Complex instanton gas approximation for the Hubbard model away of half-filling

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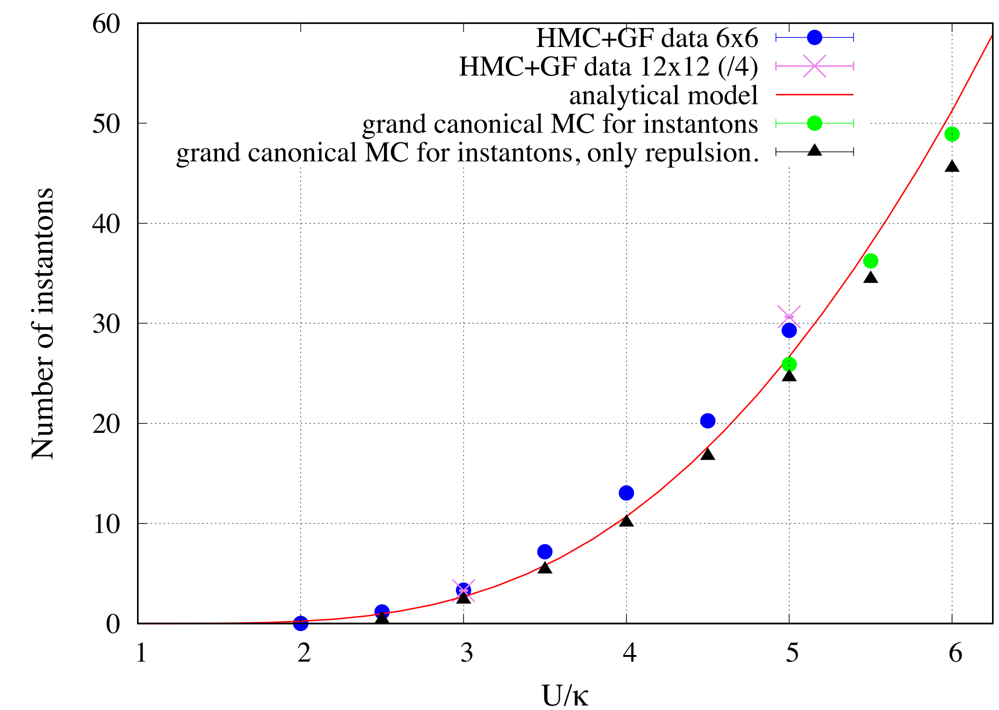
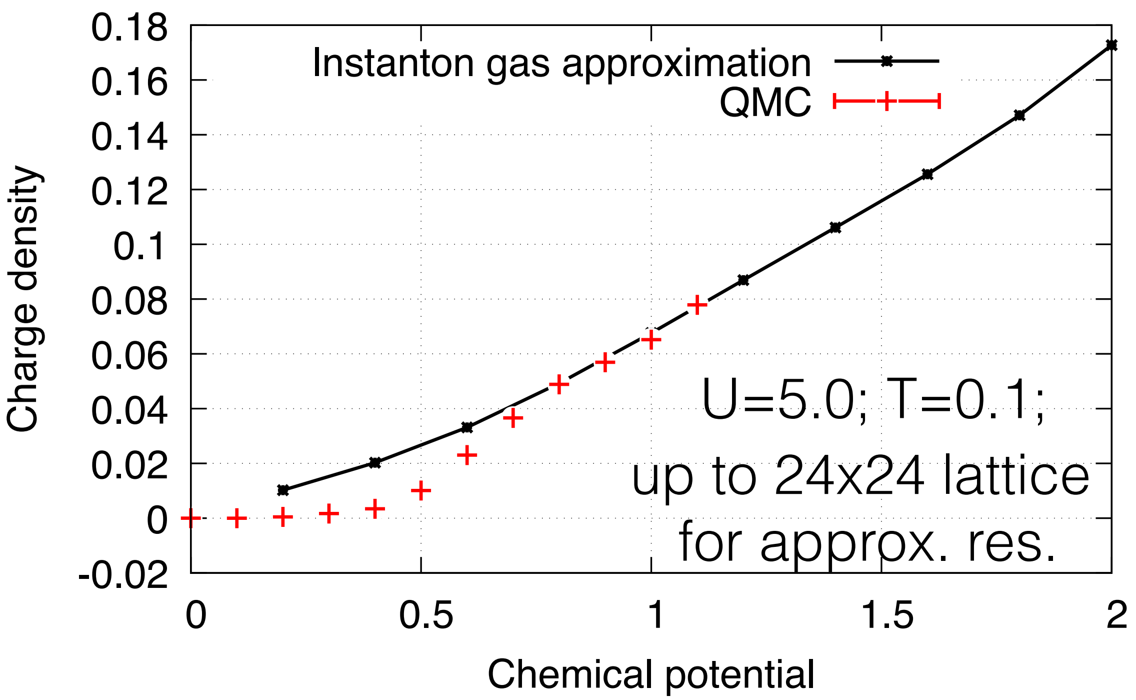
Goals

