Lefschetz thimbles approach for 2+1D Hubbard model: study of saddle points and benchmark calculations

arXiv: 1906.02726, 1906.07678, 1712.02188

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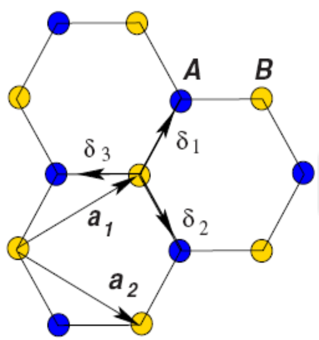
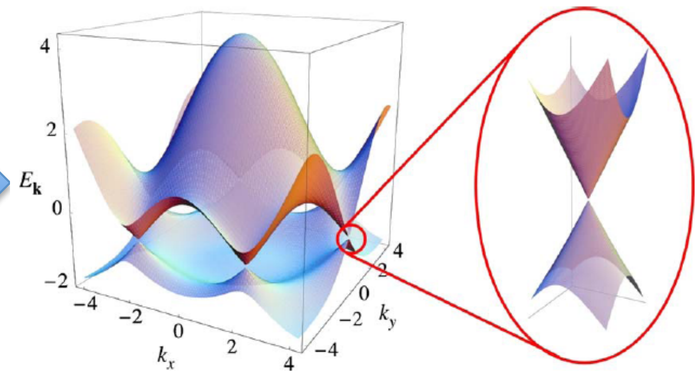
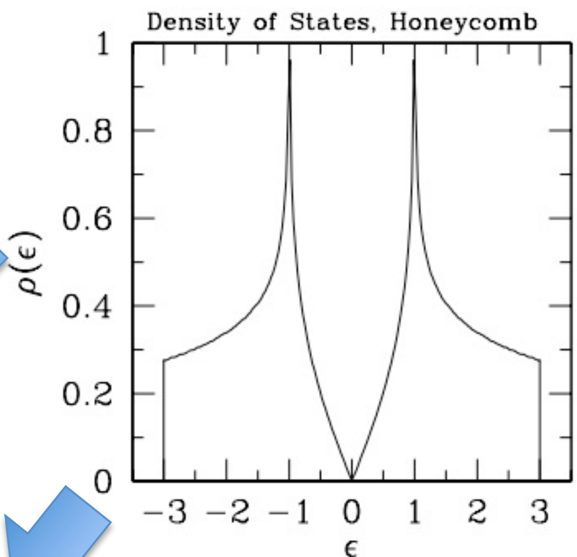
Hubbard model on hexagonal lattice

Nearest-neighbor hoppings + local interaction:

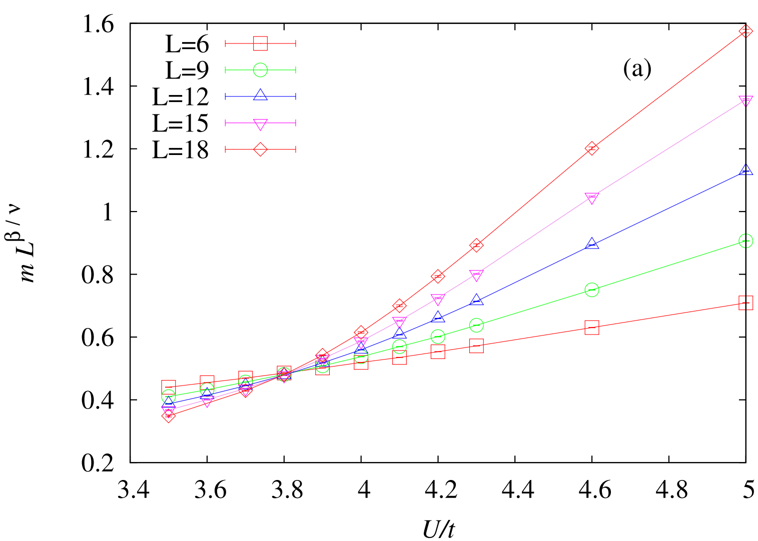
$$\hat{H} = -\kappa \sum_{\langle x,y\rangle,\sigma} (\hat{c}^{\dagger}_{x\sigma}\hat{c}_{y\sigma} + h.c.) + U \sum_{x} \hat{n}_{x\uparrow}\hat{n}_{x\downarrow} - \left(\frac{U}{2} - \mu\right) \sum_{x} (\hat{n}_{x\uparrow} + \hat{n}_{x\downarrow} - 1)$$







van Hove singularity in density of states at μ=κ



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

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

Quantum Monte Carlo

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

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:

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

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

$$\alpha = 0 \ldots 1$$

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

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

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

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

Fierz identities

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

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

Similar identity for relativistic fermions:

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

Applied for NJL model:

$$\mathcal{L} = \bar{\psi} i\gamma_\mu \partial^\mu \psi + G\left[(\bar{\psi}\psi)(\bar{\psi}\psi) - (\bar{\psi}\gamma_5\psi)(\bar{\psi}\gamma_5\psi)\right]$$

$$= \bar{\psi} i\gamma_\mu \partial^\mu \psi - \frac{G}{2}\left[(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi) - (\bar{\psi}\gamma_5\gamma^\mu\psi)(\bar{\psi}\gamma_5\gamma^\mu\psi)\right]$$

$$= \bar{\psi} i\gamma_\mu \partial^\mu \psi + \alpha G\left[(\bar{\psi}\psi)(\bar{\psi}\psi) - (\bar{\psi}\gamma_5\psi)(\bar{\psi}\gamma_5\psi)\right] - (1-\alpha)\frac{G}{2}\left[(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi) - (\bar{\psi}\gamma_5\gamma^\mu\psi)(\bar{\psi}\gamma_5\gamma^\mu\psi)\right]$$

Sign Problem

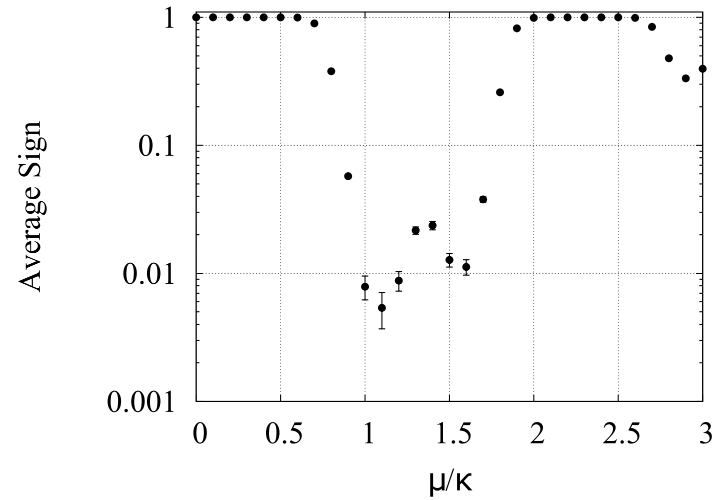
Reweighting:

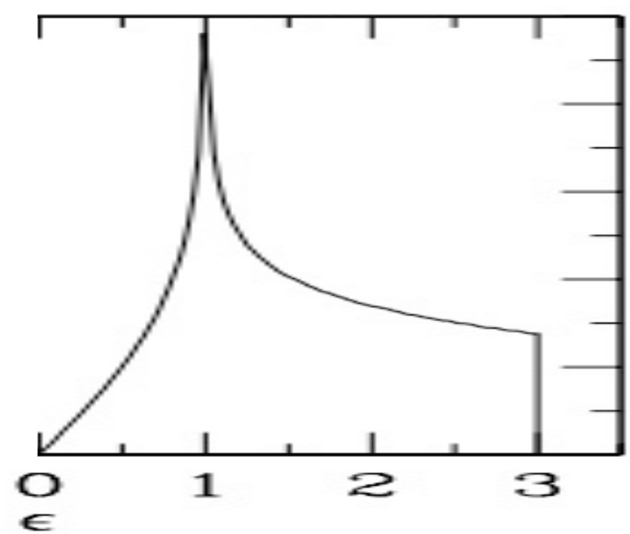
$$\mathcal{Z}_{\mathrm{pq}} = \int \mathcal{D}\Phi\, e^{-S_R[\Phi]}$$

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

$$= \frac{\frac{1}{\mathcal{Z}_{\mathrm{pq}}} \int \mathcal{D}\Phi\, \mathcal{O}[\Phi]\, \frac{e^{-S[\Phi]}}{e^{-S_R[\Phi]}}\, e^{-S_R[\Phi]}}{\frac{1}{\mathcal{Z}_{\mathrm{pq}}} \int \mathcal{D}\Phi\, \frac{e^{-S[\Phi]}}{e^{-S_R[\Phi]}}\, e^{-S_R[\Phi]}} = \frac{\langle \mathcal{O} e^{-iS_I} \rangle_{S_R}}{\langle e^{-iS_I} \rangle_{S_R}}$$

"optimal setup" for BSS-QMC: spin-coupled discrete auxiliary fields (4x4 lattice):





Lefschetz Thimbles decomposition

$$\mathcal{Z}(\beta, \mu, \dots) = \int_{\mathbb{R}^N} d^N x e^{-S(\beta,\mu,\dots,x)}$$

$$S = S_\alpha - \ln(\det M_{el.} \det M_{h.})$$

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

$$\left.\frac{\partial S}{\partial x}\right|_{x=z_\sigma(\beta,\mu,\dots)} = 0$$

Saddle points in complex space, with thimbles and anti-thimbles attached to them:

$$x \in \mathcal{I}_\sigma : x(\tau) = x, x(\tau \to -\infty) \to z_\sigma$$

$$x \in \mathcal{K}_\sigma : x(\tau) = x, x(\tau \to +\infty) \to z_\sigma$$

Intersection number:

$$k_\sigma = \langle \mathcal{K}_\sigma, \mathbb{R}^N \rangle$$

$$\frac{dx}{d\tau} = \overline{\frac{\partial S}{\partial x}}$$

Integral over thimble (manifold in complex space defined by Gradient Flow equations)

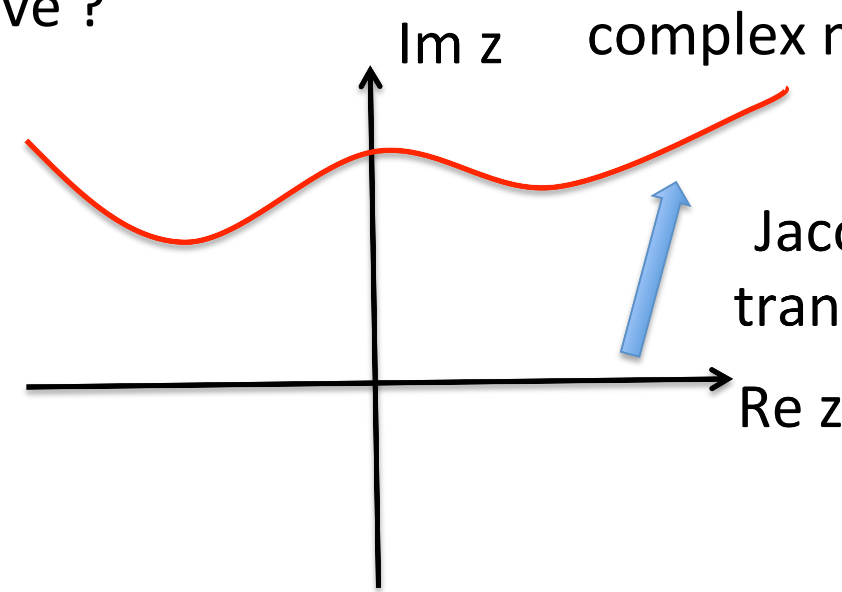
Witten, arXiv: 1009.6032, 1001.2933

Splitting of the Sign Problem

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

How many relevant thimbles do we have ?

How severe are the fluctuations of the complex measure ?

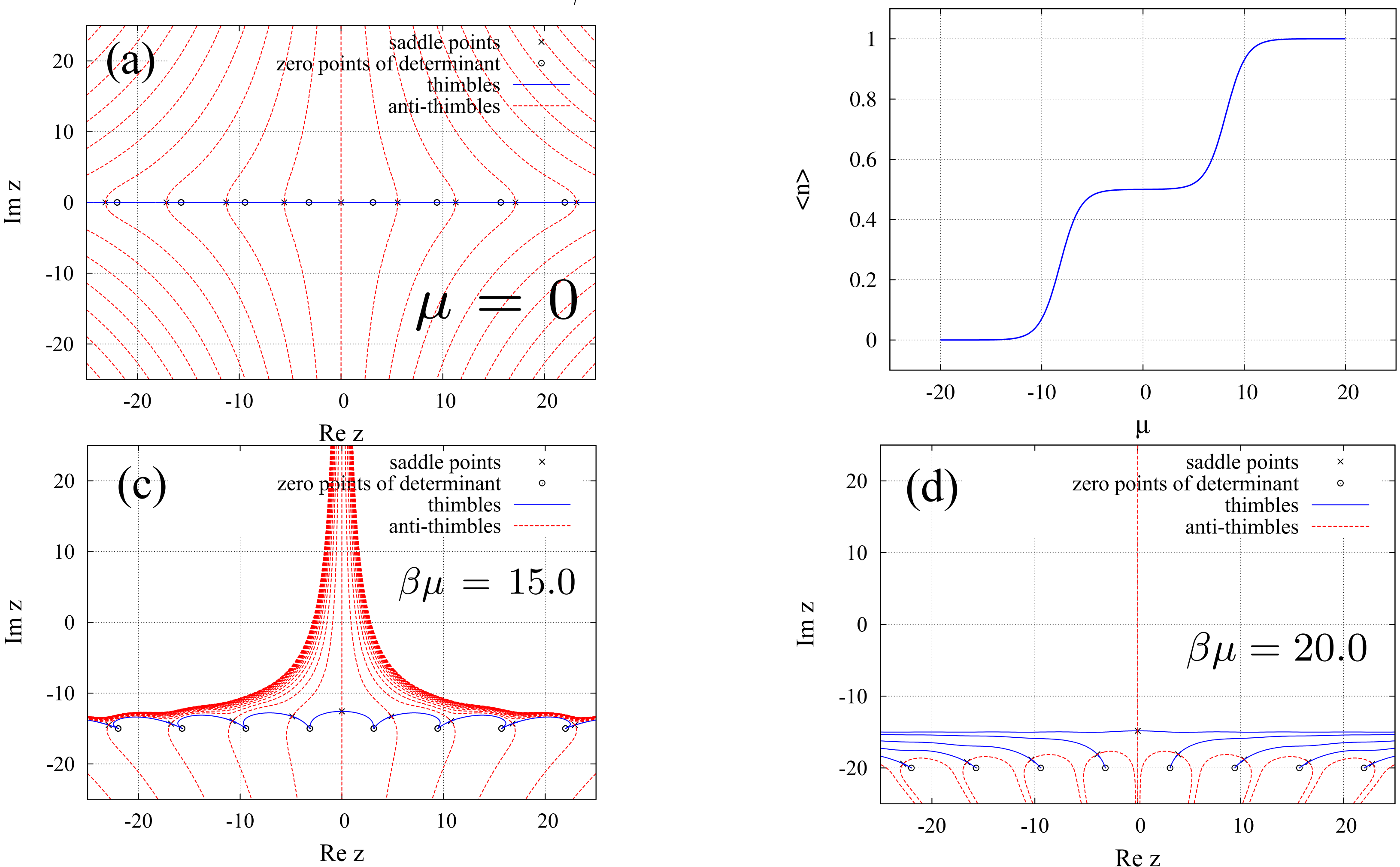


Jacobian of the transition z(x) - ?

