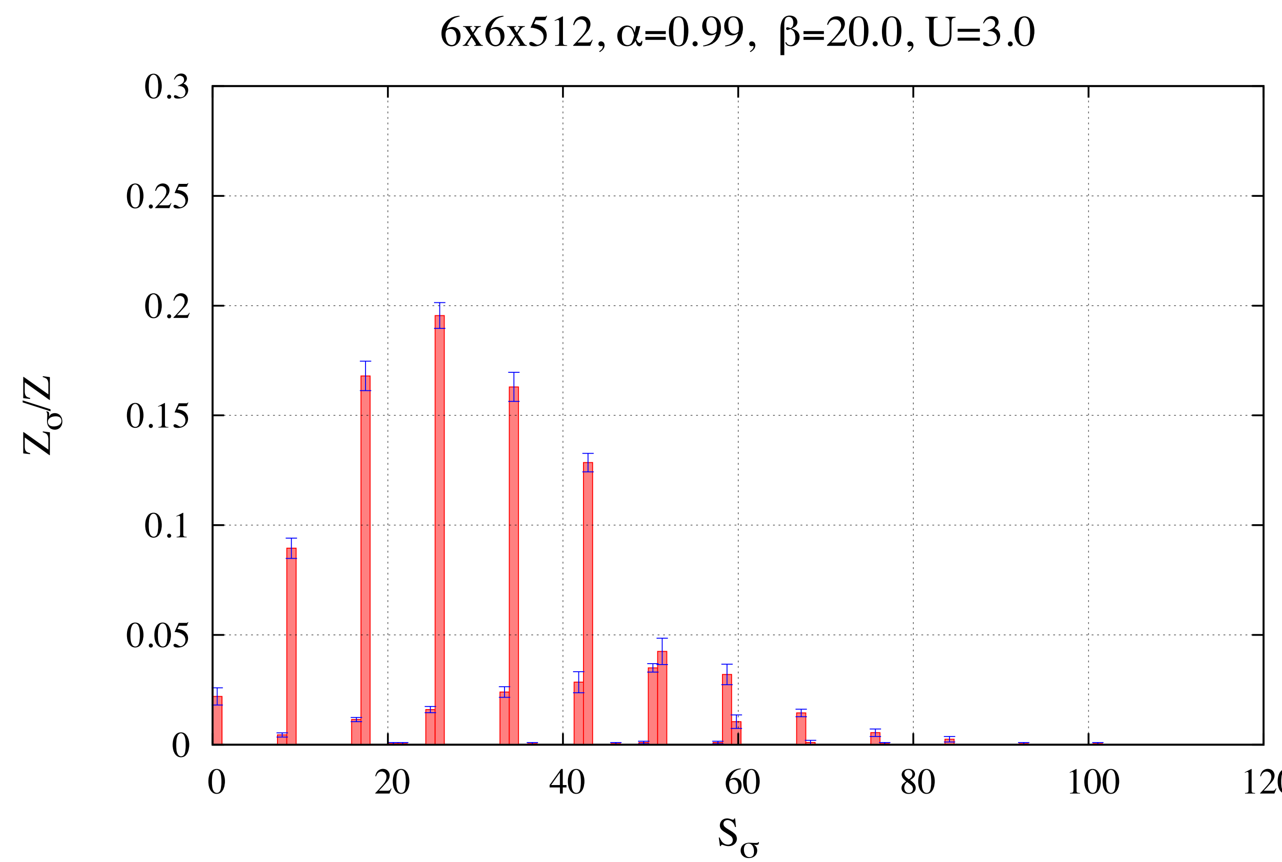
Examples of the thimbles decomposition for the Hubbard model on hexagonal lattice(2)