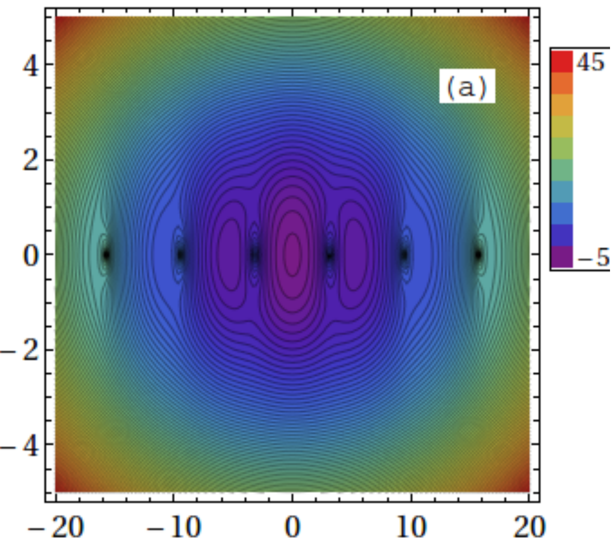
Thimbles for one-site Hubbard model (one-field formalism)

$\hat{H}_{1site} = U\hat{n}_\uparrow \hat{n}_\downarrow$ + Gaussian HS transformation $U\beta = 15.0$

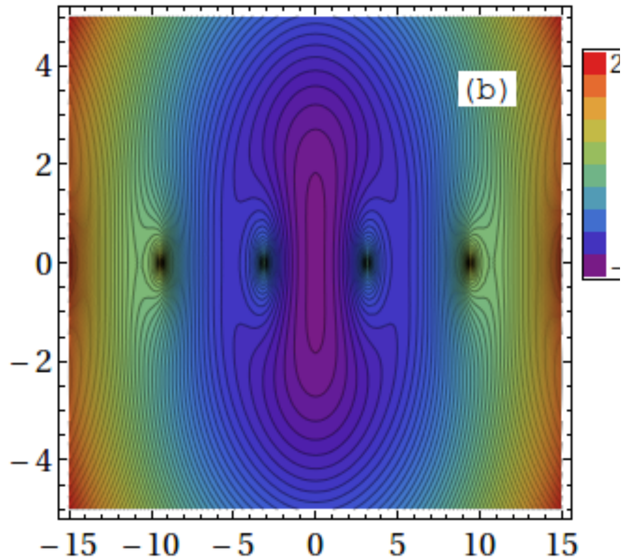
$$S(x) = \frac{x^2}{2\beta U} - \ln\left((1+e^{ix-\beta\mu})(1+e^{-ix+\beta\mu})\right)$$



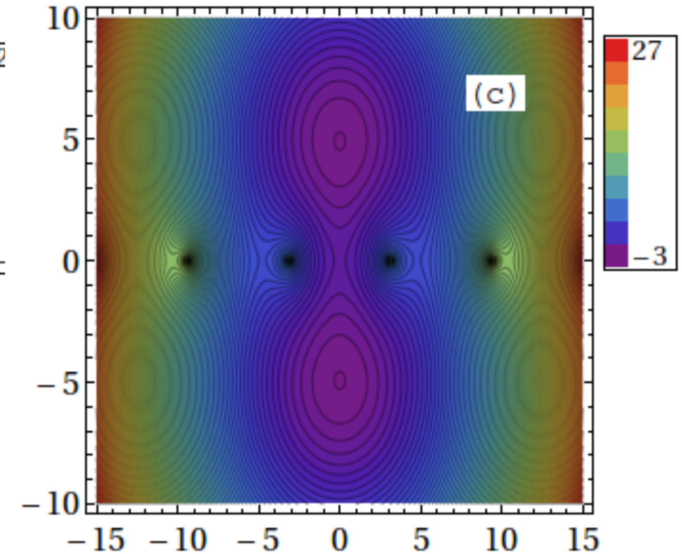
Thimbles for one-site Hubbard model (two-field formalism, half-filling)



α=0.95

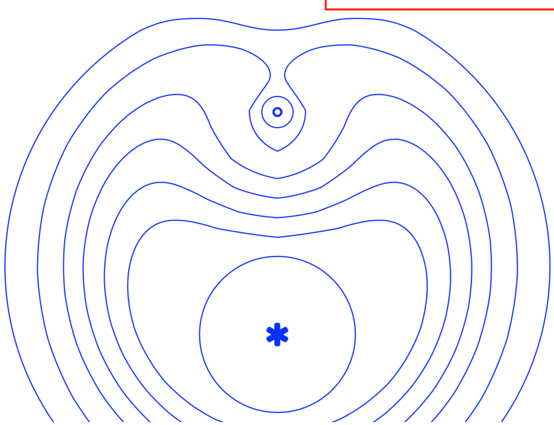


α=0.8



α=0.5

Only trivial saddle point at α ≈ 0.78…0.88

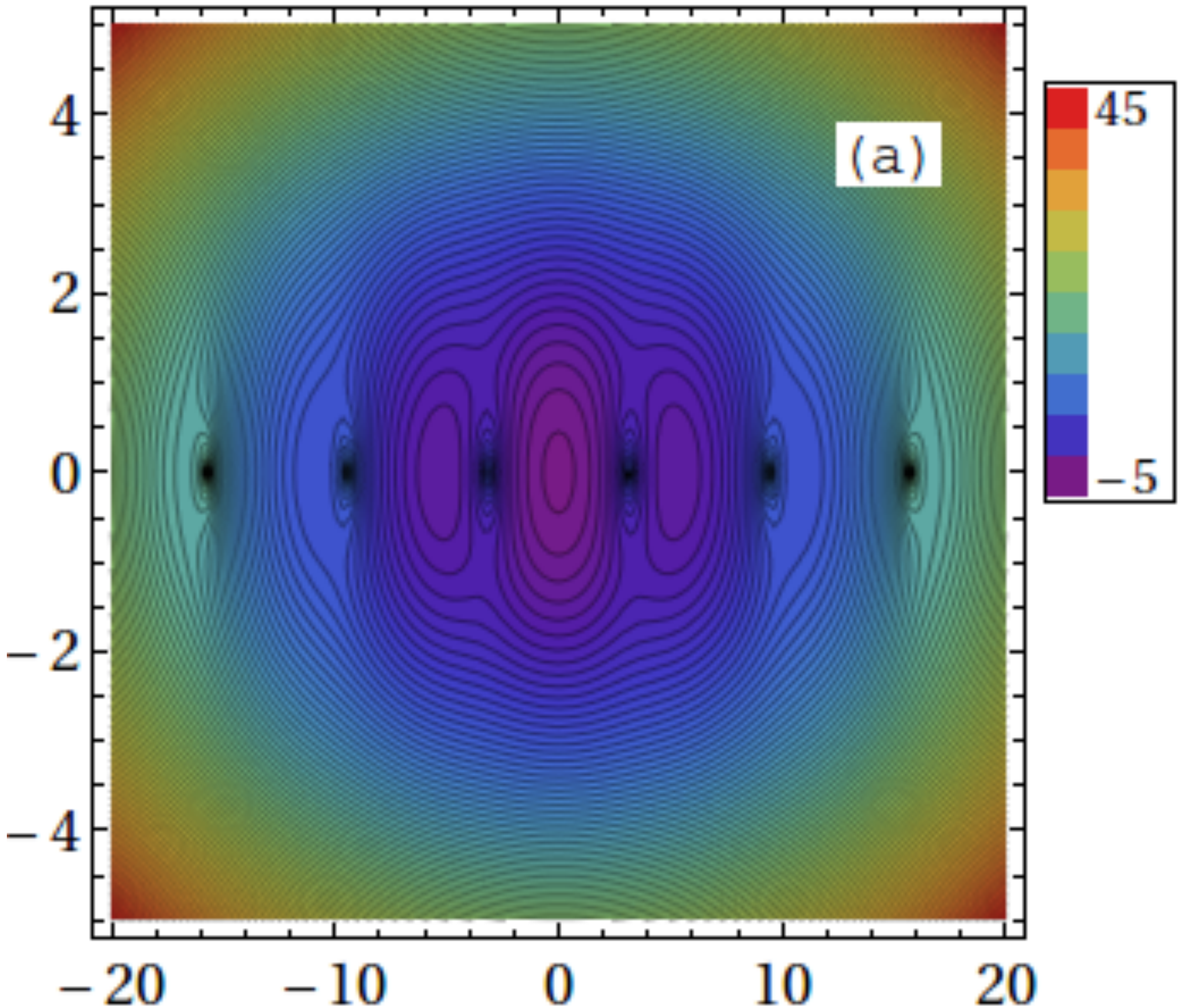


Irrelevant saddle embedded into relevant thimble

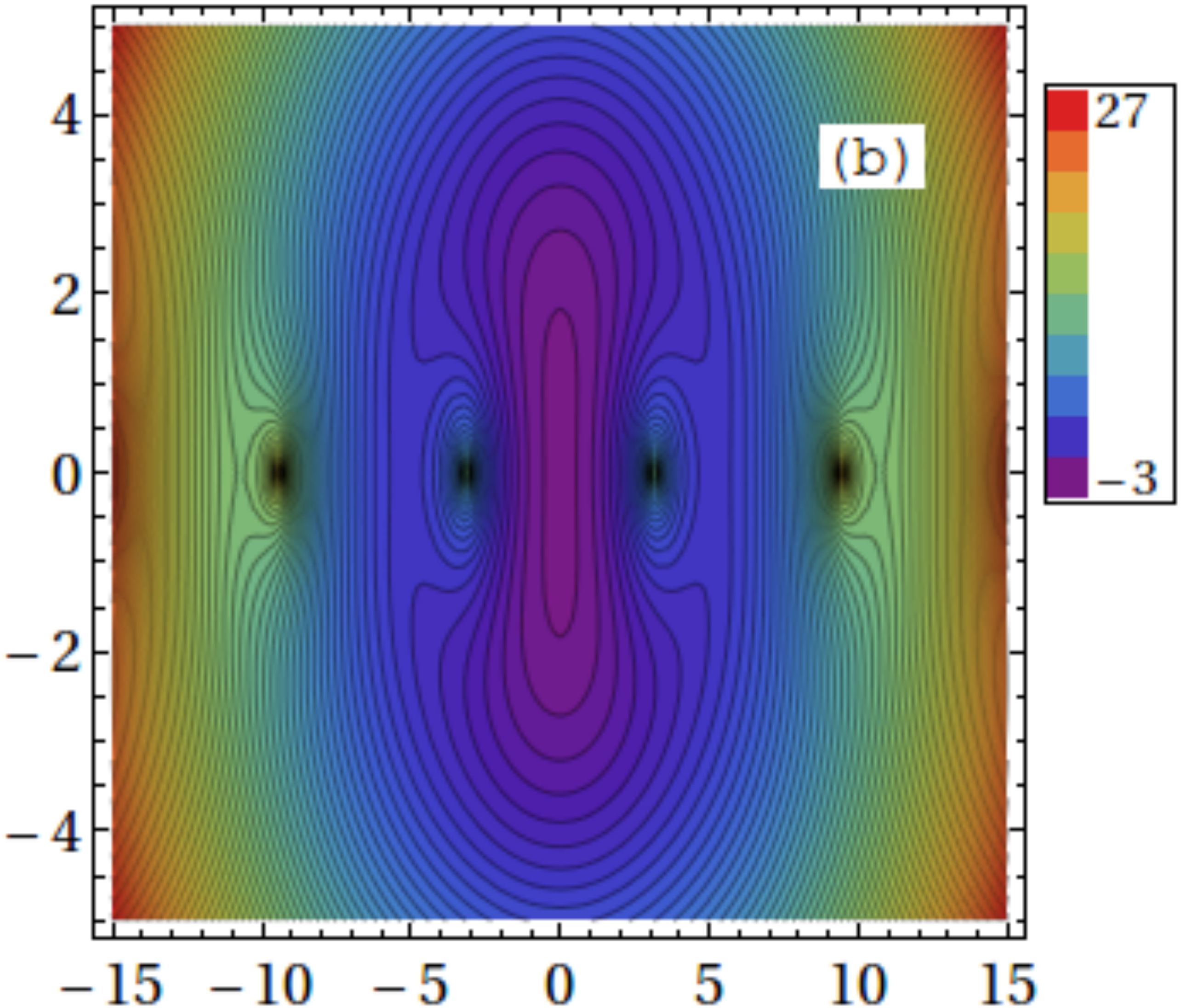
$$\dim(\mathbb{R}^N \cap \mathcal{K}_\sigma) = \mathcal{N}_\sigma > 0$$

Stokes phenomenon at half-filling

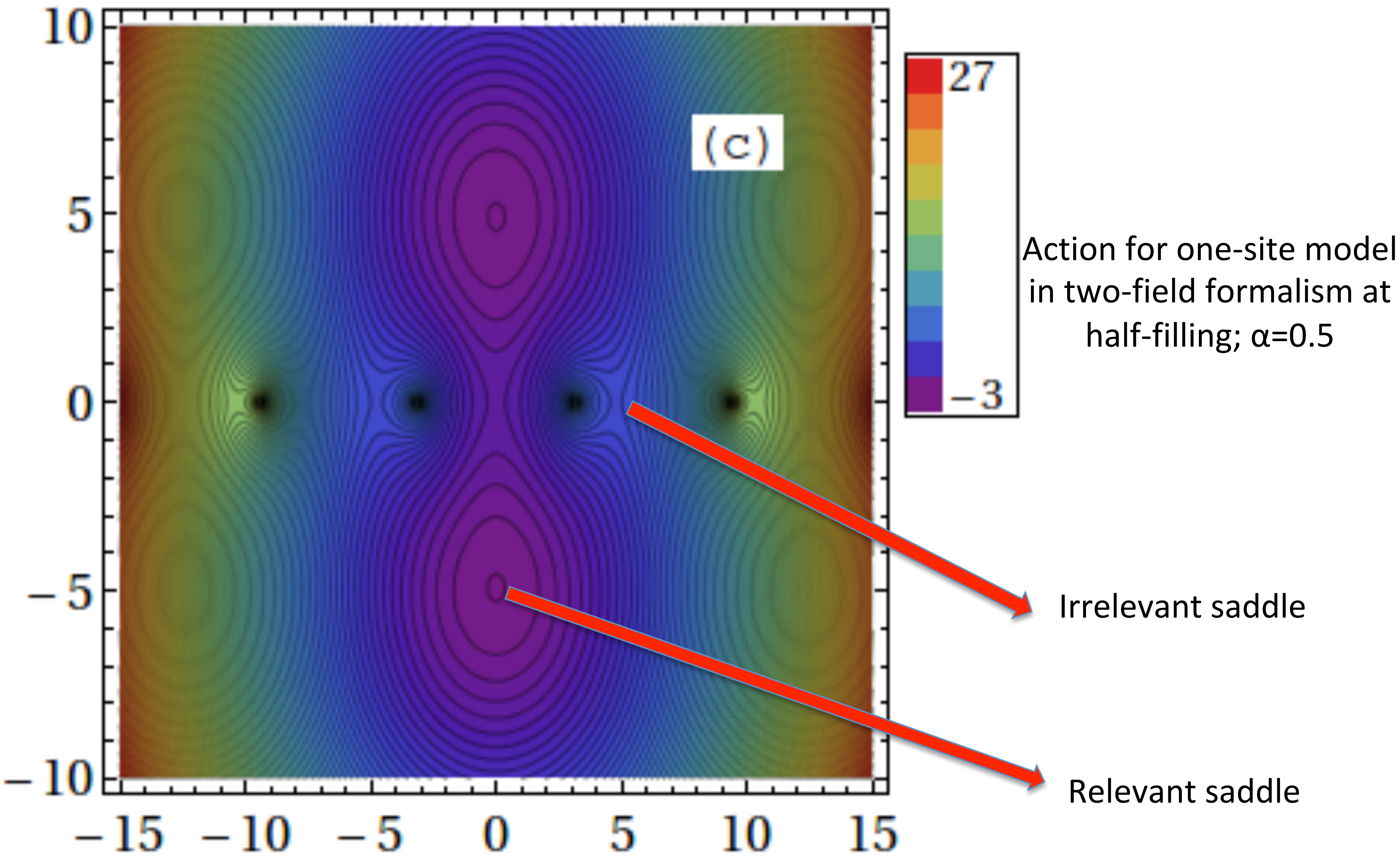
Relevant saddles points are the local minima of the action if we are bounded within R^N



Action for one-site model in two-field formalism at half-filling; $\alpha=0.95$



Action for one-site model in two-field formalism at half-filling; α=0.8


(c)
27
−3
Action for one-site model in two-field formalism at half-filling; α=0.5
Irrelevant saddle
Relevant saddle
10
5
0
−5
−10
−15
−10
−5
0
5
10
15

What happens in thermodynamic and continuum limit?

What do we need to go to large lattice?

$$\mathcal{Z}(\beta, \mu, \ldots) = \int_{\mathbb{R}^N} d^N x e^{-S(\beta,\mu,\ldots,x)}$$

$$\mathcal{Z} = \sum_\sigma k_\sigma e^{-i \operatorname{Im} S(z_\sigma)} \int_{\mathcal{I}_\sigma} d^N x e^{-\operatorname{Re} S(x)}$$

$$\left.\frac{\partial S}{\partial x}\right|_{x=z_\sigma(\beta,\mu,\ldots)} = 0$$

$$\frac{dx}{d\tau} = \overline{\frac{\partial S}{\partial x}}$$

$$S = S_\alpha - \ln(\det M_{el.} \det M_{h.})$$

Fast solution of GF equations with fermionic determinants is essential.

$$\det M^\dagger M = \int d\bar{Y} dY \, e^{-\bar{Y}(M^\dagger M)^{-1} Y}$$

Stochastic calculation of fermionic determinant doesn't work: not precise enough, the phase is not conserved.

Exact fermionic forces (1)

General form of the fermionic operator:

$N_s \times N_s$ Blocks

$$M = \begin{pmatrix} I & D_1 & & & & \\ & I & D_2 & & & \\ & & I & D_3 & & \\ & & & \ddots & \ddots & \\ & & & & I & D_{2N_t-1} \\ D_{2N_t} & & & & & I \end{pmatrix}$$

Also staggered fermions in axial gauge.

$$D_{2k} = \pm \begin{pmatrix} e^{i\phi_1^k} & & \\ & \ddots & \\ & & e^{i\phi_{N_s}^k} \end{pmatrix}$$

Interaction with Hubbard fields (antiperiodic boundary conditions for fermions)

Exponential transfer matrix preserves the spin symmetry (arXiv:1610.09855):

$$D_{2k-1} = -e^{-\Delta\tau\ h}$$

Conventional discretization:

$$D_{2k-1} = -1 + \Delta\tau\ h$$

Exact fermionic forces (2)

$$\frac{\partial \ln \det M}{\partial \phi_{x,t}} = \mathrm{Tr}\left(M^{-1} \frac{\partial M}{\partial \phi_{x,t}} \right)$$

$$M = \begin{pmatrix} I & D_1 & & & & \\ & I & D_2 & & & \\ & & I & D_3 & & \\ & & & \ddots & \ddots & \\ & & & & I & D_{2N_t-1} \\ D_{2N_t} & & & & & I \end{pmatrix}$$

We need blocks of lattice propagator just below the main diagonal

$$\bar{g}_m = {D_m}^{-1}(I - g_m)$$

Iterations for the blocks at the main diagonal

$$g_{m+1} = {D_m}^{-1} g_m D_m$$

The algorithm can be taken from BSS-QMC. See the description of ALF package (F. Assaad et al): arXiv:1704.00131

But: we can not go through the entire lattice: "stabilization" is needed

Schur solver

Basic idea – highly specialized version of sparse LU decomposition.

arXiv:1803.05478

$$X \equiv X^{(1)} = \begin{pmatrix} X_1^{(1)} \\ X_2^{(1)} \\ \vdots \\ X_{K_1-1}^{(1)} \\ X_{K_1}^{(1)} \end{pmatrix}, \qquad Y \equiv Y^{(1)} = \begin{pmatrix} Y_1^{(1)} \\ Y_2^{(1)} \\ \vdots \\ Y_{K_1-1}^{(1)} \\ Y_{K_1}^{(1)} \end{pmatrix} \qquad M^{(1)}X^{(1)} = Y^{(1)}$$

$$P^\dagger_{K_l} X^{(l)} = \begin{pmatrix} {U_X}^{(l)} \\ {L_X}^{(l)} \end{pmatrix} \qquad P^\dagger_{K_l} Y^{(l)} = \begin{pmatrix} {U_Y}^{(l)} \\ {L_Y}^{(l)} \end{pmatrix} \qquad P^\dagger_{K_l} \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_{K-1} \\ X_{K_l} \end{pmatrix} = \begin{pmatrix} X_1 \\ X_3 \\ \vdots \\ X_{K_l-1} \\ X_2 \\ X_4 \\ \vdots \\ X_{K_l} \end{pmatrix} \qquad P_{K_l} \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_{K_l-1} \\ X_{K_l} \end{pmatrix} = \begin{pmatrix} X_1 \\ X_{K_l/2+1} \\ X_2 \\ X_{K_l/2+2} \\ \vdots \\ X_{K_l/2} \\ X_{K_l} \end{pmatrix}$$

$$M^{(l)}X^{(l)} = Y^{(l)}$$

$$\begin{pmatrix} I & D_1^{(l+1)} & & & \\ & I & D_2^{(l+1)} & & \\ & & \ddots & \ddots & \\ & & & I & D_{K_{l+1}-1}^{(l+1)} \\ D_{K_{l+1}}^{(l+1)} & & & & I \end{pmatrix}$$

$$\begin{aligned} X^{(l+1)} &:= {L_X}^{(l)}, \\ Y^{(l+1)} &:= {L_Y}^{(l)} - Q^{(l)}{U_Y}^{(l)}. \end{aligned} \qquad Q^{(l)} = \begin{pmatrix} 0 & D_2^{(l)} & & \\ & \ddots & \ddots & \\ & & \ddots & D_{K_l-2}^{(l)} \\ D_{K_l}^{(l)} & & & 0 \end{pmatrix}.$$

$$\begin{aligned} D_k^{(l+1)} &:= -D_{2k}^{(l)} D_{2k+1}^{(l)}, \quad k = 1 \ldots K_{l+1}-1, \\ D_{K_{l+1}}^{(l+1)} &:= -D_{K_l}^{(l)} D_1^{(l)}. \end{aligned}$$

$$R^{(l)} = \begin{pmatrix} D_1^{(l)} & & & \\ & D_3^{(l)} & & \\ & & \ddots & \\ & & & D_{K_l-1}^{(l)} \end{pmatrix}$$

$$X^{(l-1)} = P_{l-1} \begin{pmatrix} {U_Y}^{(l-1)} - R^{(l-1)}X^{(l)} \\ X^{(l)} \end{pmatrix} \qquad l_{\max} = 6 - 8$$

Schur solver for QCD

Staggered fermions (almost the same for Wilson fermions):

$$S = \sum_x \Big\{ \sum_{\nu=2}^{4} \alpha_{x,\nu} \left[(\bar\psi_x U_{x,\nu} \psi_{x+\hat\nu}) - (\bar\psi_{x+\hat\nu} U^\dagger_{x,\nu} \psi_x \right] + \Big[(\bar\psi_x U_{x,1} e^{\mu} \psi_{x+\hat 1}) - (\bar\psi_{x+\hat 1} U^\dagger_{x,1} e^{-\mu} \psi_x \Big] + M(\bar\psi\psi) \Big\}$$

Unitary transformation + constant multiplier:

$$M(U) = \begin{pmatrix} 1 & \omega_1 & 0 & 0 & 0 & \dots \\ 0 & 1 & \delta_1 & 0 & 0 & \dots \\ 0 & 0 & 1 & \omega_2 & 0 & \dots \\ 0 & 0 & 0 & 1 & \delta_2 & \dots \\ \vdots & & & & \ddots & \\ -\delta_{N_t} & 0 & 0 & & \dots & 1 \end{pmatrix}$$

hoppings in k-th time slice + mass term

$$\omega_k = \begin{pmatrix} B_k & 1 \\ 1 & 0 \end{pmatrix}$$

$$\delta_k = \begin{pmatrix} \mathrm{diag}(U_{x,1}) e^{\mu} & 0 \\ 0 & \mathrm{diag}(U_{x,1}) e^{\mu} \end{pmatrix}$$

$$x = \{k, \vec r\}$$

Additional complications:

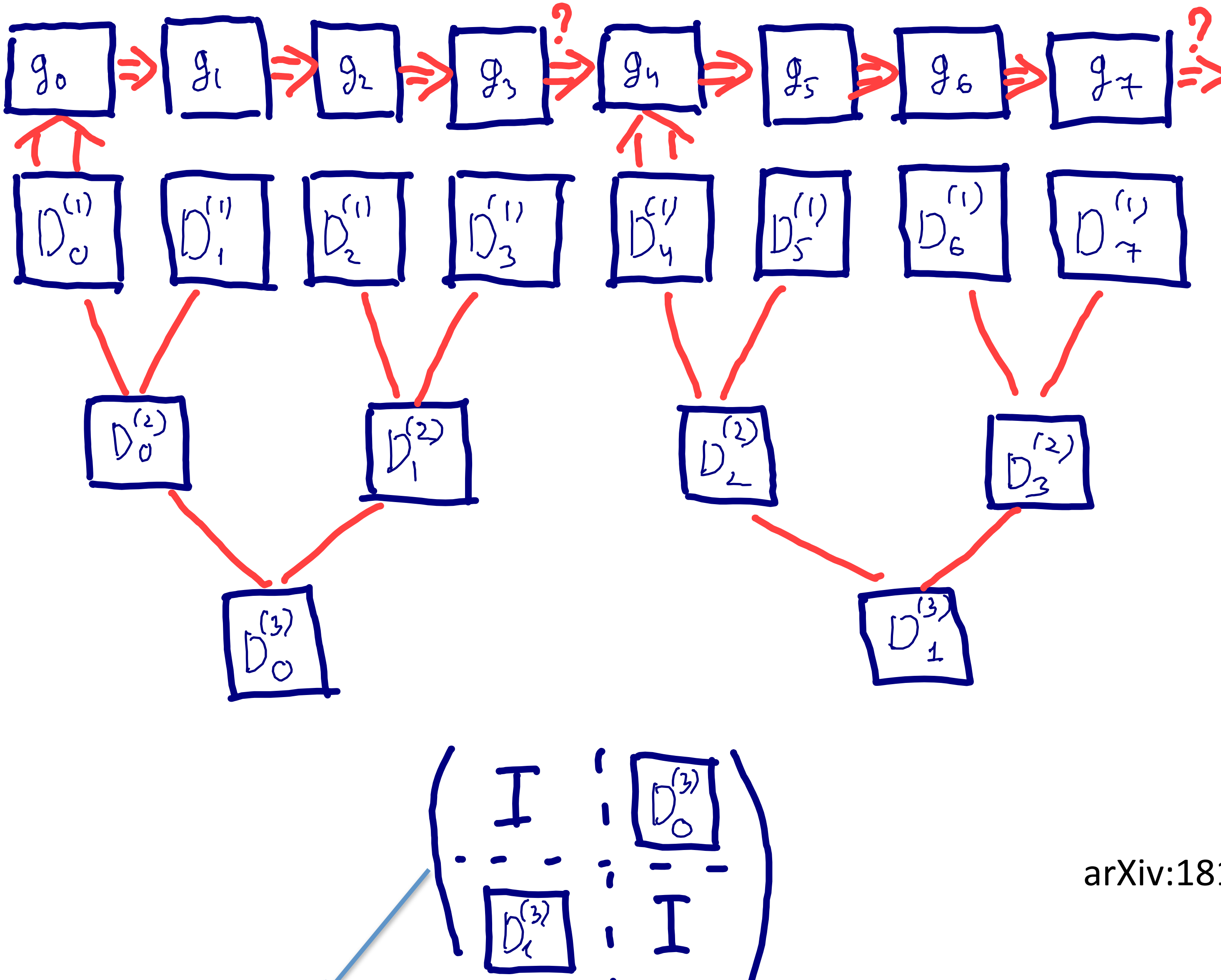
$$\bar g_m = {D_m}^{-1} (I - g_m)$$

$$g_{m+1} = {D_m}^{-1} g_m D_m$$

$$D_k \to \omega_k,\ \delta_k$$

ω_k^{-1} is needed for each time slice. But it doesn't change the overall $N_s^3 N_t$ scaling.

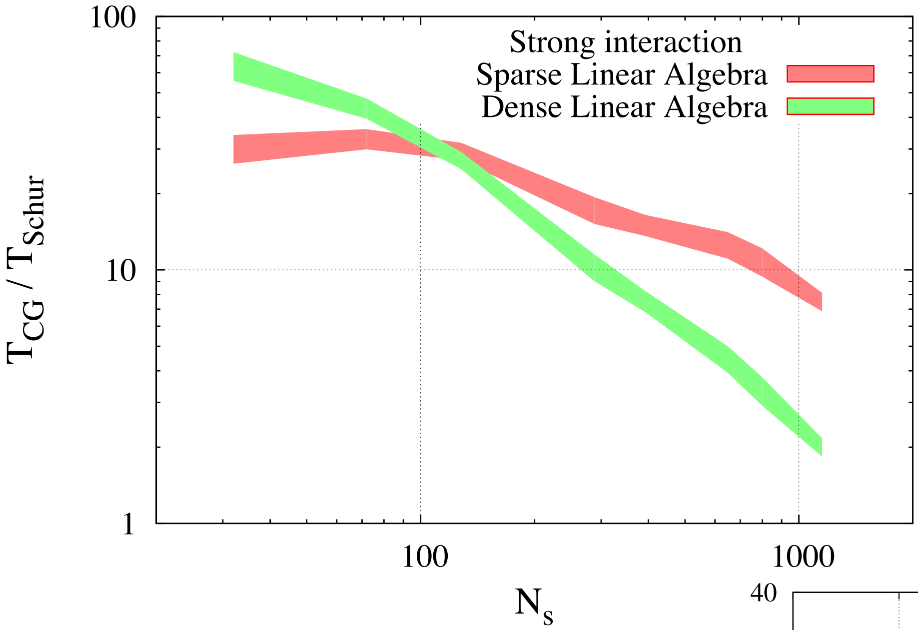
Calculation of propagators

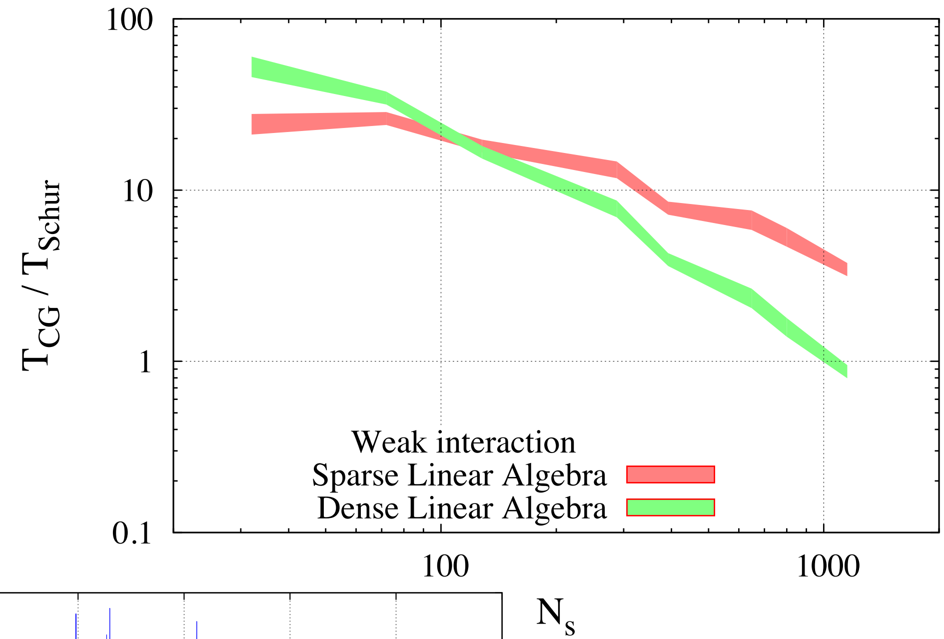


arXiv:1812.06435

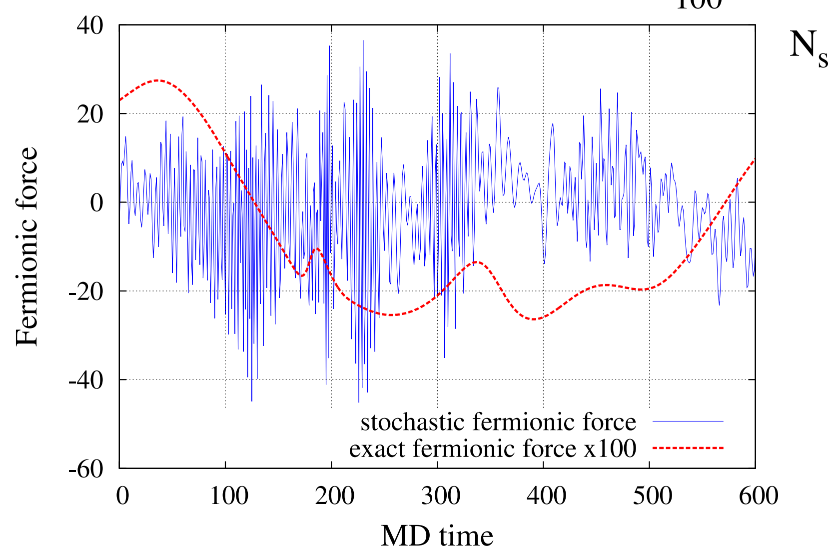
Proceed with sparse LU decomposition and reverse iterations

Schur solver vs CG





Side effect: smooth fermionic forces

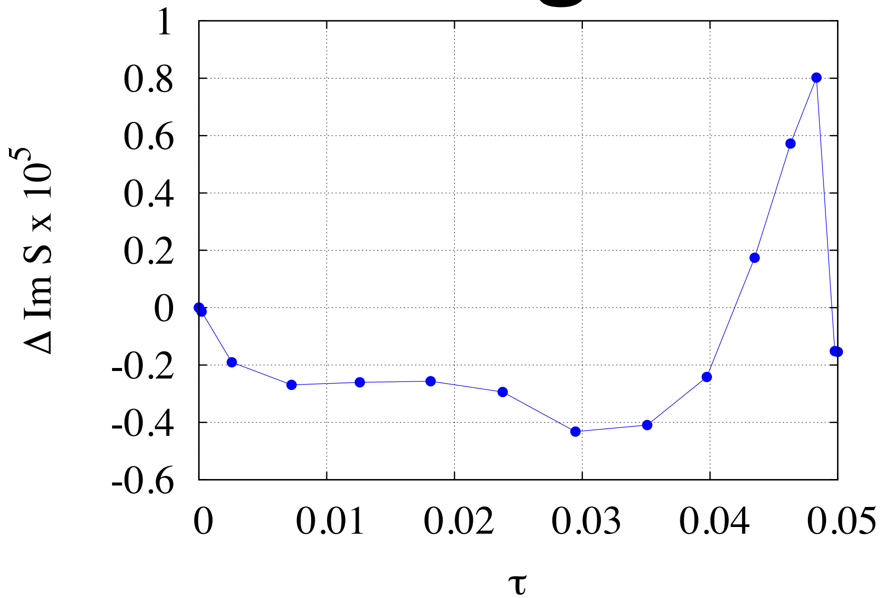


arXiv:1812.06435

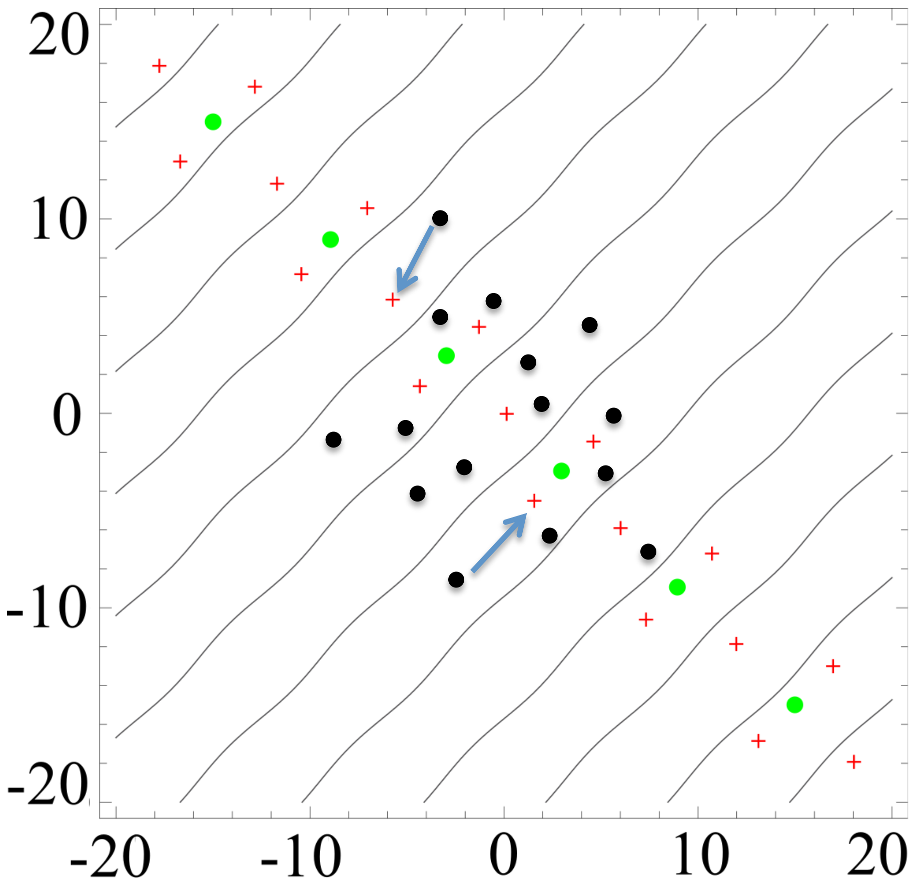
CG is advantageous only at very large lattices (e.g. we use it for 2x102x102x160 lattice to compute Fermi velocity renormalization)