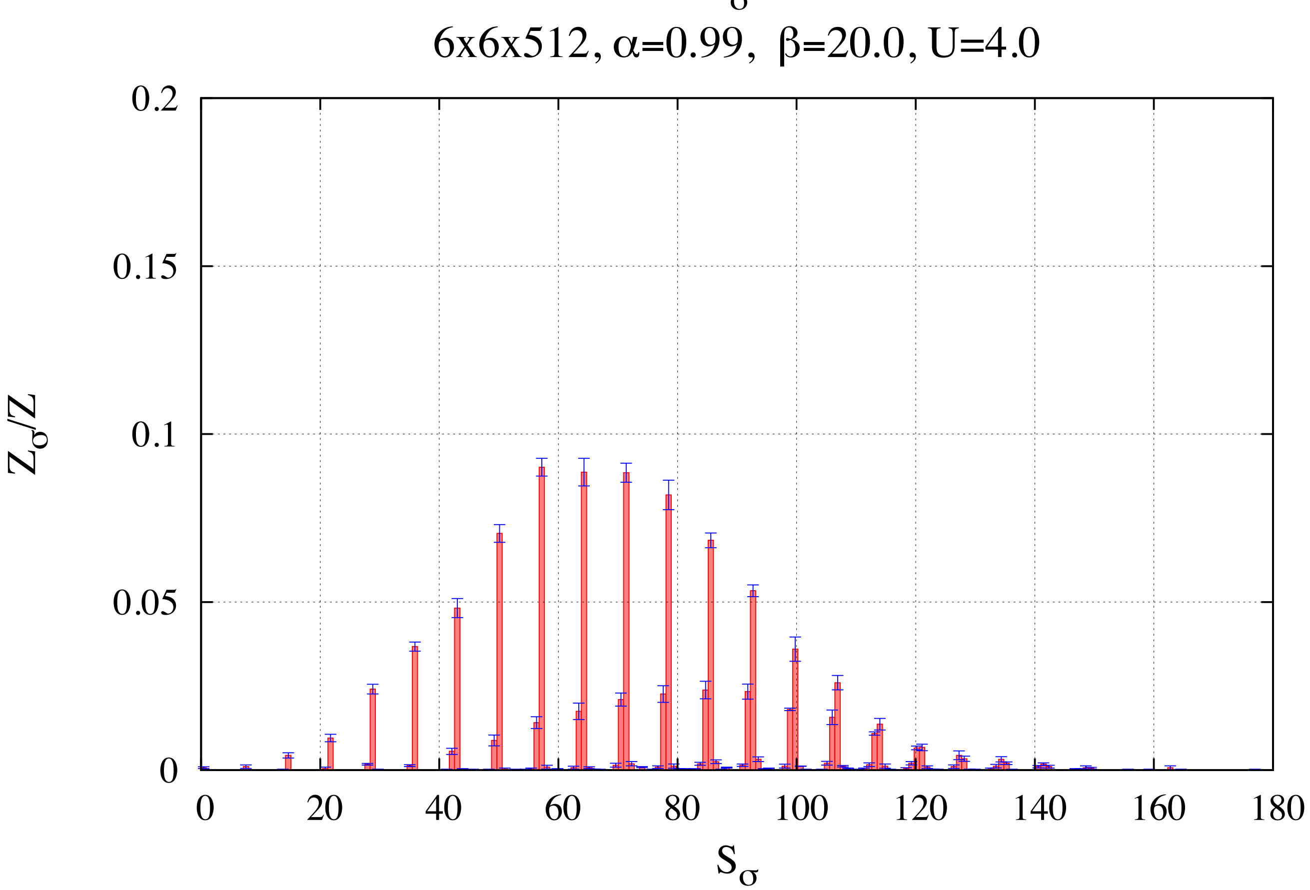


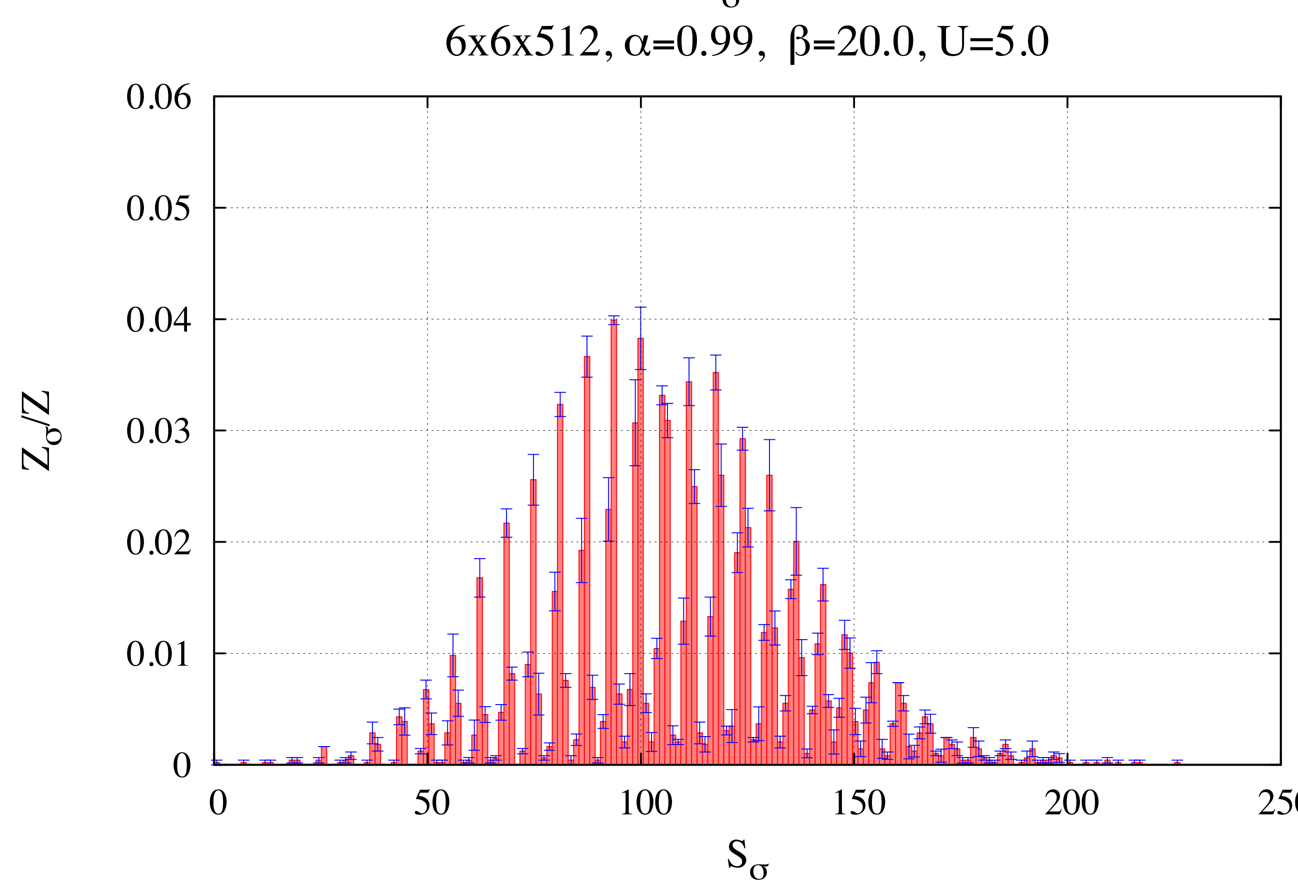
Spin-coupled auxiliary field

Examples of the thimbles decomposition for the Hubbard model on hexagonal lattice(2)



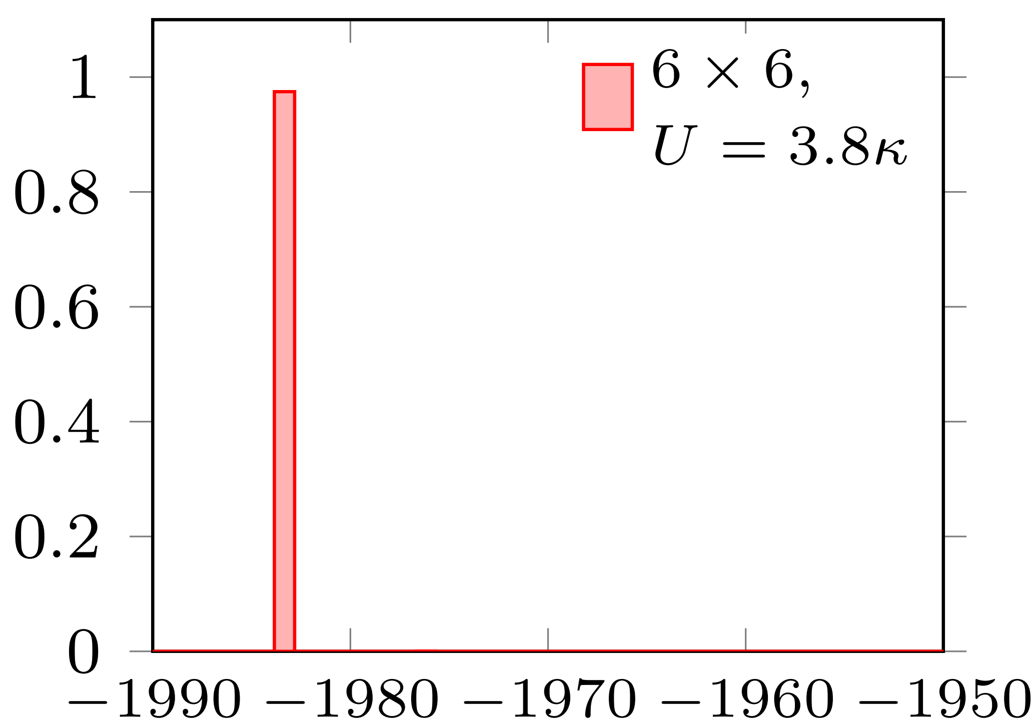


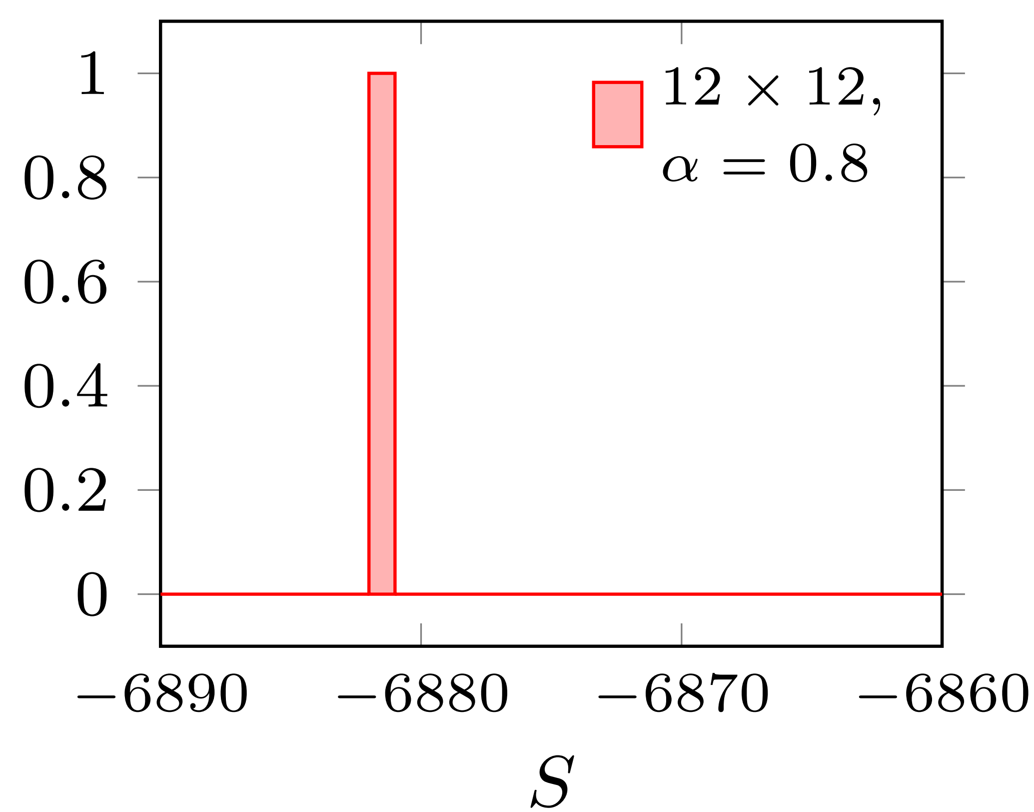




Examples of the thimbles decomposition for the Hubbard model on hexagonal lattice(2)

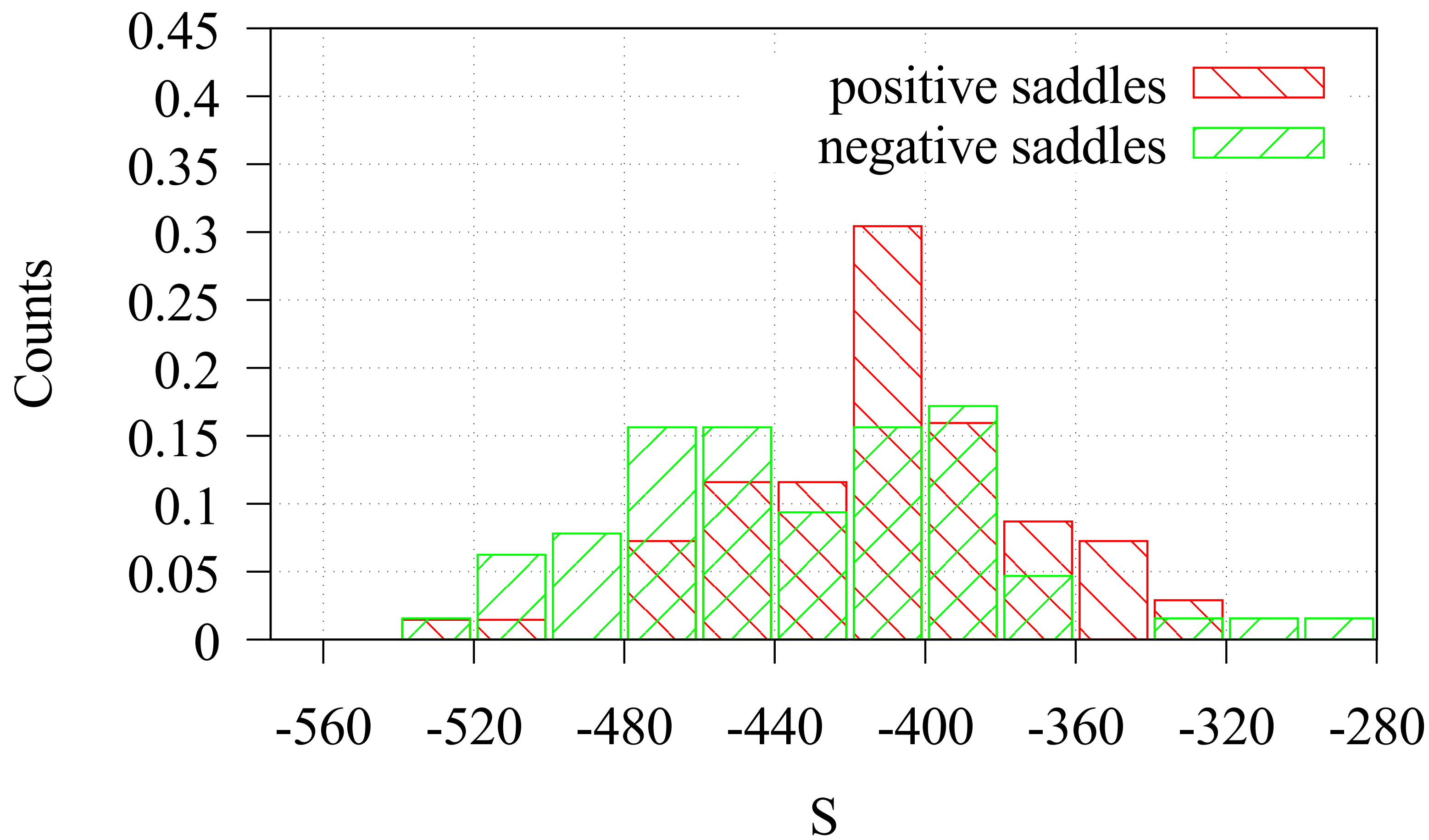
Mixed regime: both field are present. One-thimble regime possible even at strong coupling.