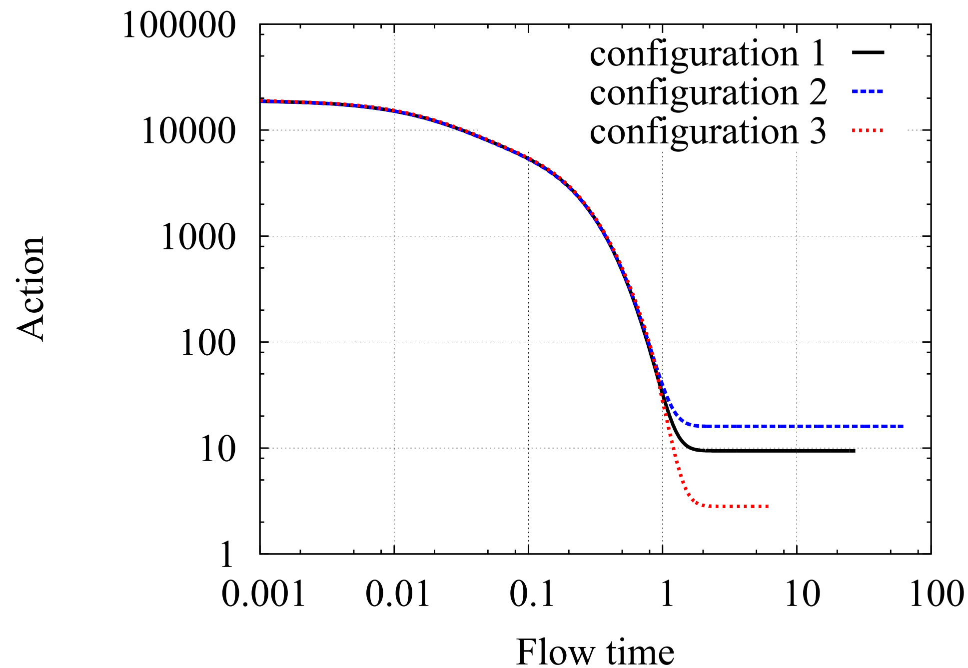
Saddle points at half-filling

Phase conservation:

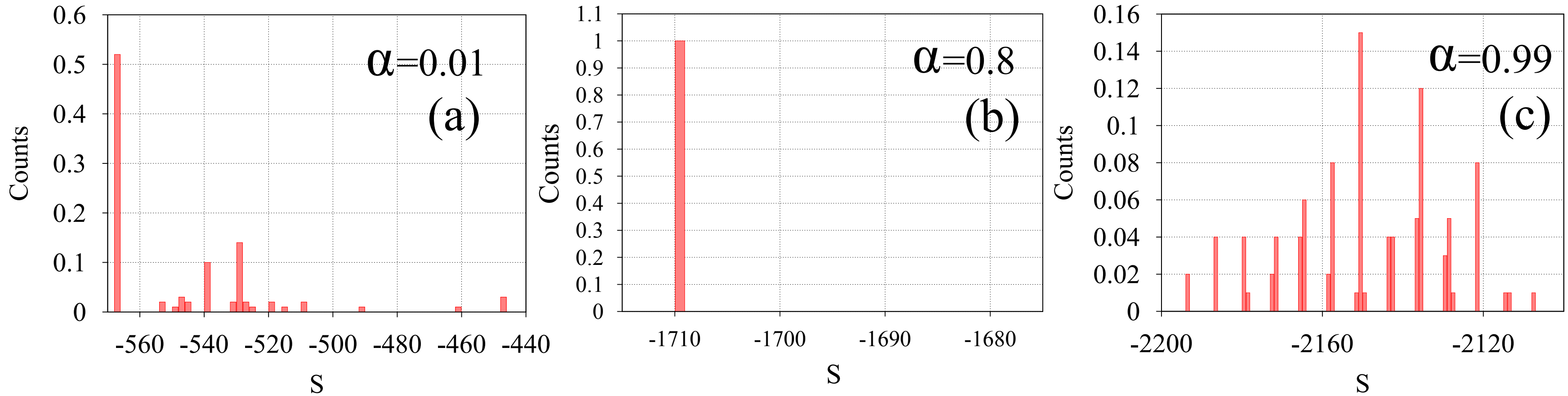


2-site Hubbard model

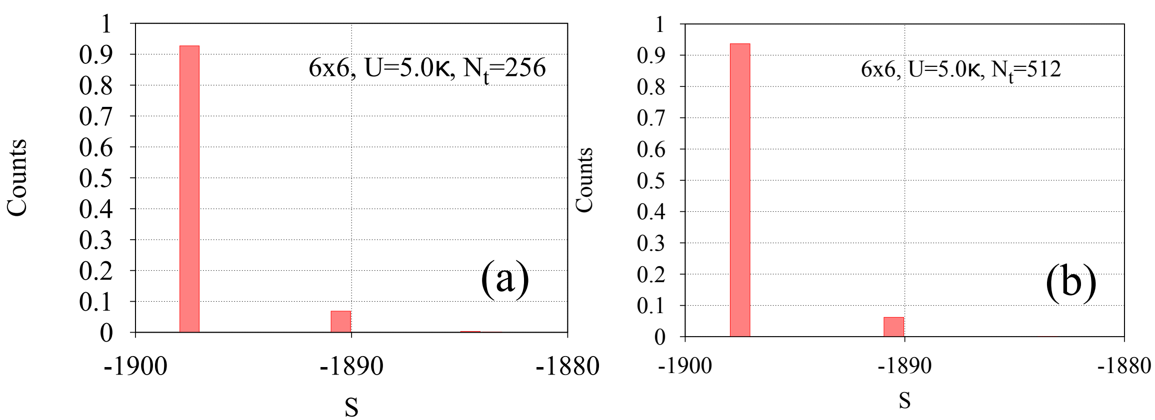




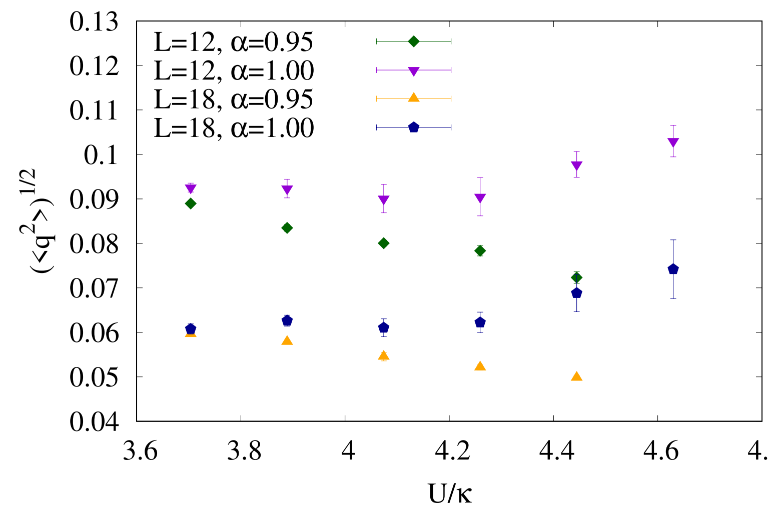
Continuum limit and α-dependence



Continuum limit:

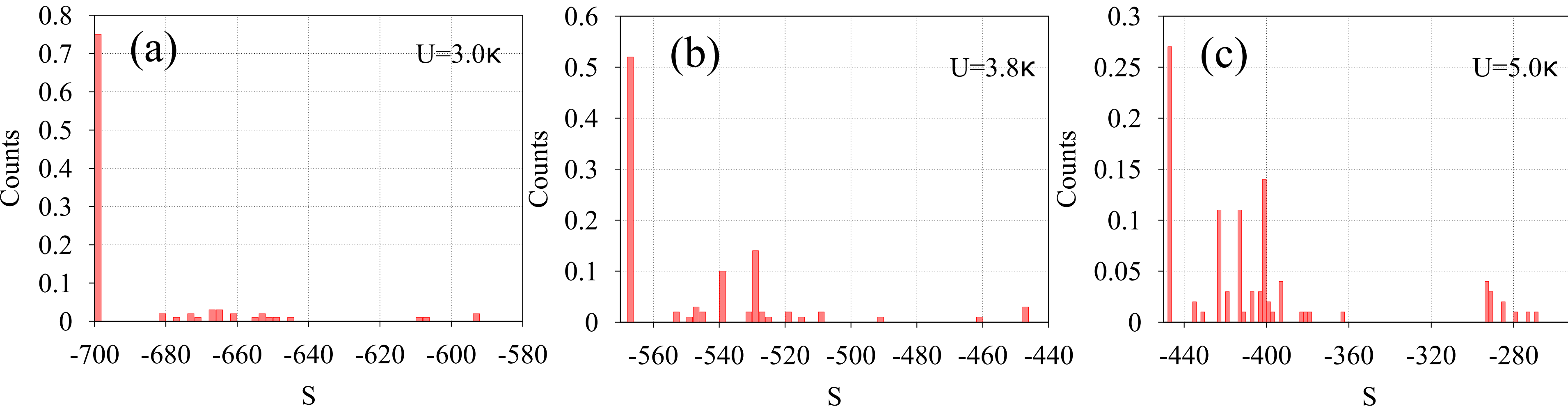


α=0.9

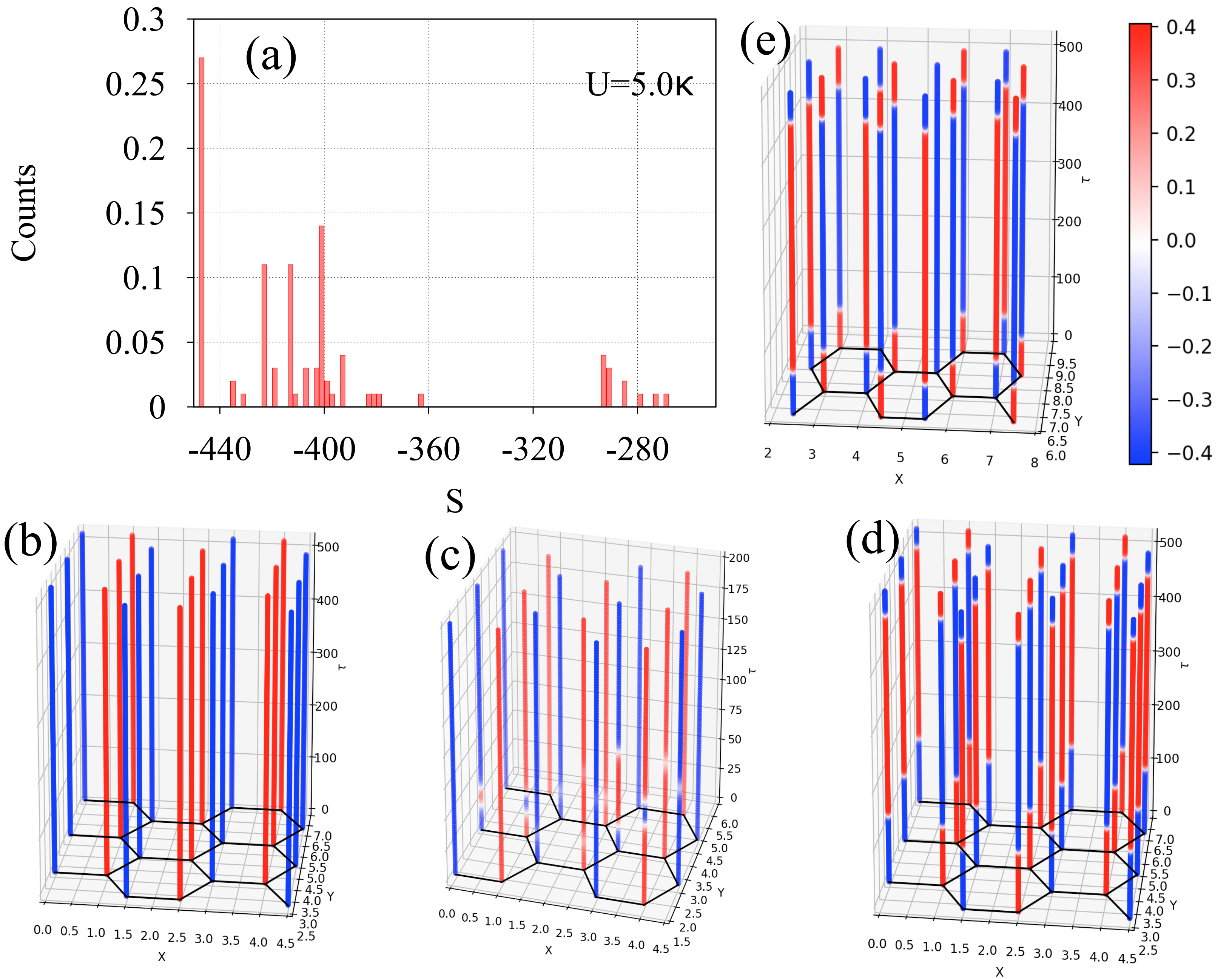


Ergodicity issues at α=0.0 and α=1.0. arXiv:1807.07025

Dominant spin-coupled field

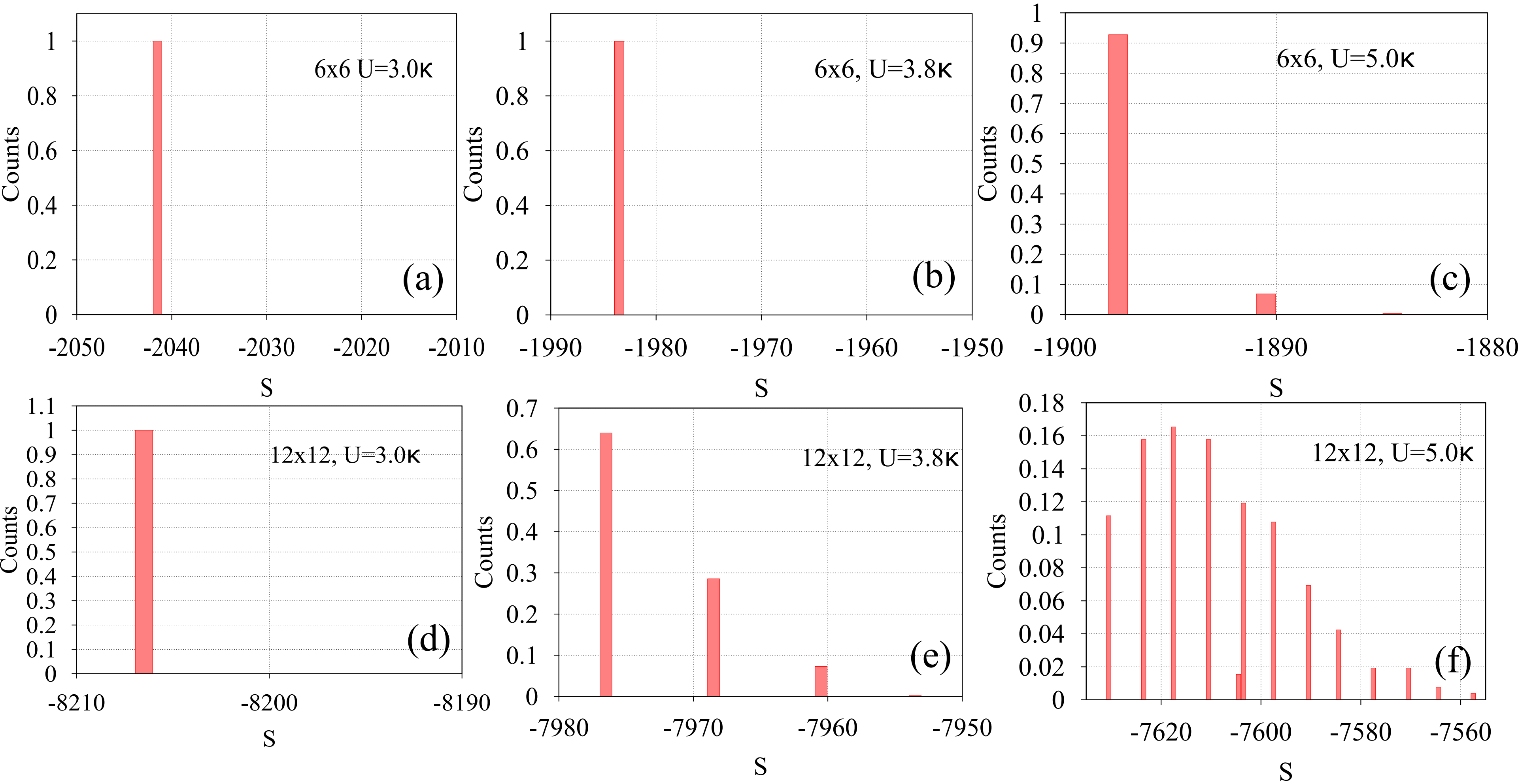


6x6 lattice, α=0.01

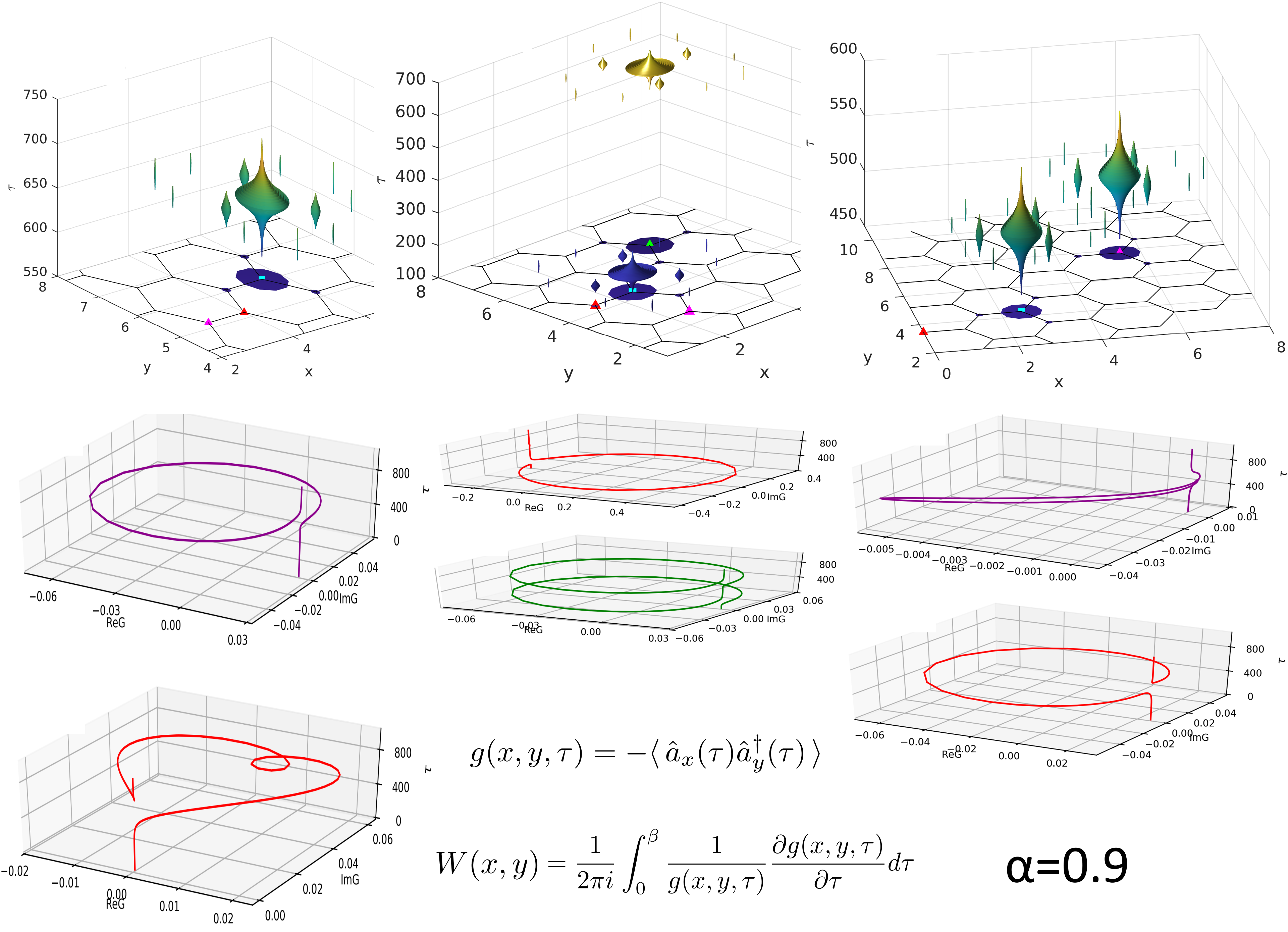


6x6 lattice, α=0.01

Dominant charge-coupled field



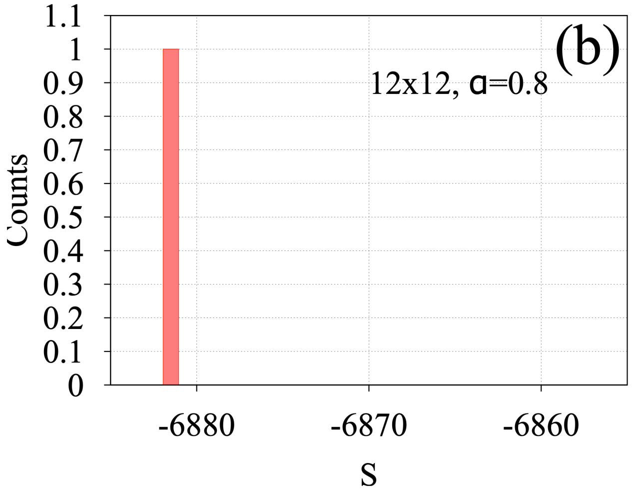
α=0.9

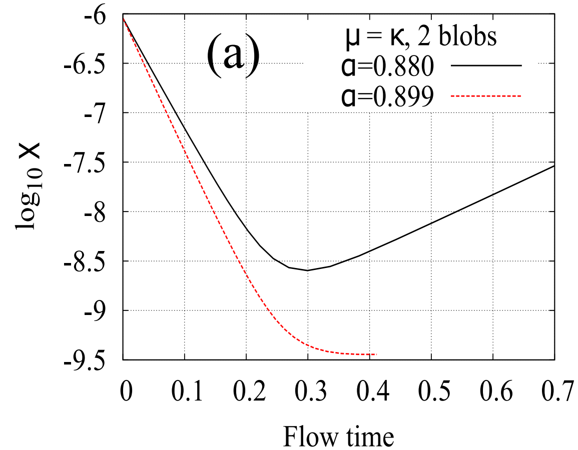


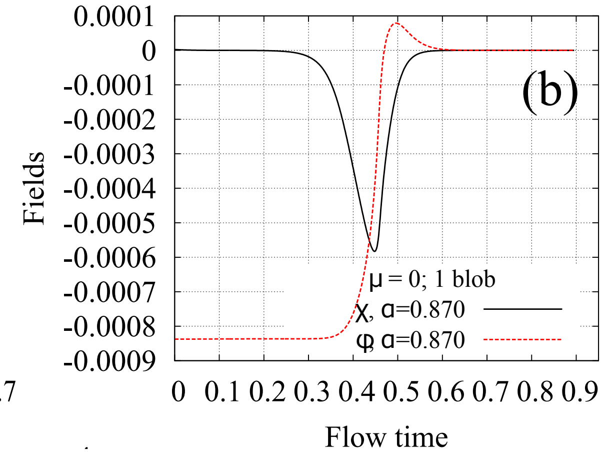
$$g(x,y,\tau) = -\langle\, \hat{a}_x(\tau)\hat{a}_y^{\dagger}(\tau)\,\rangle$$

$$W(x,y) = \frac{1}{2\pi i}\int_0^{\beta} \frac{1}{g(x,y,\tau)}\frac{\partial g(x,y,\tau)}{\partial \tau}d\tau$$

Optimal regime: α=0.8

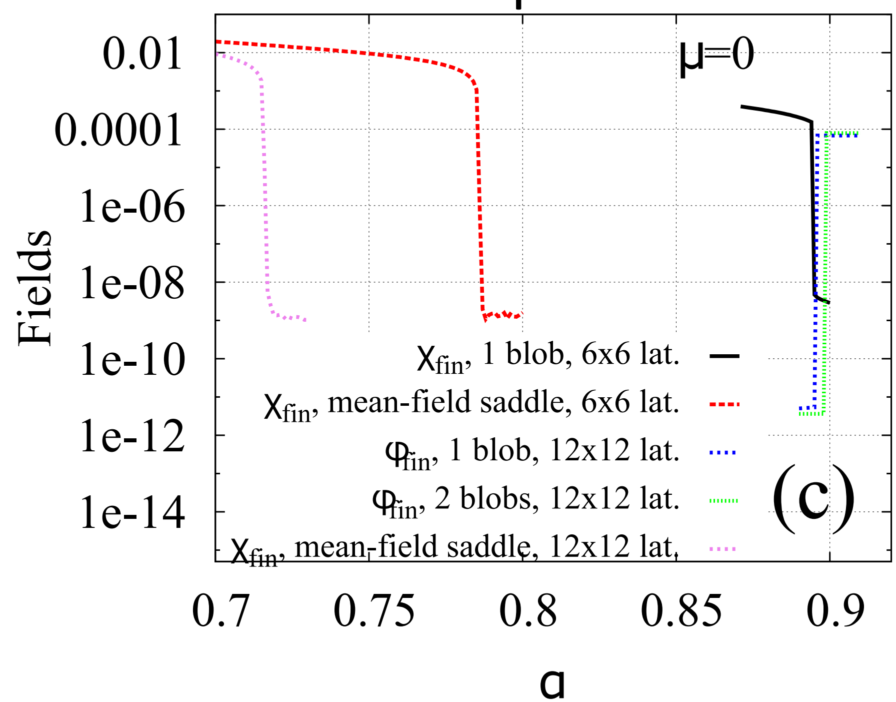






U=3.8

Flow examples

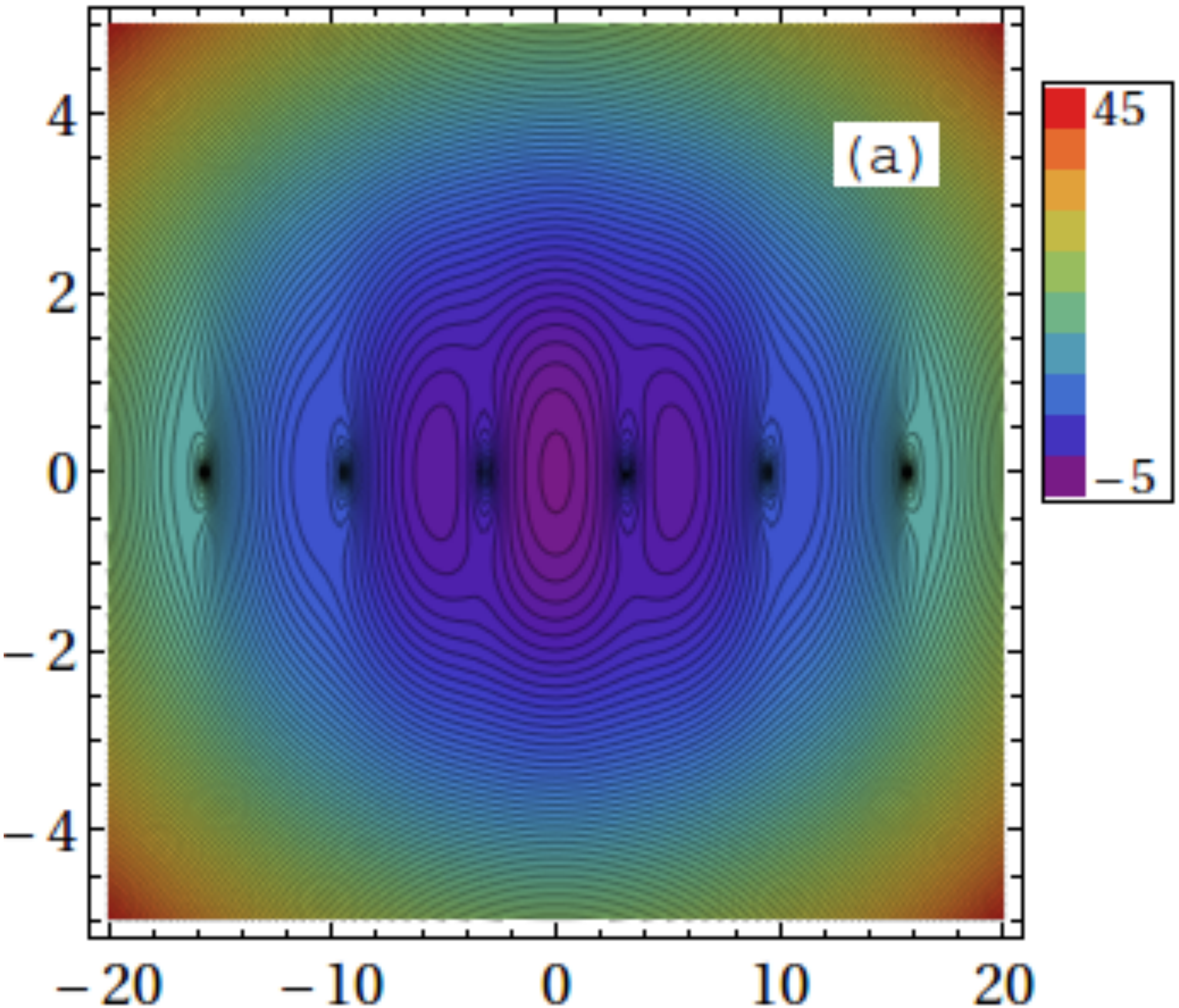


Summary

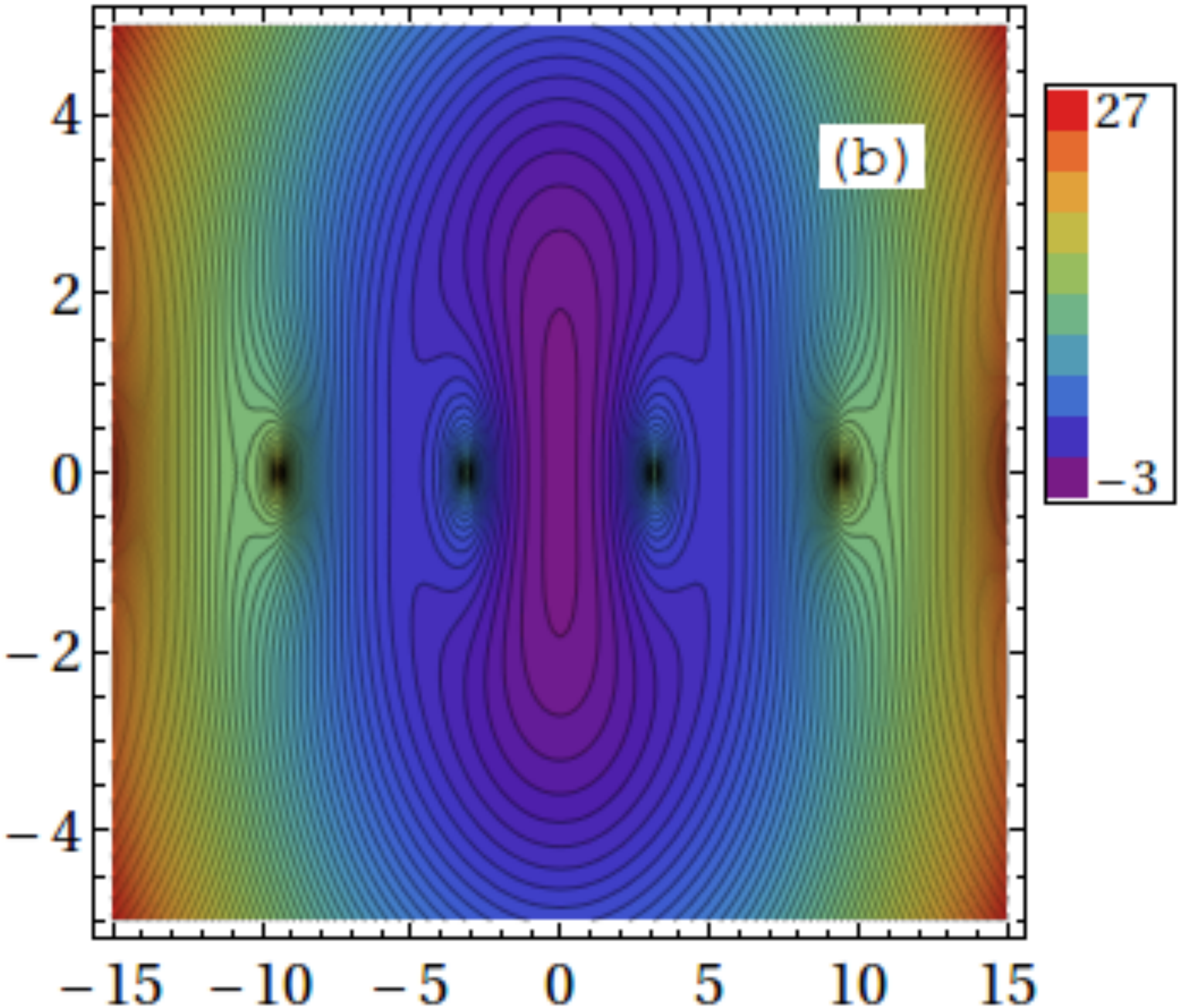
1) Optimal regime with only 1 important saddle exists at intermediate values of alpha parameter.
2) If charge-coupled field dominates, it is possible to build complete semi-analytical saddle point approximation.