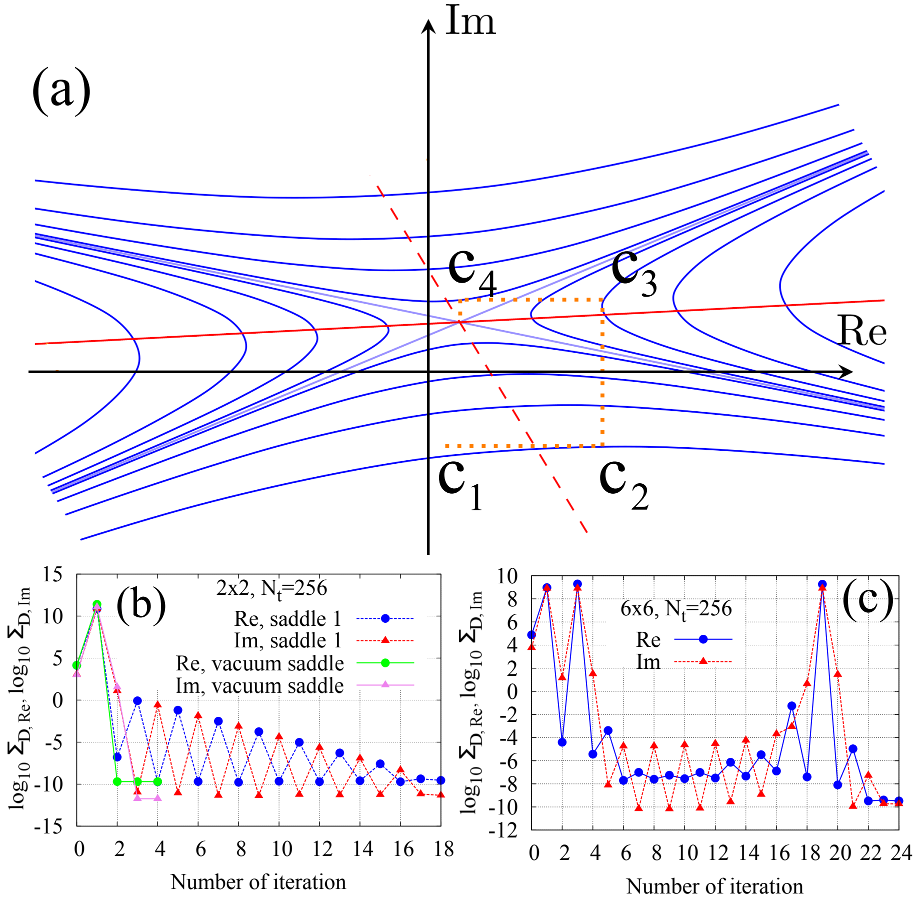
It means that we can use unphysical degrees of freedom in the path integral representation to optimize the structure of thimbles decomposition.

Connection to the sign problem(1)

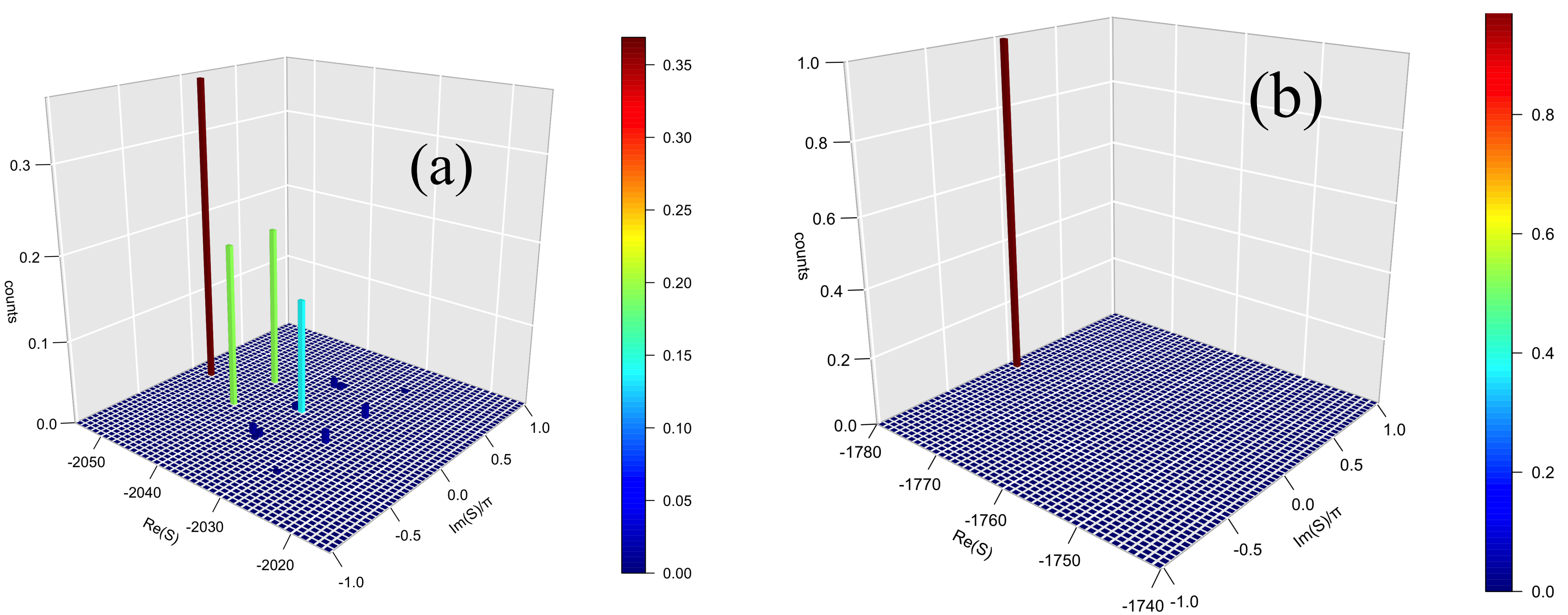


Spin-coupled field: only real saddle points (due to fermionic determinant being real)

Connection to the sign problem(2)



Mixed case (both charge- and spin-coupled fields): complex saddle points.
a) general scheme of the search algorithm; b) c) examples of iterations



a) α=0.9;
b) α=0.8

Summary(1)