Stokes phenomenon at half-filling

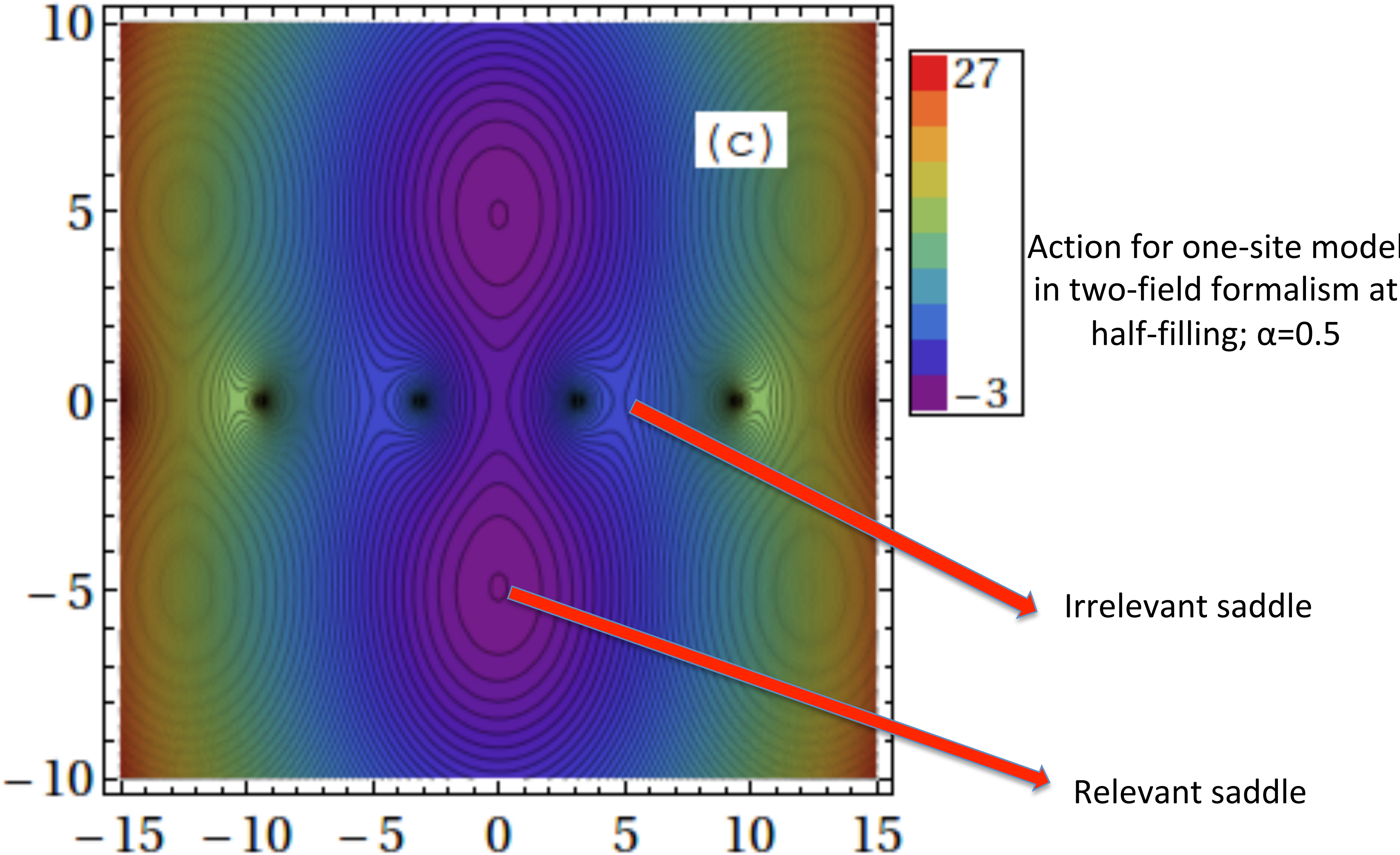
Relevant saddles points are the local minima of the action if we are bounded within R^N



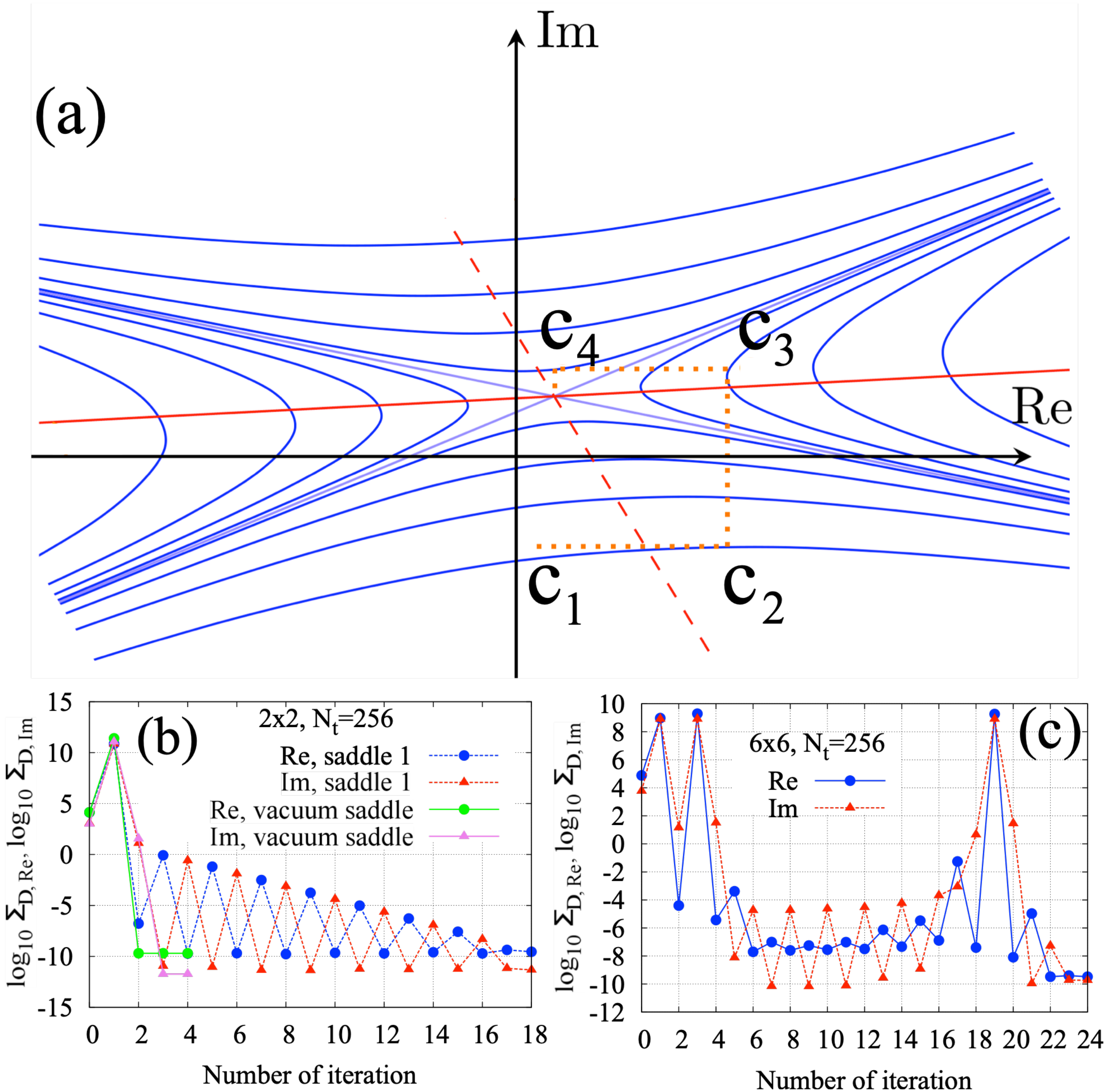
Action for one-site model in two-field formalism at half-filling; $\alpha=0.95$



Action for one-site model in two-field formalism at half-filling; α=0.8


(c)
27
−3
Action for one-site model in two-field formalism at half-filling; α=0.5
Irrelevant saddle
Relevant saddle
10
5
0
−5
−10
−15
−10
−5
0
5
10
15

Saddles points away of half-filling



U=3.8

α=0.9

Saddles points away of half-filling: convergence of iterations

$$\partial^2 \mathrm{Re} S / \partial \Phi_i^{(R)} \partial \Phi_j^{(R)} \qquad \partial^2 \mathrm{Re} S / \partial \Phi_i^{(R)} \partial \Phi_j^{(I)}$$

Hessian matrix at saddle point:

$$\Gamma = \begin{pmatrix} A & C \\ C & B \end{pmatrix}$$

$$\partial^2 \mathrm{Re} S / \partial \Phi_i^{(R)} \partial \Phi_j^{(I)} \qquad \partial^2 \mathrm{Re} S / \partial \Phi_i^{(I)} \partial \Phi_j^{(I)}$$

A and (-B) should be positive-definite, also the eigenvalues of the matrix:

$$A^{-1} C B^{-1} C$$

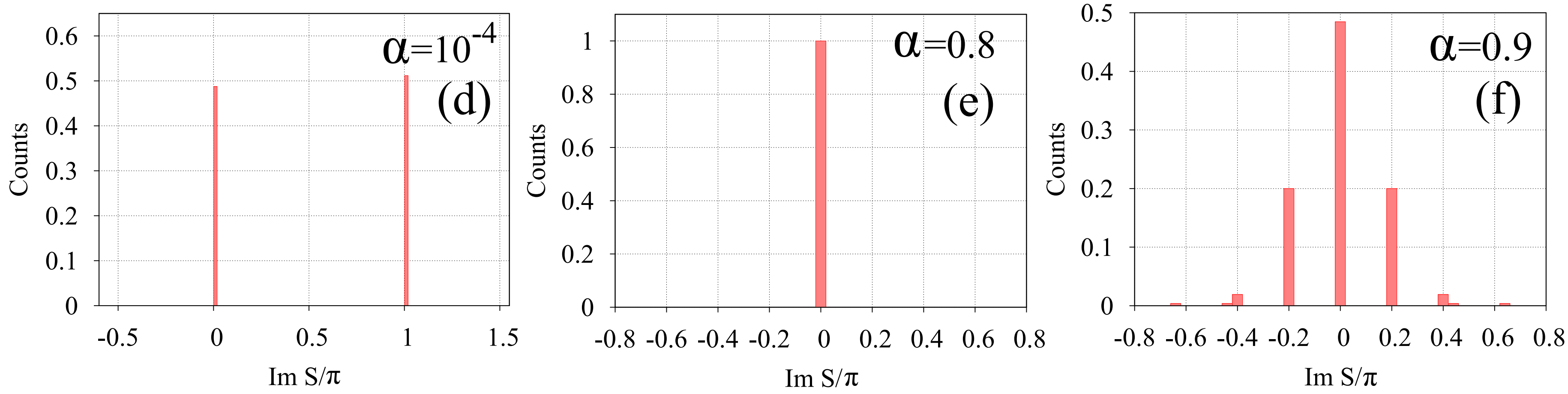
should satisfy the condition:

$$|\lambda_i| < 1$$

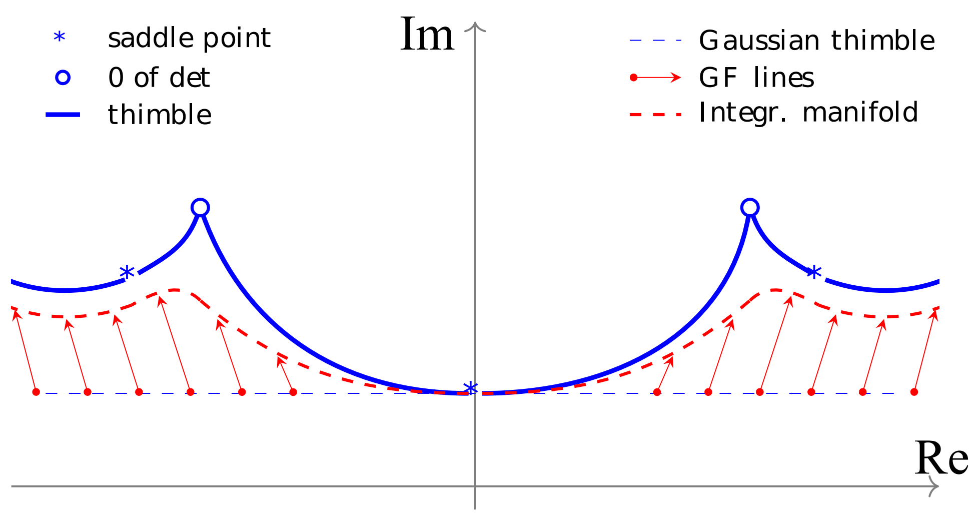
In 1D case in means:

$$|\arg \partial^2 S|_{z_\sigma}| < \pi/4$$

α-dependence at van Hove singularity



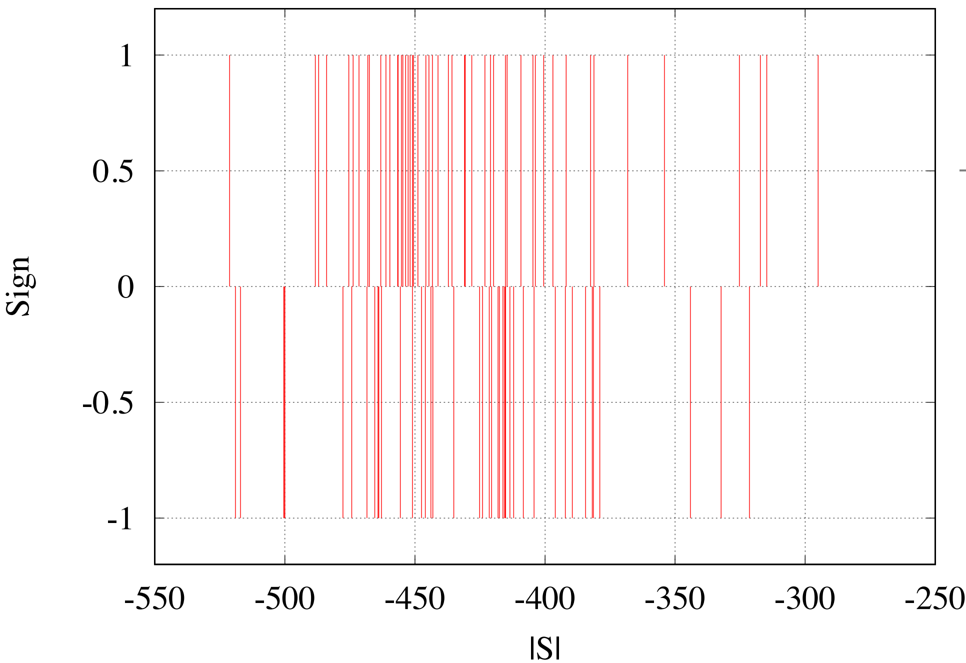
U=3.8

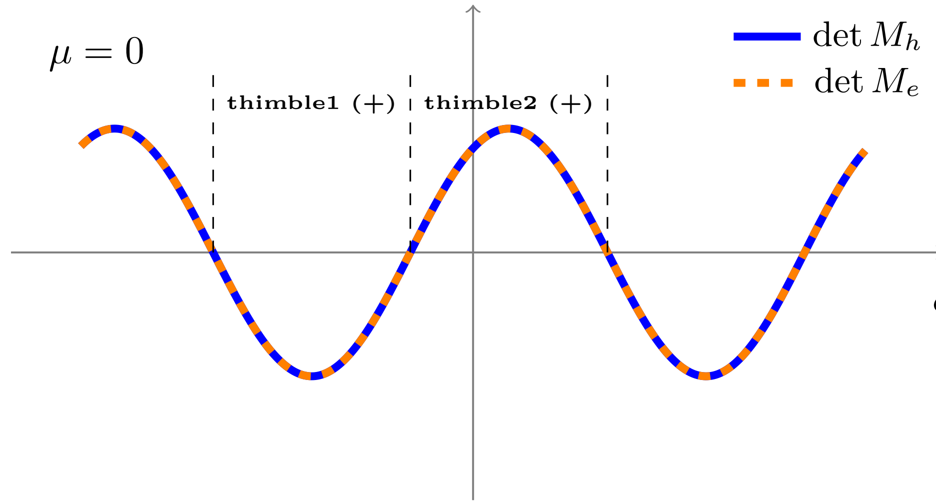


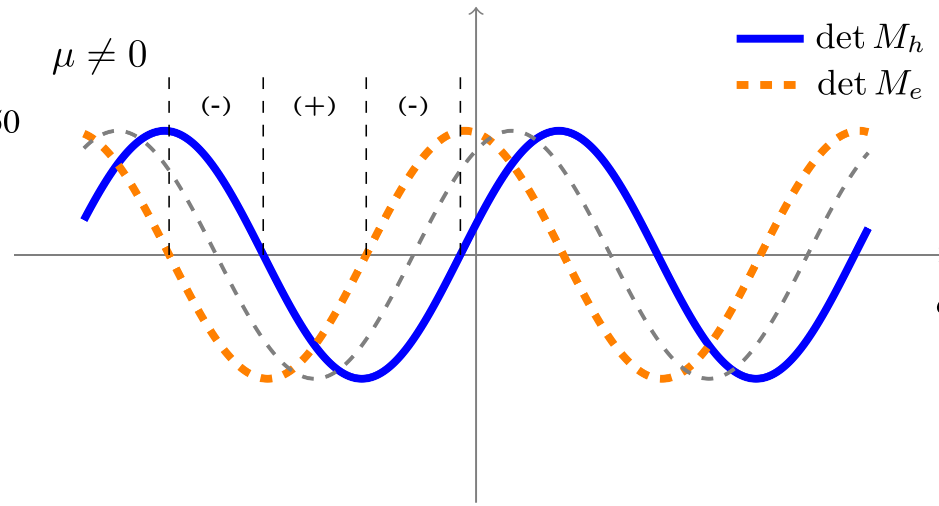
Search iterations are launched starting from Gaussian thimble attached to vacuum:

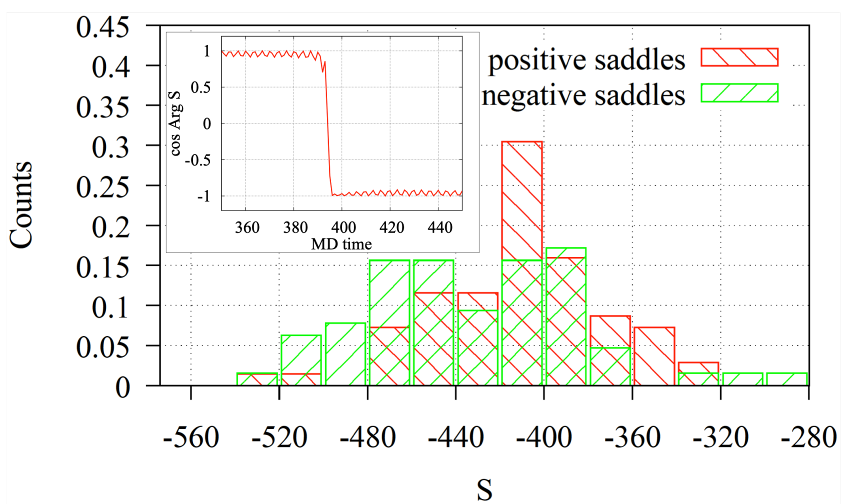
The distribution is not exact!