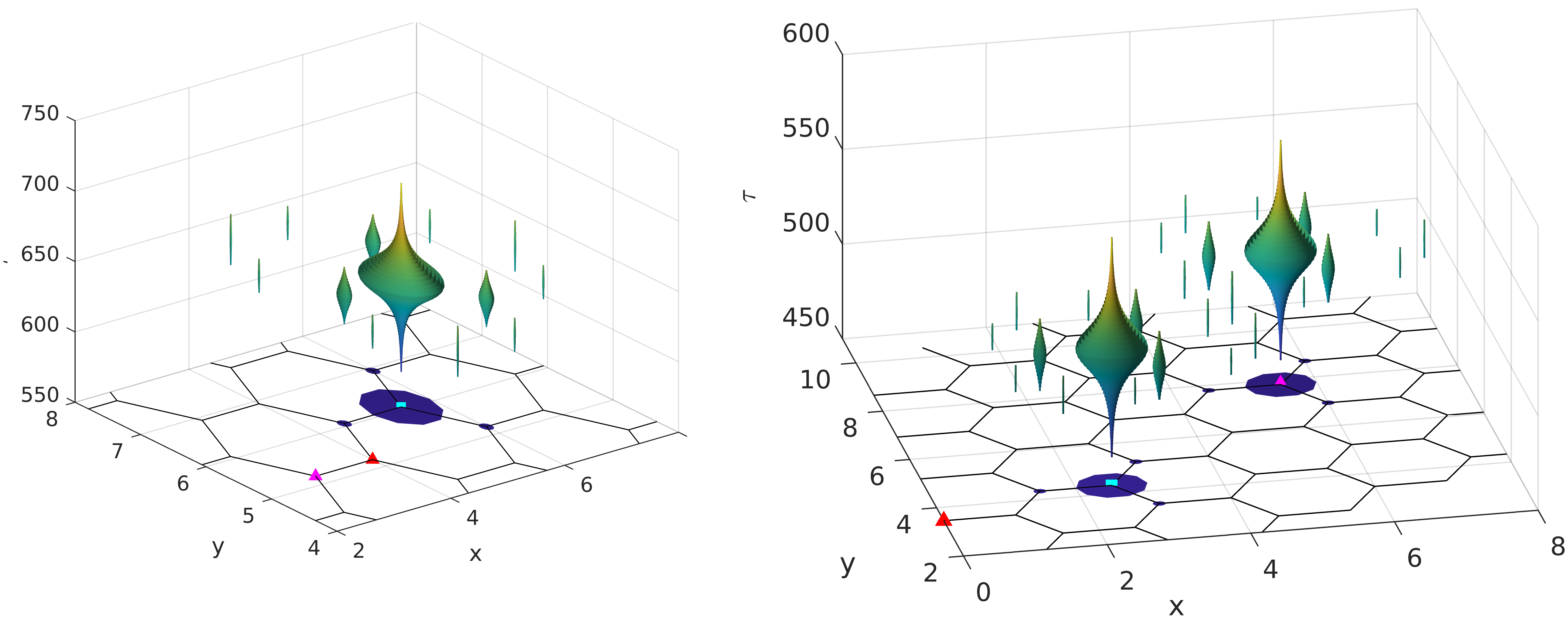
Using non-iterative solvers we can compute exact derivatives of the fermonic determinant with respect to bosonic fields. It allows us to solve the gradient flow equations for relatively large lattices taking into account the fermonic back reaction on bosonic fields.

Thus, we can find both real and complex saddle points and describe the structure of the thimbles decomposition approaching thermodynamic limit.

Using this information we can optimize the structure of the thimbles decomposition, which is actually formulation-dependent.
In particular, we demonstrated that at least in one example of strongly correlated model with lattice fermions, we can find the representation where only one thimble survives in thermodynamic limit even at the phase transition or in the strong coupling regime.

TODO algorithms for sampling following curved manifolds in complex space

Instantons for charge-coupled auxiliary field



Saddle point field configurations are localised both in space and Euclidean time, hence many-instanton saddles are equidistant in action

Analytical description of instantons with fermonic back reaction (1)

$$S = \frac{\sum_{x,\tau} (\varphi_x^\tau)^2}{2U\Delta\tau} - \ln\det\left(I + \prod_\tau e^{-\Delta\tau H}\{e^{i\varphi_x^\tau}\}\right) - \ln\det\left(I + \prod_\tau e^{-\Delta\tau H}\{e^{-i\varphi_x^\tau}\}\right)$$

$$\frac{\partial S}{\partial \varphi_x^\tau} = \frac{\varphi_x^\tau}{U\Delta\tau} - \left[\bar{g}_{xx}^\tau i e^{i\varphi_x^\tau} - i(\bar{g}_{xx}^\tau)^* e^{-i\varphi_x^\tau}\right] = 0$$

(saddle point)

$\Rightarrow$ we need to add equations for $\bar{g}_{xx}^\tau$ to close the system:

$$\bar{g}^{\tau+1} = \{e^{-i\varphi_x^{\tau+1}}\} e^{\Delta\tau H} \bar{g}^\tau \{e^{i\varphi_x^\tau}\} e^{-\Delta\tau H}$$

$$\Rightarrow \varphi_x^\tau = -U \,\mathrm{Im}\, \bar{g}_{xx}^\tau$$

Analytical description of instantons with fermonic back reaction (2)

Final system of equations for propagator in continuous time:

$$\boxed{\varphi_x^\tau = -U\,\mathrm{Im}\,\bar{g}^\tau_{xx}}$$

$$\begin{cases} \dot{\bar{g}}_{xx}(\tau) = -\varkappa \sum\limits_{\langle x,y\rangle} \left(\bar{g}_{xy} - \bar{g}_{yx}\right) \\ \dot{\bar{g}}_{xy}(\tau) = iU\,\bar{g}_{xy}\left(\mathrm{Im}\,\bar{g}_{xx} - \mathrm{Im}\,\bar{g}_{yy}\right) - \varkappa\left(\sum\limits_{\langle z_1,y\rangle} \bar{g}_{xz_1} - \sum\limits_{\langle z_2,x\rangle} \bar{g}_{z_2 y}\right) \end{cases}$$

Same equations can be obtained from

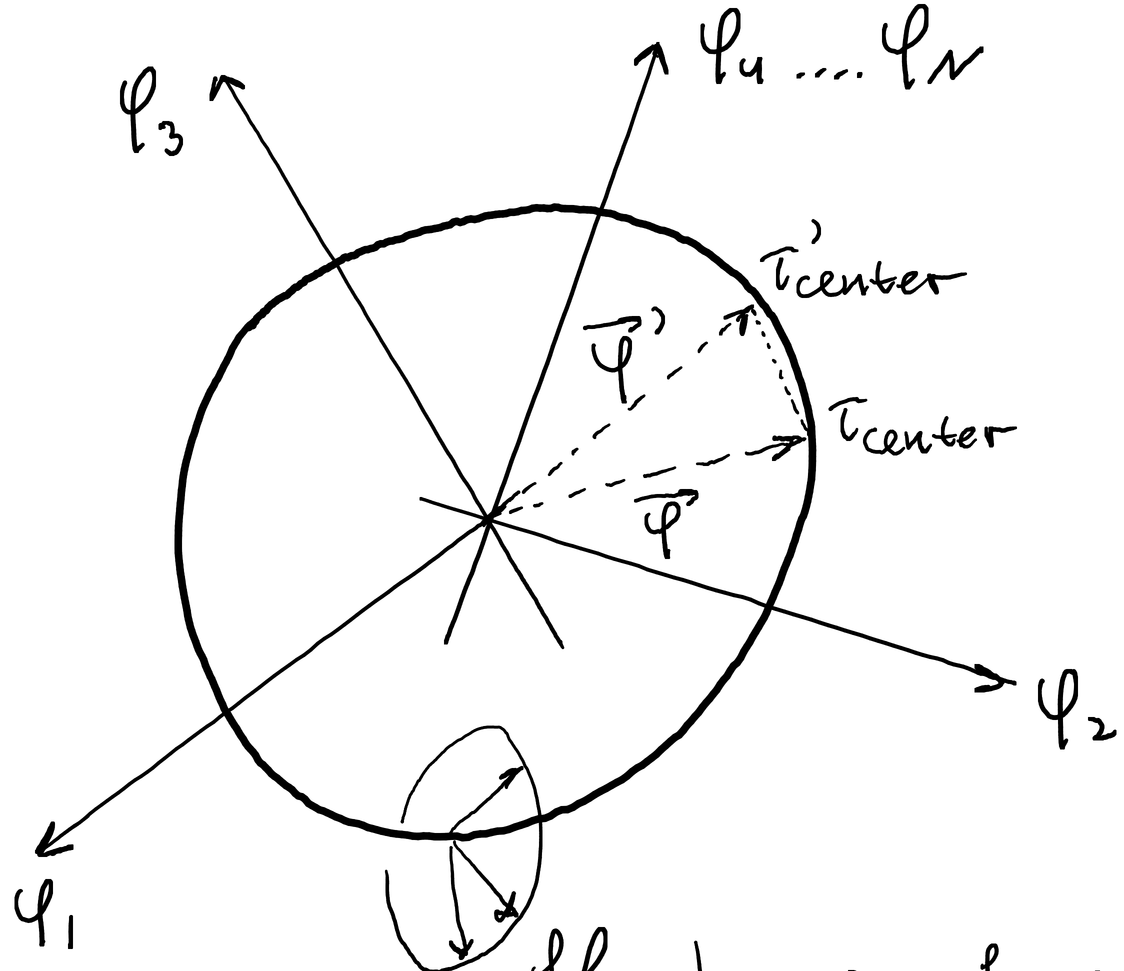
$$\frac{d\hat{A}}{d\tau} = [\hat{H}, \hat{A}]; \quad \hat{A} = \hat{a}^+_x a_y; \quad \hat{b}^+_x b_y; \text{ etc.}$$

$$\begin{cases} \dfrac{d(\hat{a}^+_x \hat{a}_x)}{d\tau} = -\varkappa \sum\limits_{x,y} \left(\hat{a}^+_y \hat{a}_x - \hat{a}^+_x \hat{a}_y\right) \\ \dfrac{d(\hat{a}^+_x \hat{a}_y)}{d\tau} = U\,\hat{a}^+_y \hat{a}_x \left(\hat{b}^+_x \hat{b}_x - \hat{b}^+_y b_y\right) - \varkappa\left(\sum\limits_{\langle z_1,y\rangle} \hat{a}^+_{z_1} \hat{a}_x - \sum\limits_{\langle z_2, x\rangle} \hat{a}^+_y \hat{a}_{z_2}\right) \end{cases}$$