Dominant spin-coupled field





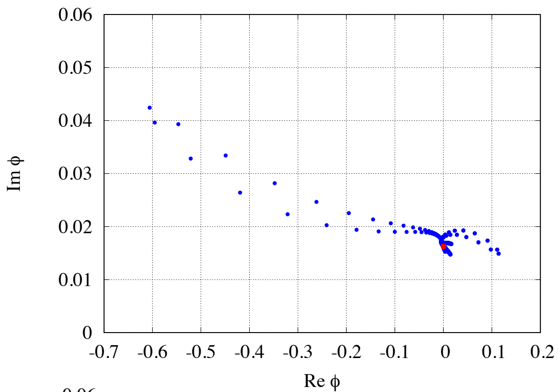




6x6 lattice, N_t=256, U=3.8, β=20.0, μ=1.0, α=0.0001

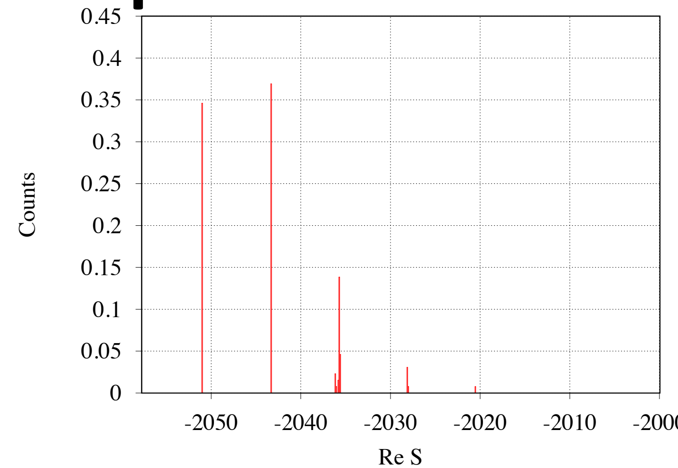
Dominant charge-coupled field

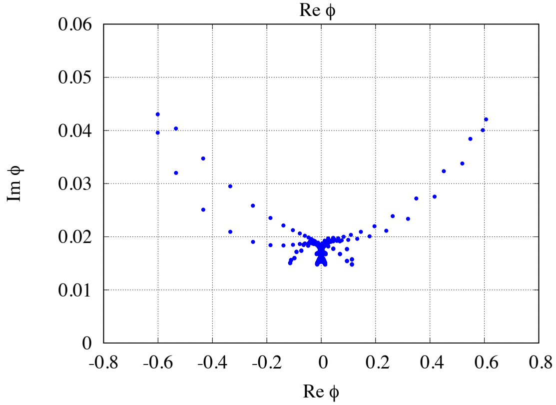
α=0.9, 6x6x256 lattice, U=3.8, β=20.0, μ=1.0



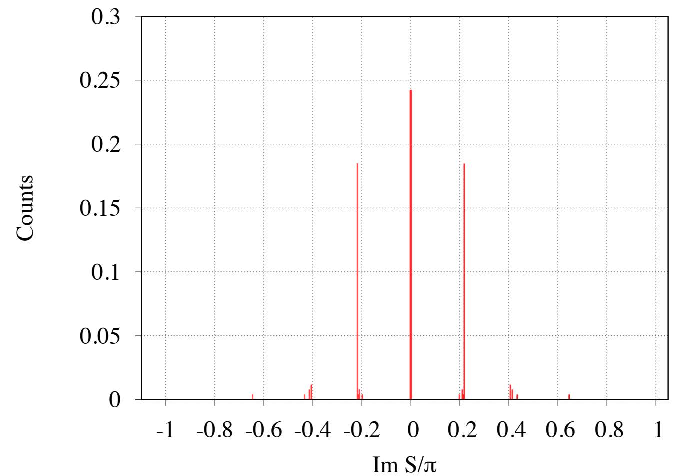
Different classes of saddle points:

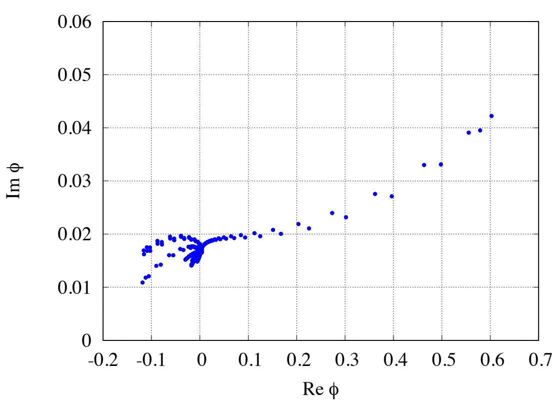
“0” and “↓”





“↑↓”



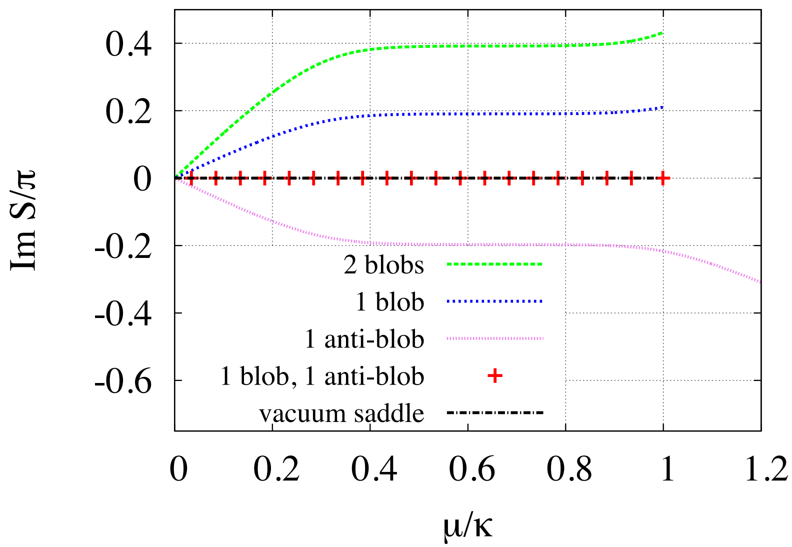


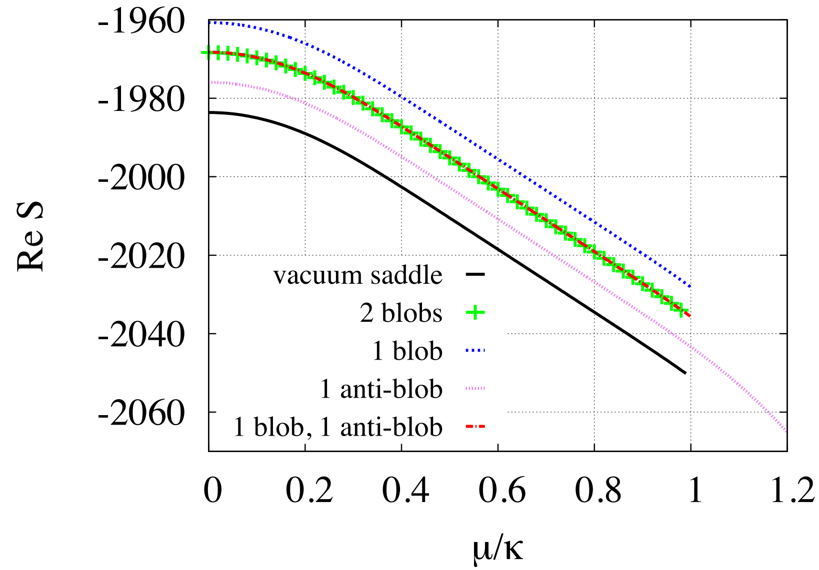
“↑↑”

Within the saddle point approximation, saddles with smaller phases will always dominate within the class with fixed weight: more variants with smaller phase (↑↑ and ↓↓ vs ↓↑ + ↑↓).

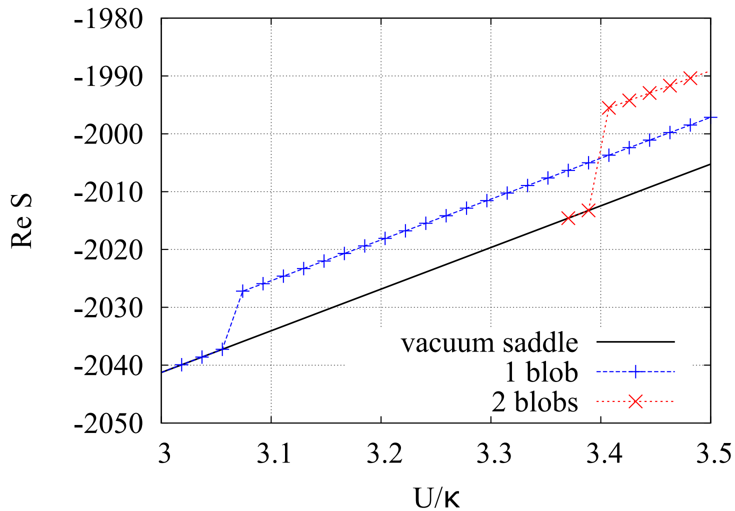
Saddle points and phase transitions

Dependence of saddle points on chemical potential:



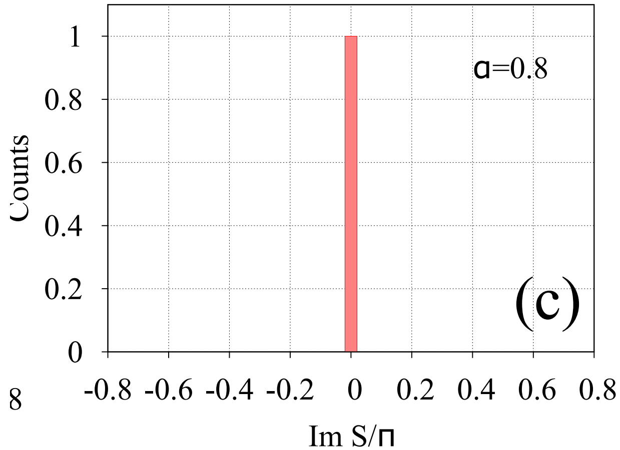


Dependence of saddle points on interaction strength:

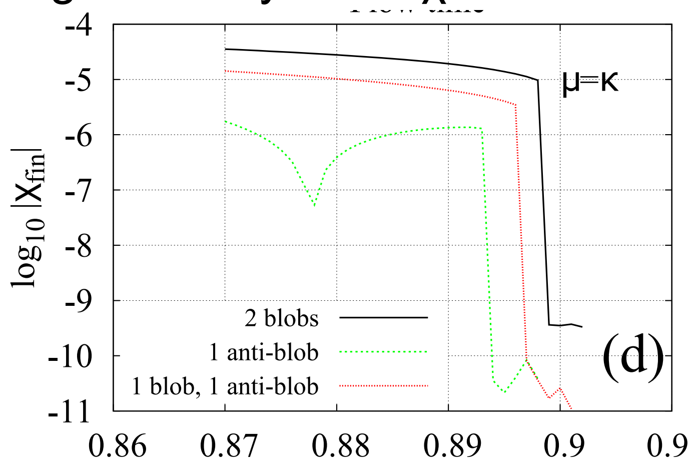


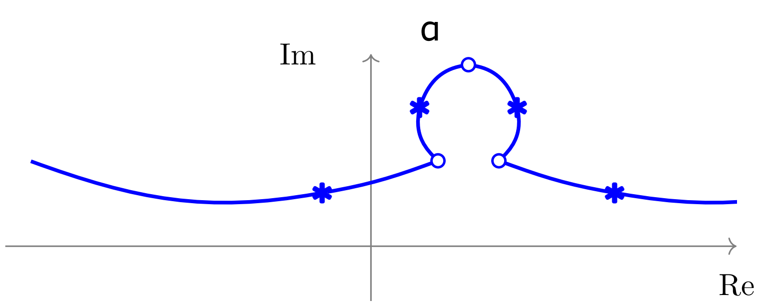
α=0.9

Optimal regime: α=0.8

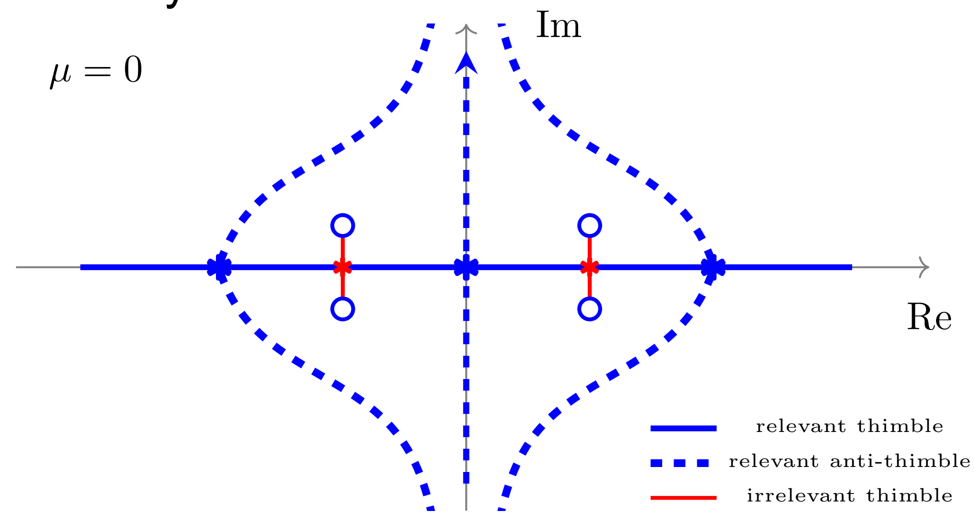


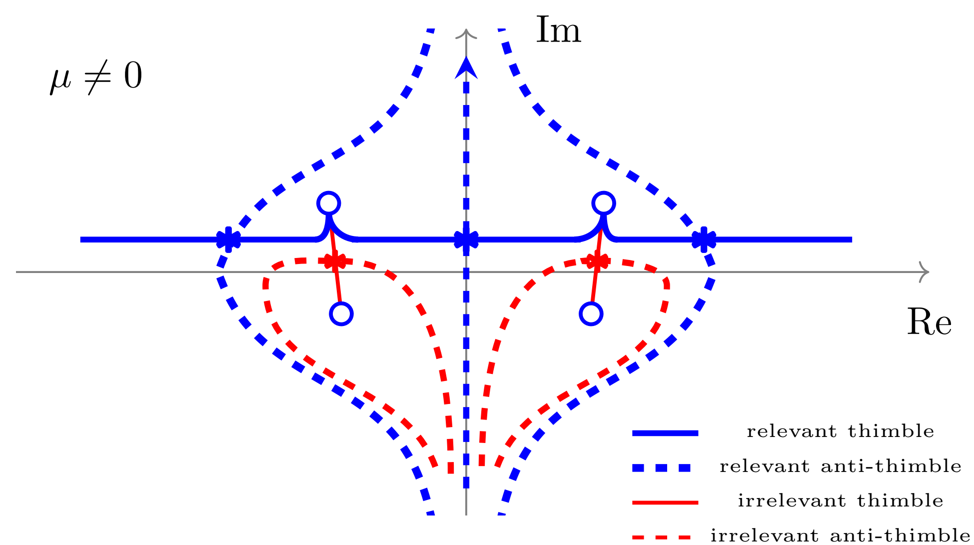
Again decay in Re χ direction:





Non-vacuum saddles are either irrelevant or "vertically oriented"





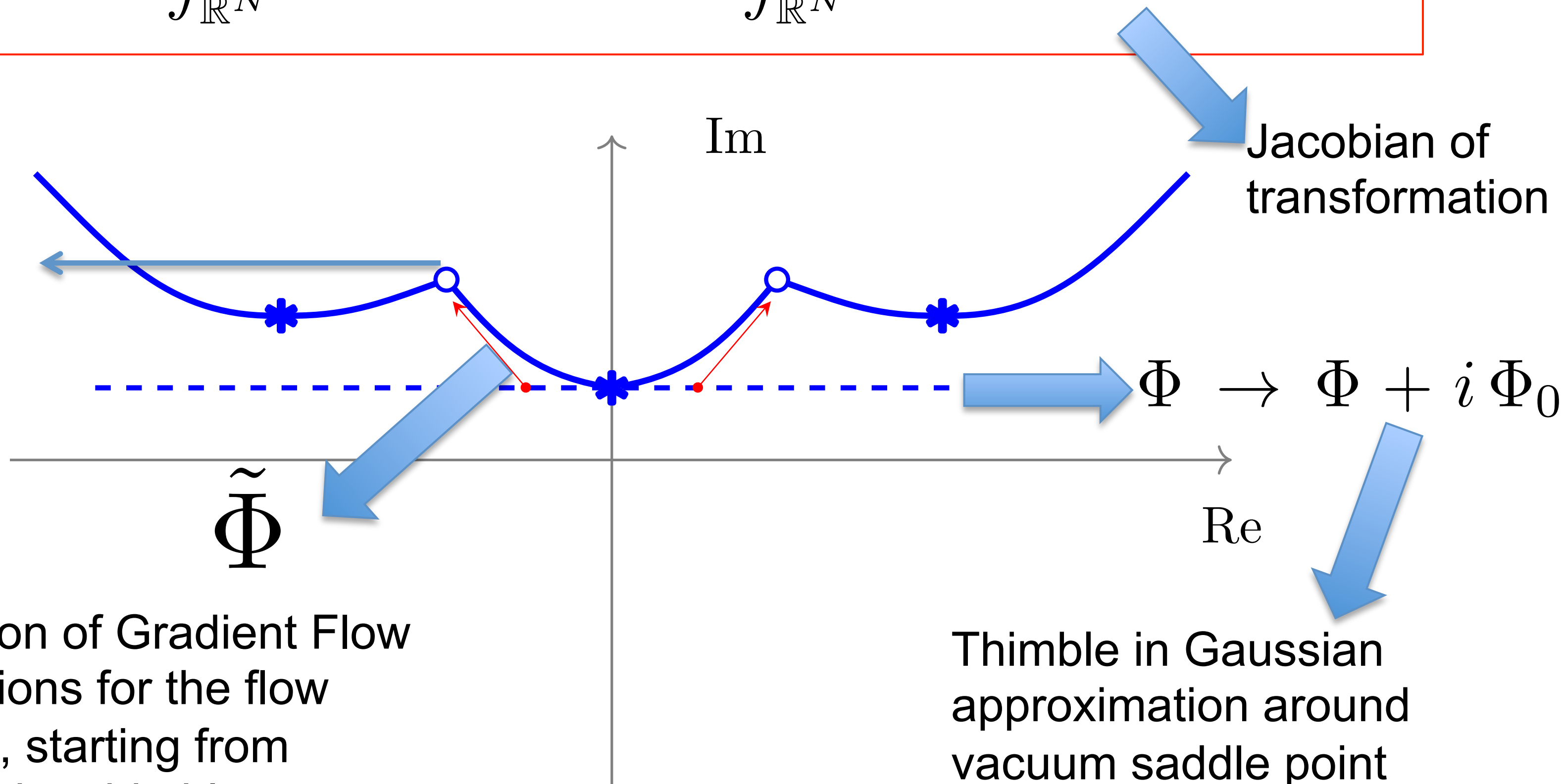
HMC with gradient flow

Approximates thimble with solution of Gradient Flow equations (following arXiv: 1609.01730):

$$\mathcal{Z} = \int_{\mathbb{R}^N} \mathcal{D}\Phi e^{-S[\Phi + i\Phi_0]} = \int_{\mathbb{R}^N} \mathcal{D}\Phi e^{-S[\tilde{\Phi}]} \det J.$$

Jacobian of transformation

Zeros of determinant can cause ergodicity issues



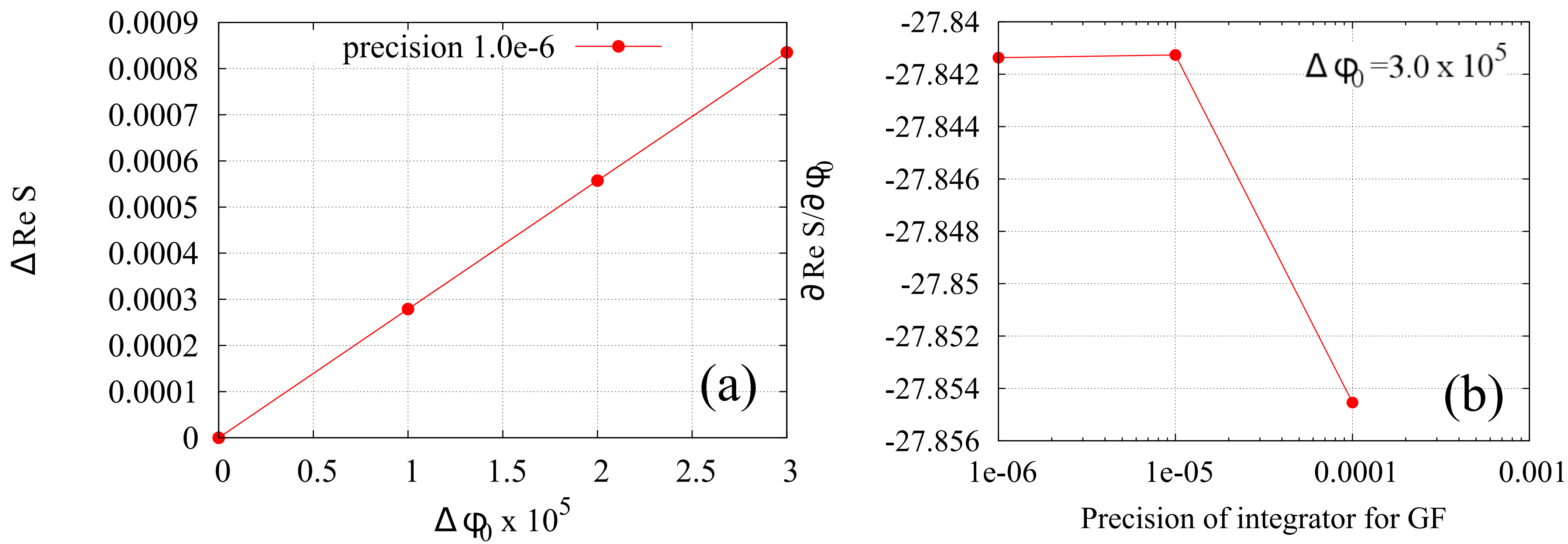
Solution of Gradient Flow equations for the flow time τ, starting from Gaussian thimble

Thimble in Gaussian approximation around vacuum saddle point

$$\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O} e^{i\,\mathrm{Im}(-S + \ln\det J) + \mathrm{Re}(\ln\det J)} \rangle}{\langle e^{i\,\mathrm{Im}(-S + \ln\det J) + \mathrm{Re}(\ln\det J)} \rangle}$$

HMC with gradient flow: calculation of derivatives

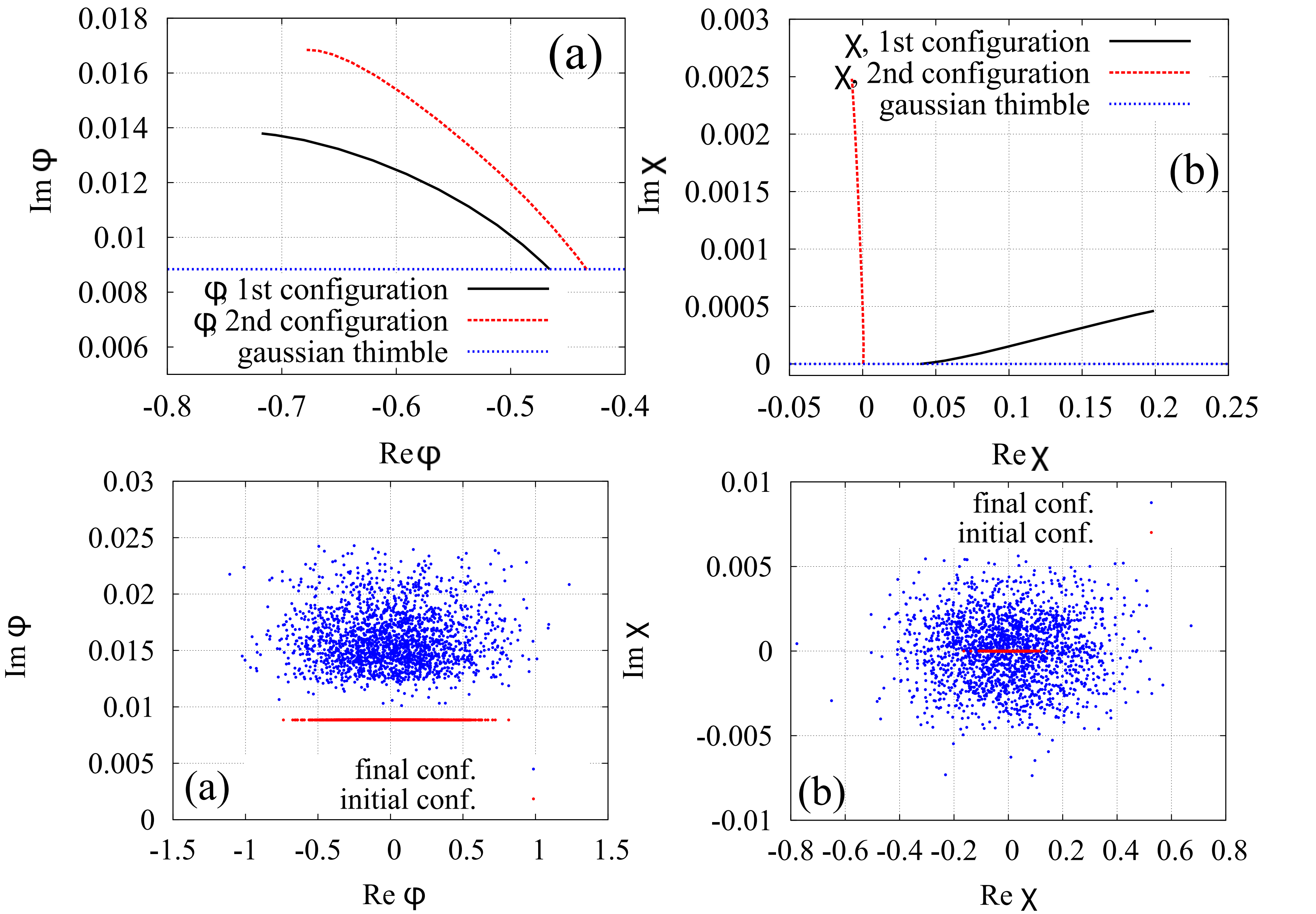
$$\partial \mathrm{Re} S[\tilde{\Phi}(\Phi + \Phi_0)] / \partial \Phi_i$$



Gradient Flow equations are solved for all individual shifts of auxiliary fields, to compute derivatives of the final action with respect to initial fields. Molecular dynamics for initial fields uses these derivatives.

Scaling: $C_\tau C_{MD} N_s^4 N_t^2$ instead of $N_s^3 N_t^1$ in BSS-QMC

HMC with gradient flow: examples



HMC with gradient flow: benchmarks (1)

2x2x256 lattice, U=2.0, β=20.0, μ=1.0

	Kinetic energy	**Spin-spin correlation**
Exact Diagonalization	19.5781	-0.14624
BSS-QMC (ALF)	19.587±0.002	-0.1466 ± 0.0008
HMC with flow α=1.0	19.65 ±0.31	-0.112 ± 0.0069
HMC with flow α=0.8	19.52 ± 0.17	-0.142 ± 0.0062

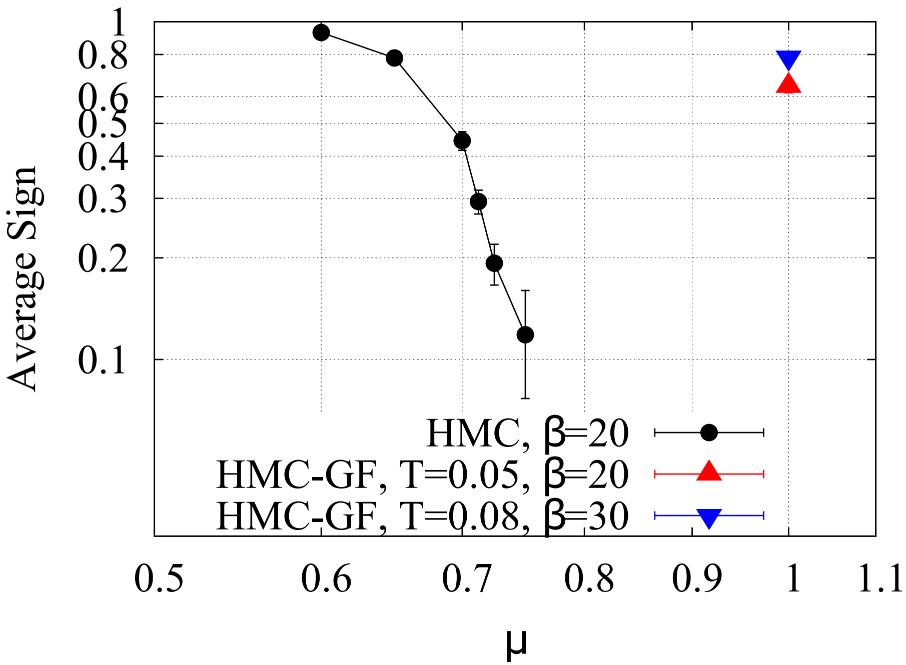
Comparison of observables with BSS-QMC and Ex. Diag.

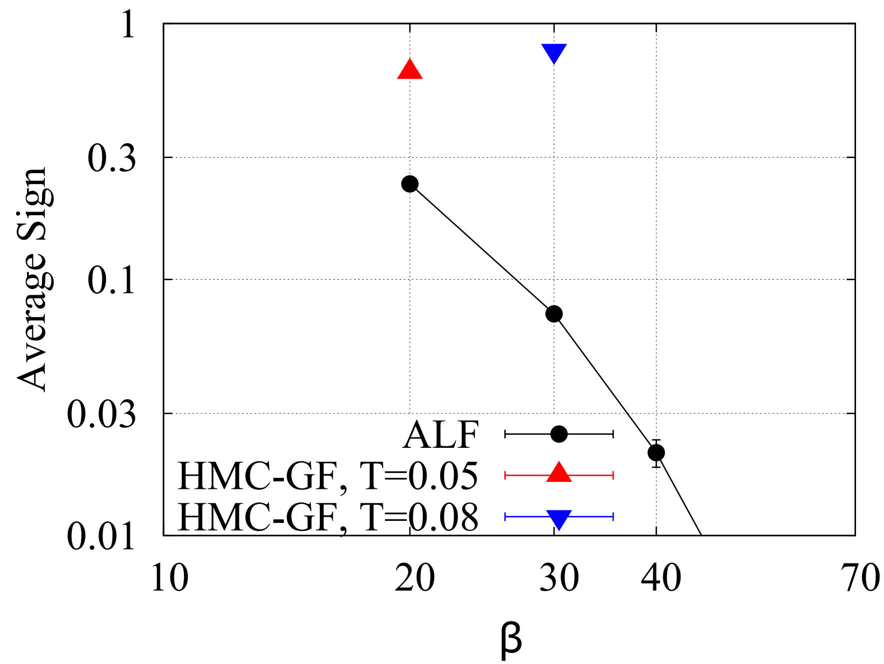
	cos Im S	**cos Arg J**	**Sign$_\Sigma$**
BSS-QMC (ALF)	0.2363 ± 0.0032		0.2363 ± 0.0032
HMC with flow α=1.0	0.9627± 0.0038	0.427 ± 0.014	0.351 ± 0.015
HMC with flow α=0.8	0.797 ± 0.022	0.915 ± 0.008	0.644 ± 0.028

Comparison of average sign with BSS-QMC for discrete fields

HMC with gradient flow: benchmarks (2)

2x2x2x256, 2x2x2x384 lattice; U=2.0, β=20.0, 30.0; μ=1.0





Also, recent tests on 2x4x2x256 lattice showed average sign>0.7

Possible problems due to growth of fluctuations of Jacobian:

N_t=256: <cos Arg J> = 0.915+-0.008, D_J=1.115

N_t=384: <cos Arg J> = 0.823+-0.018, D_J=1.68

Summary

1) Set of algorithms for fast solution of GF equations was developed.
2) Using this set of algorithm we could find saddle points both at half-filling at non-zero chemical potential. Thus we could study the properties of saddle point decomposition approaching continuum and thermodynamic limit.
3) There is optimal regime at intermediate values of alpha around 0.8, where only vacuum is important in overall sum (at half filling this result is numerically exact).
4) In optimal regime the ergodicity issues are weak enough for HMC-CG could reproduce exact diagonalization.
5) Further directions: Hubbard model on square lattice, QCD (?)