Mean field approximation: $\langle \hat{a}^+_x \hat{a}_y \hat{b}_x \hat{b}_x \rangle = g_{xy}\, g^*_{yy}$

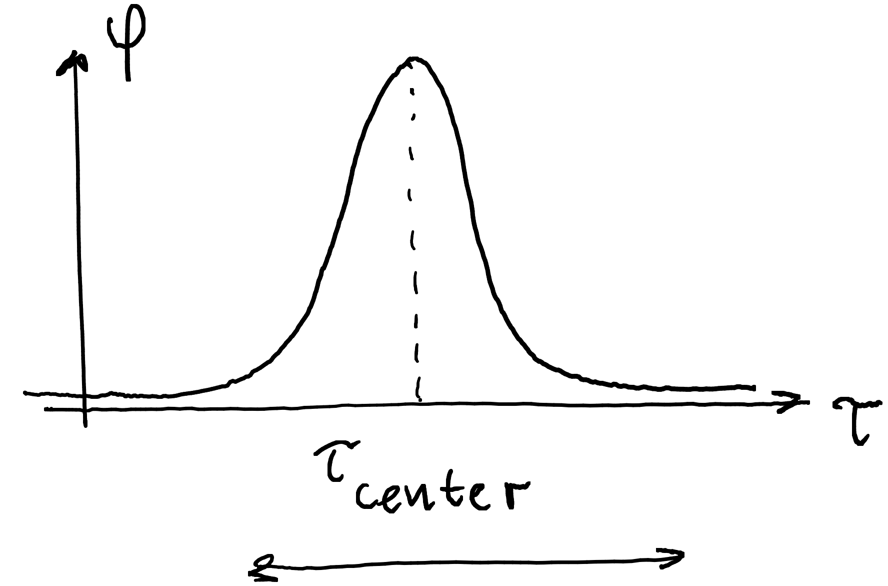
Hessians and continuum limit

Degenerate saddle:



$\mathcal{H}_\perp$ - hessian for fluctuations in perpendicular directions

det $\mathcal{H}_\perp$ is dependent on $\Delta\tau$



continuous symmetry: zero mode in hessian $\mathcal{H}$

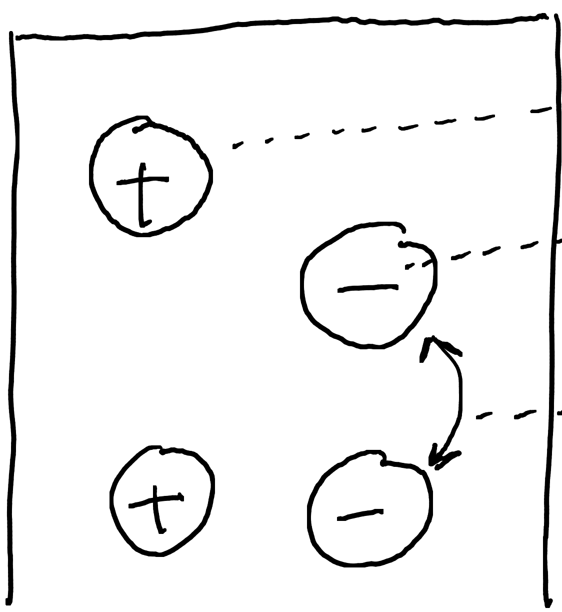
$$L = N_\tau \left| \vec{\varphi}(\tau_c) - \vec{\varphi}(\tau_c + 1) \right| \Rightarrow$$

dependent on $\Delta\tau$

However: $\boxed{L\left(\det \mathcal{H}_\perp\right)^{-1/2}}$ is $\Delta\tau$-independent

Simple analytic partition function for non-interacting instantons (1)

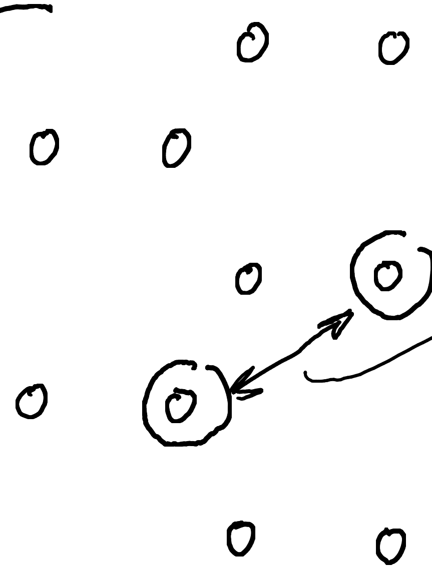
All N-instanton saddle points + gaussian fluctuations around them.



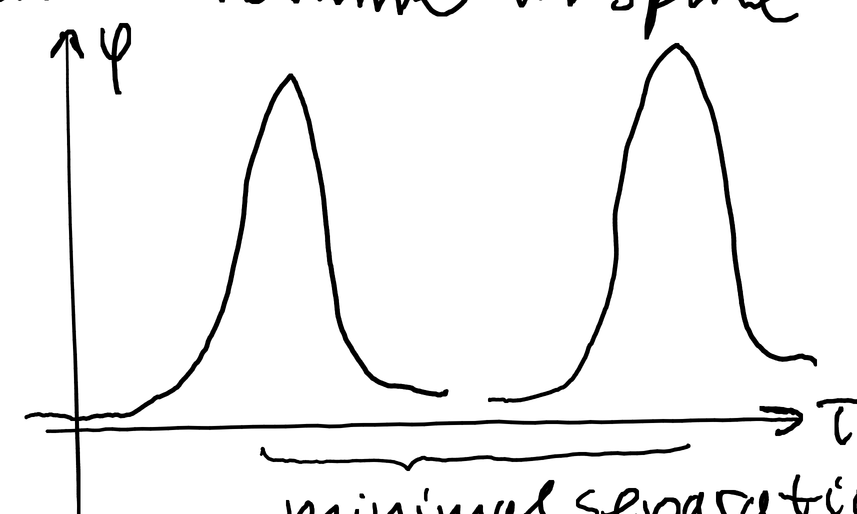
→ instanton

→ anti-instanton

→ can not occupy the same volume in space and Euclidean time:



minimal separation in space (~1)



minimal separation in time (~width of instanton)

Simple analytic partition function for non-interacting instantons (2)

$$\frac{Z}{Z_0} = 1 + \sum_{K=1}^{K_{max}} \frac{1}{K!} \underbrace{\beta N_s \left(\beta N_s - \Delta\beta X\right) \dots \left(\beta N_s - (K-1)\Delta\beta X\right)}_{\text{Volume factors}} \times$$

Z_0 → vacuum

$K!$ → equivalence of instantons

$$\times\, 2^{2K}\, e^{-S_0 K} \left(\left(\frac{\det \mathcal{H}_0}{2\pi \det \mathcal{H}_\perp} \right)^{\frac{1}{2}} \frac{L}{\beta} \right)^{K}$$

S_0: quantum of action

L → length of orbit in configuration space

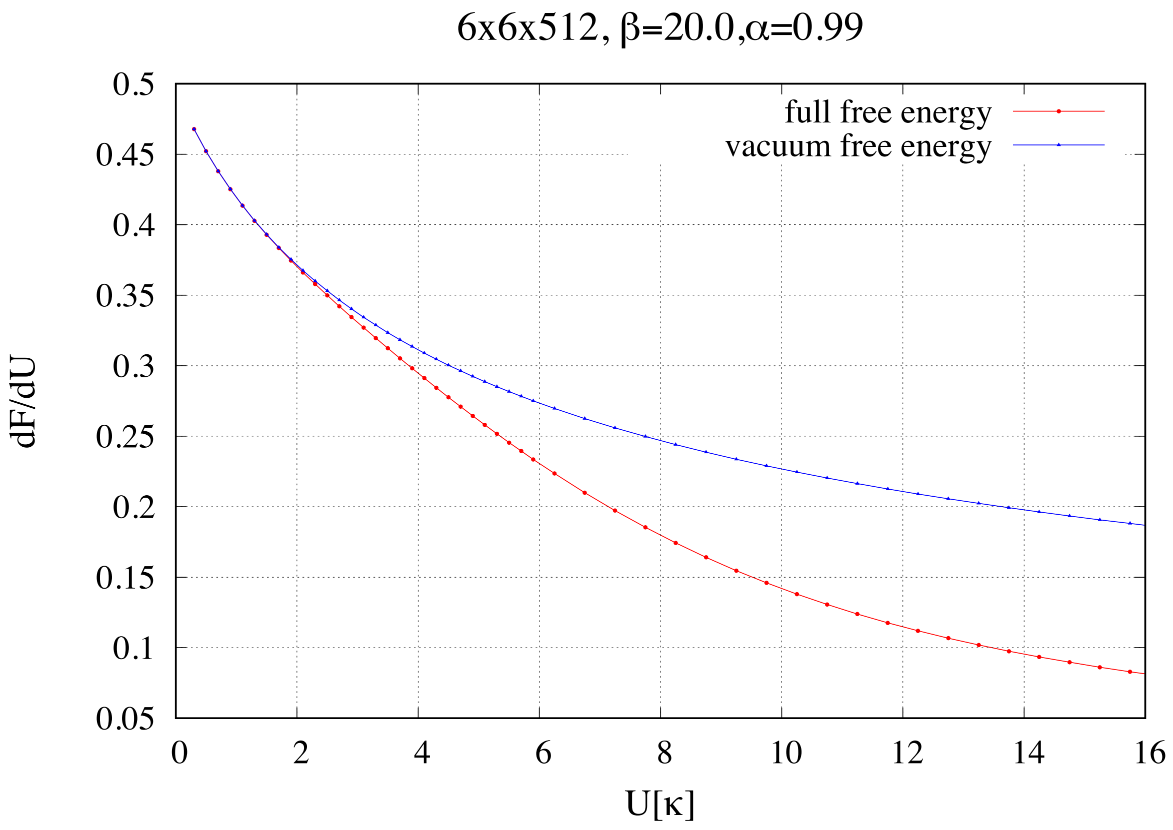
2^{2K} → combinatorial factor: Sublattice + (instanton-anti-instanton)

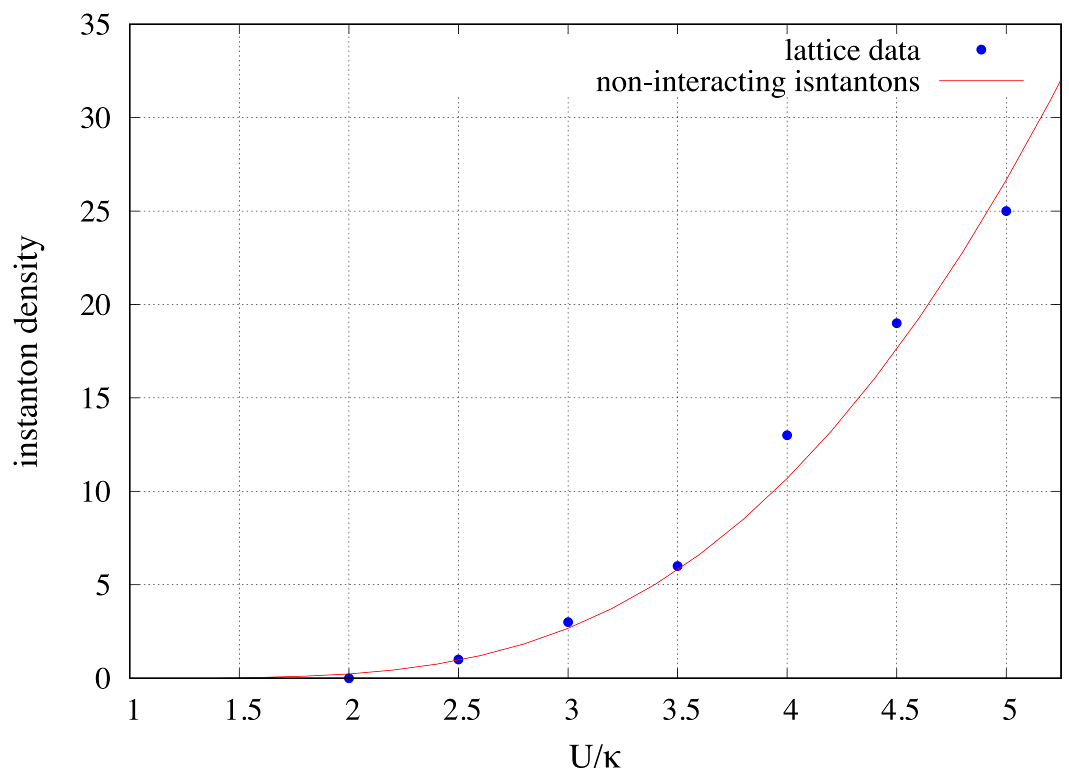
$$K_{max} \cong \frac{\beta}{\Delta\beta} \frac{N_s}{X}$$

$$\Rightarrow f = f_0 - \frac{1}{\Delta\beta X} \ln\left(1 + \frac{4 e^{-S_0} \Delta\beta X L}{\beta \sqrt{\det \mathcal{H}_\perp \det \mathcal{H}_0 \cdot 2\pi}}\right)$$

f_0 → vacuum

Double occupancy from non-interacting instantons model

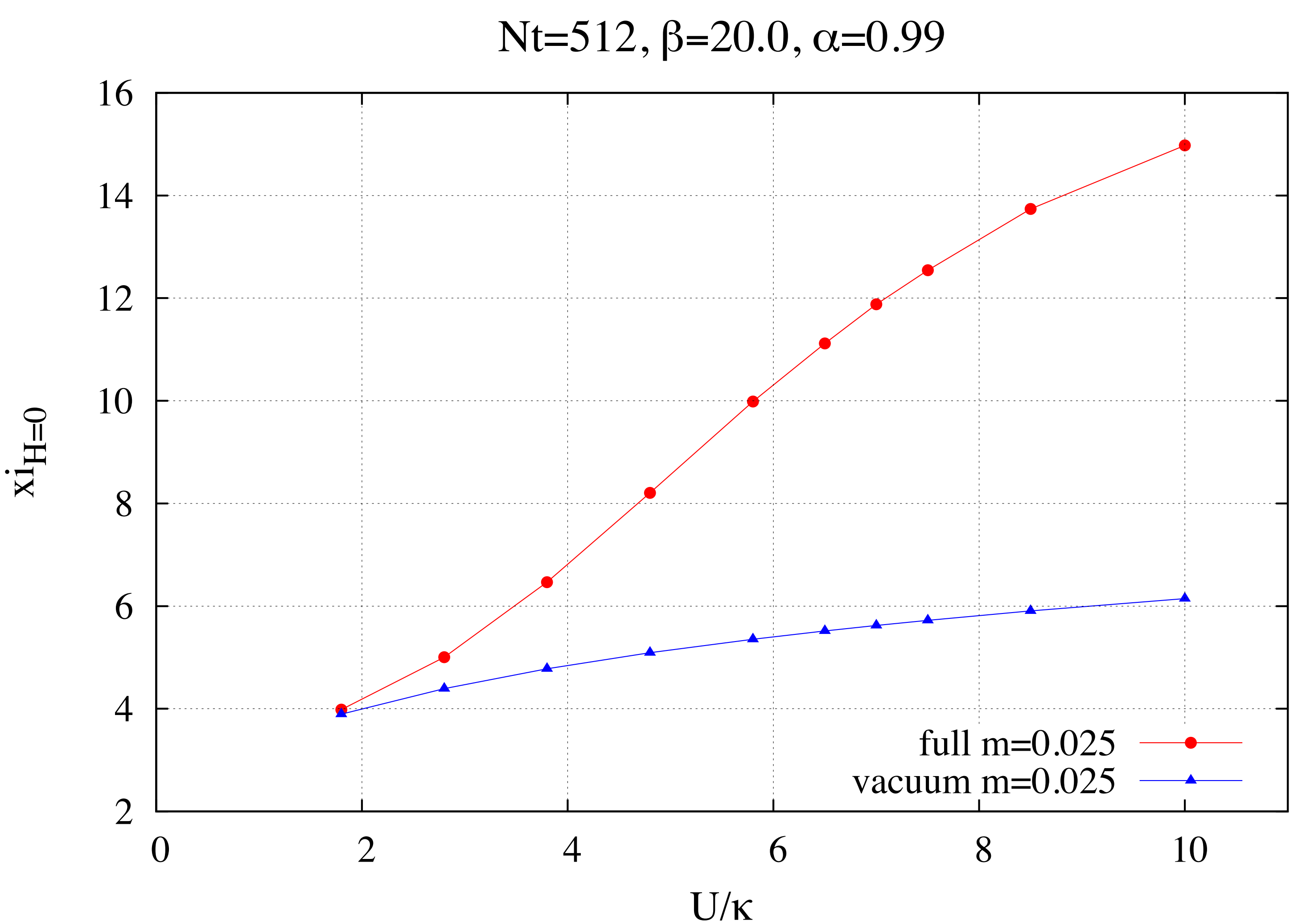




Double occupancy as the derivative of the free energy over U

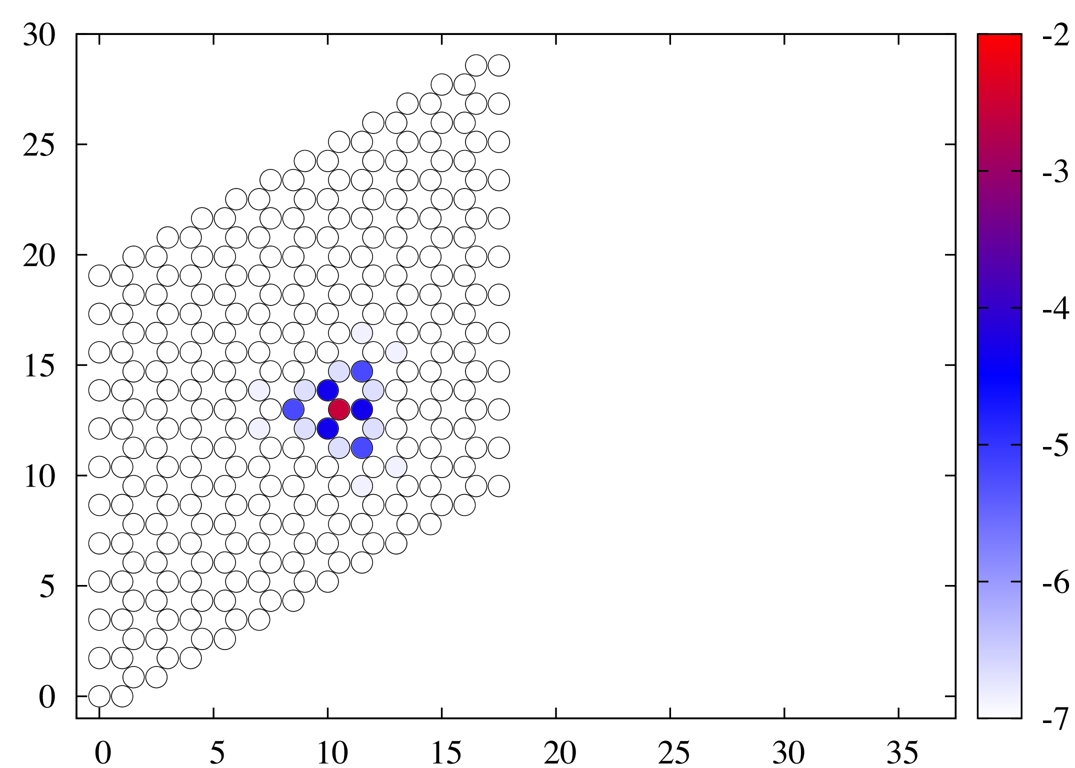
Benchmark: density of instantons

AFM susceptibility from non-interacting instantons model



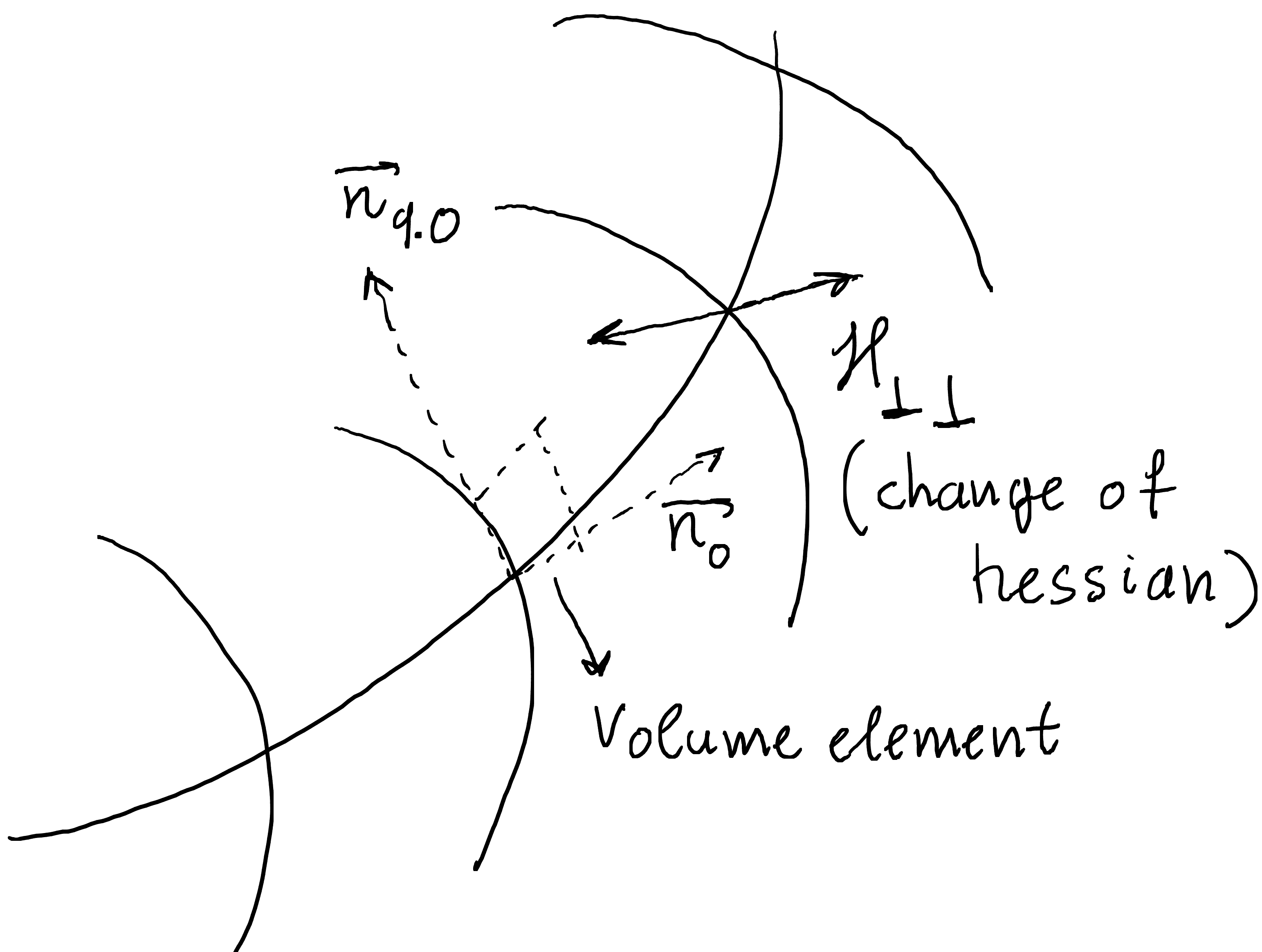
Magnetic susceptibility doesn't diverge at any point: no description of the phase transition (AFM spin ordering)

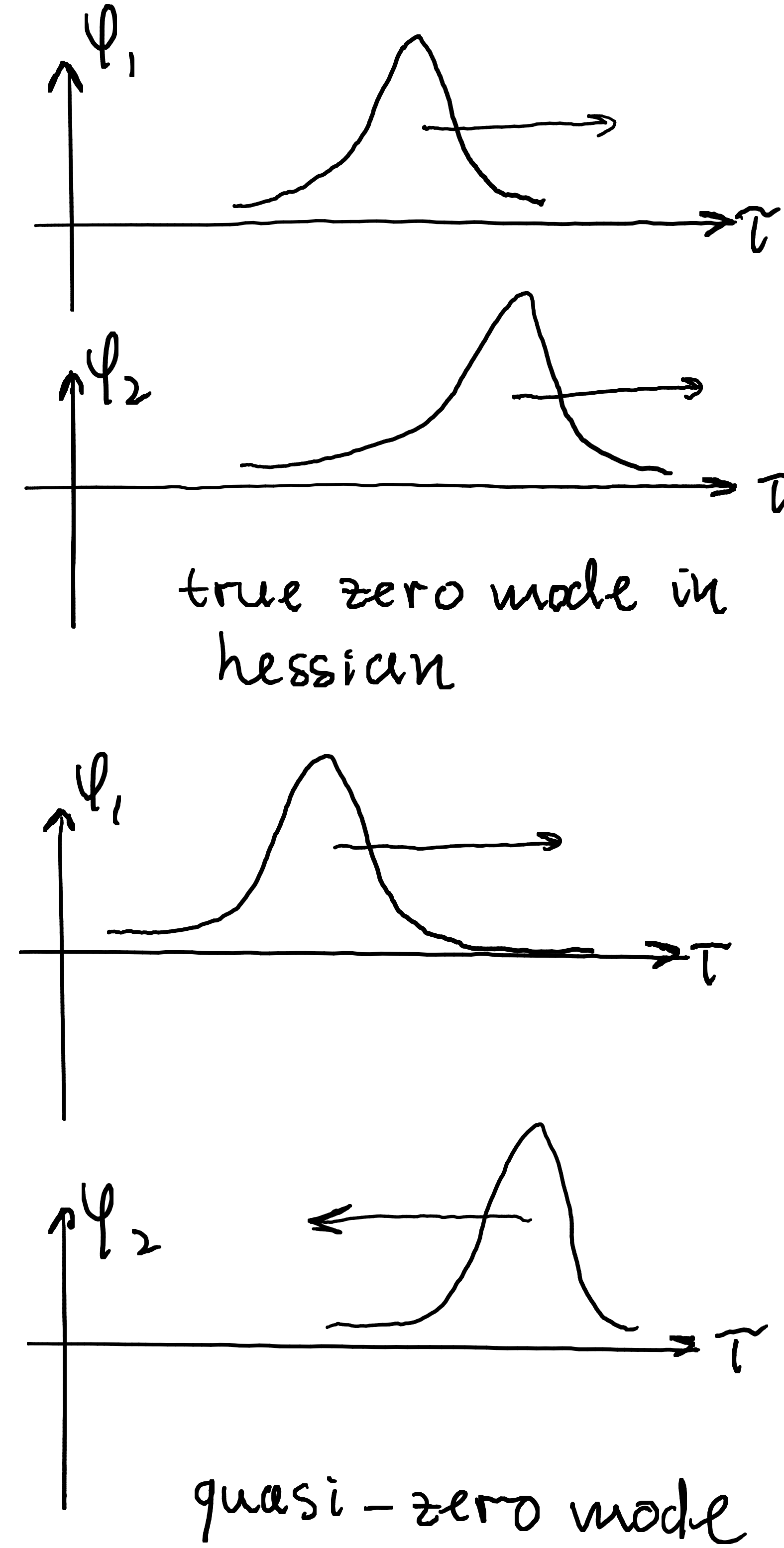
We really described spin localization, but local spins are still in paramagnetic phase



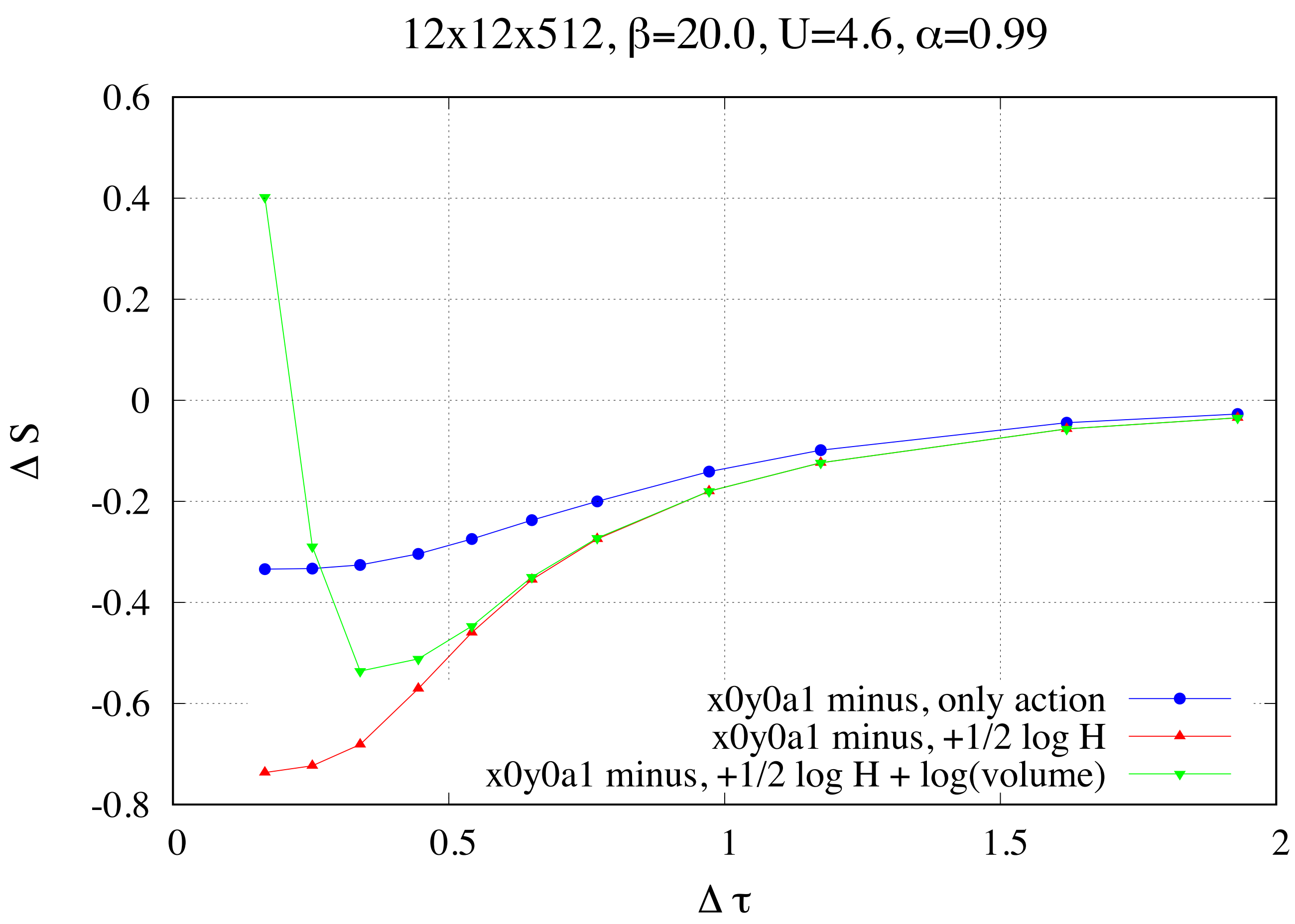
Interaction of instantons: various factors

1) change of action
2) change of Hessian
3) change of volume element

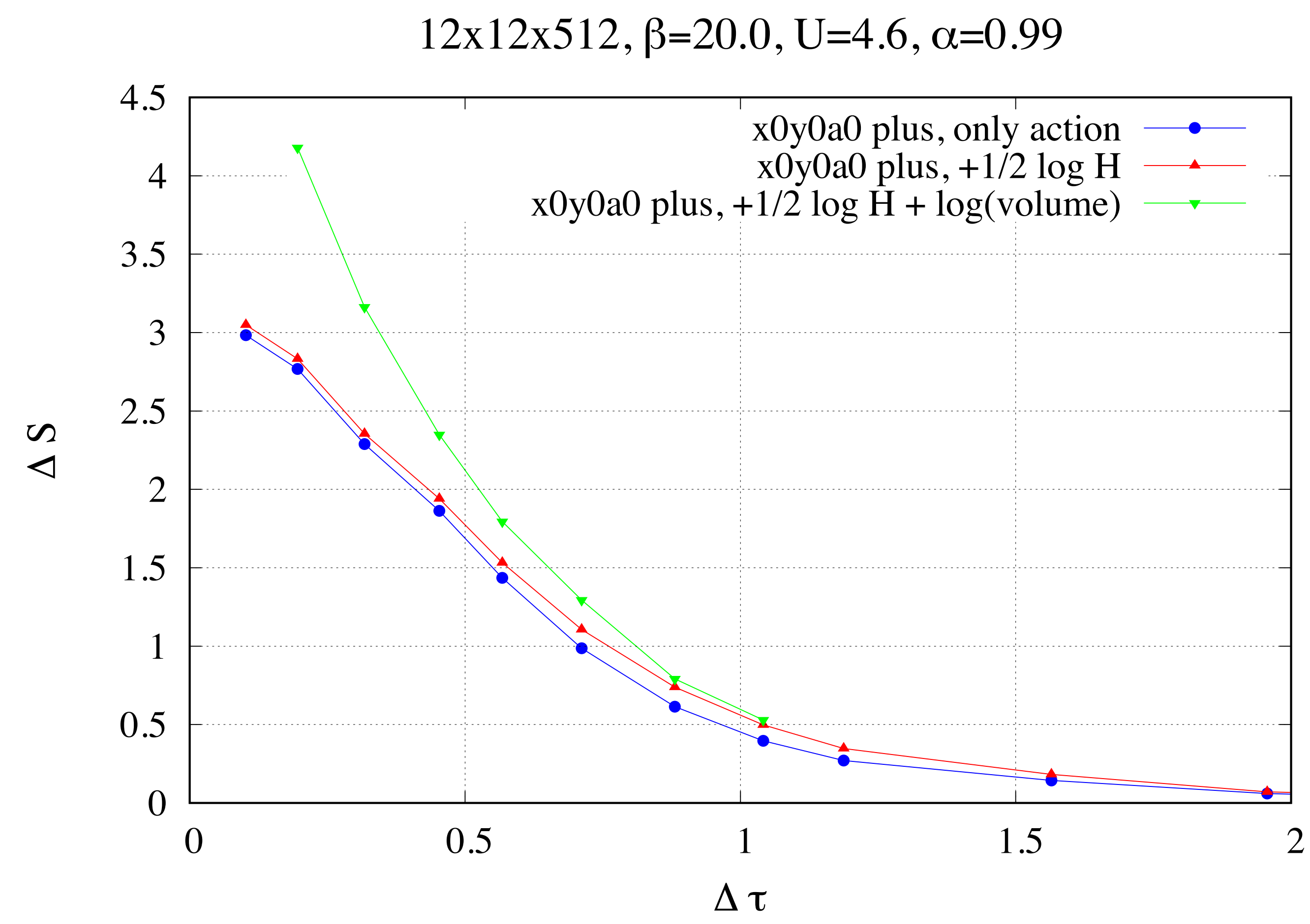




Example of interaction curves



Instanton and anti-instanton at nearest-neighbour lattice sites



Two instantons at the same lattice site

Summary (2)

The solution of gradient flow equations with fermions provided us with knowledge on both real and complex saddle points of the full action. This information can be used to construct quasi-classical approximation on the basis of saddle points field configurations and gaussian fluctuations around them.

Here we present example of such study for Hubbard model, where the detailed knowledge on the saddle points leads to the formulation of instantons gas model with either interacting or non-interacting instantons. Even simple non-interacting model already features at least some important properties of the initial quantum Hamiltonian: spin localization and growth of magnetic susceptibility. Since the saddle points do not change qualitatively away of half-filling, we can try to expand this model to non-zero chemical potential, where QMC doesn't work due to the sign problem.

Further directions: many-body interaction of instantons, tunnelling between different instanton sectors, another lattice models (QCD?)