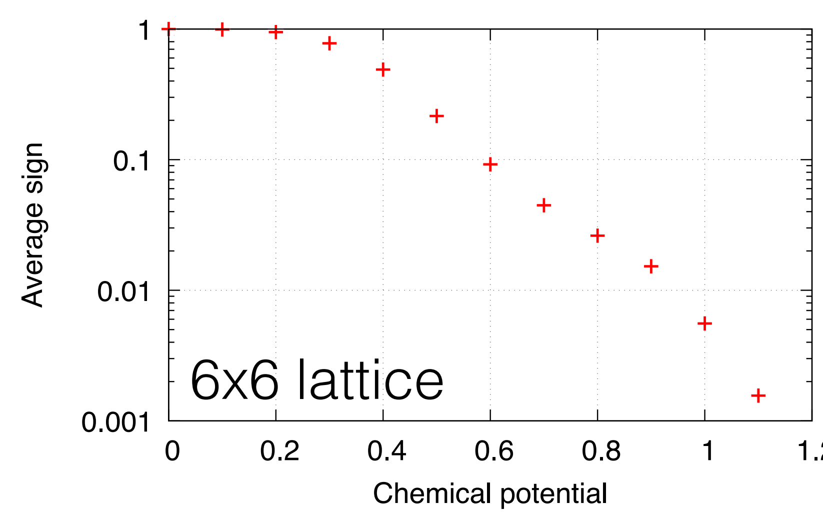
Systematic study of the thimbles decomposition of the path integral with the aim to develop an effective model predicting the phase and weight of thimbles without actual QMC simulation.

This model can be used:

1) to draw general conclusions about the difficulty of the sign problem;
2) to construct approximations extending to the regions of the phase diagram, where we are unable to perform QMC simulations.







Sign problem for the Hubbard model on bipartite lattice

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

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

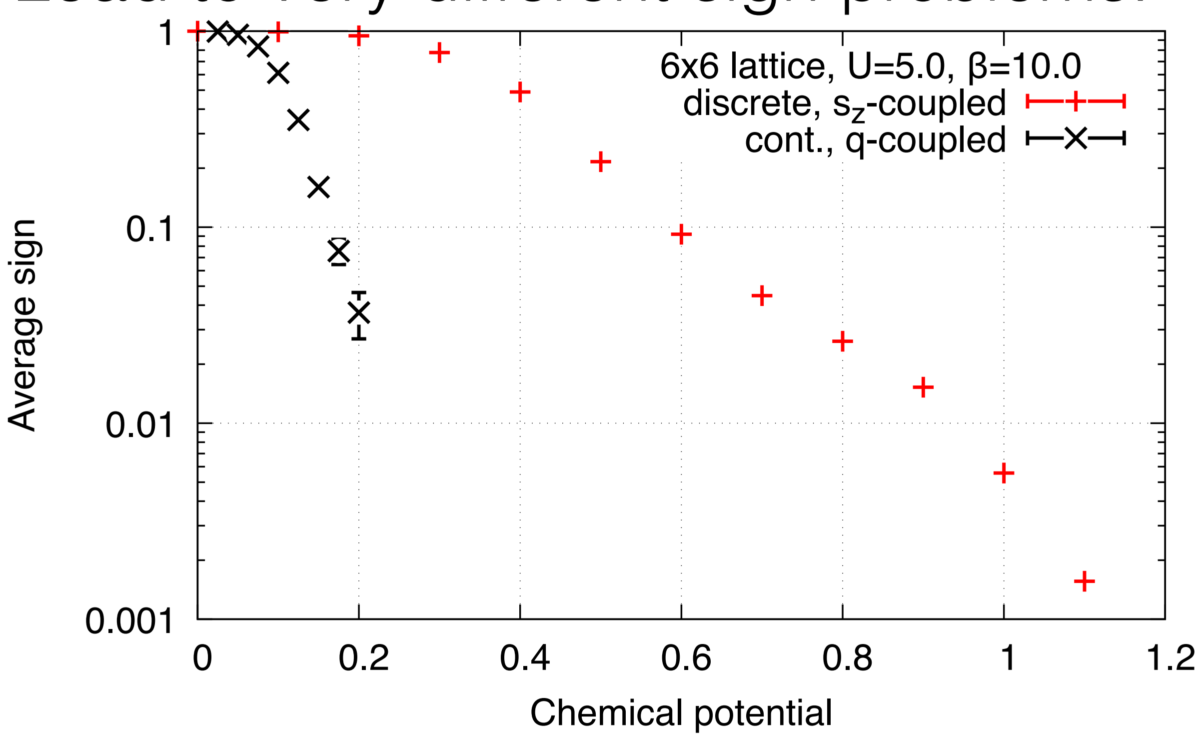
Different HS decompositions:

Discrete spin-coupled field:

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

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

Lead to very different sign problems:



Continuous charge-coupled field:

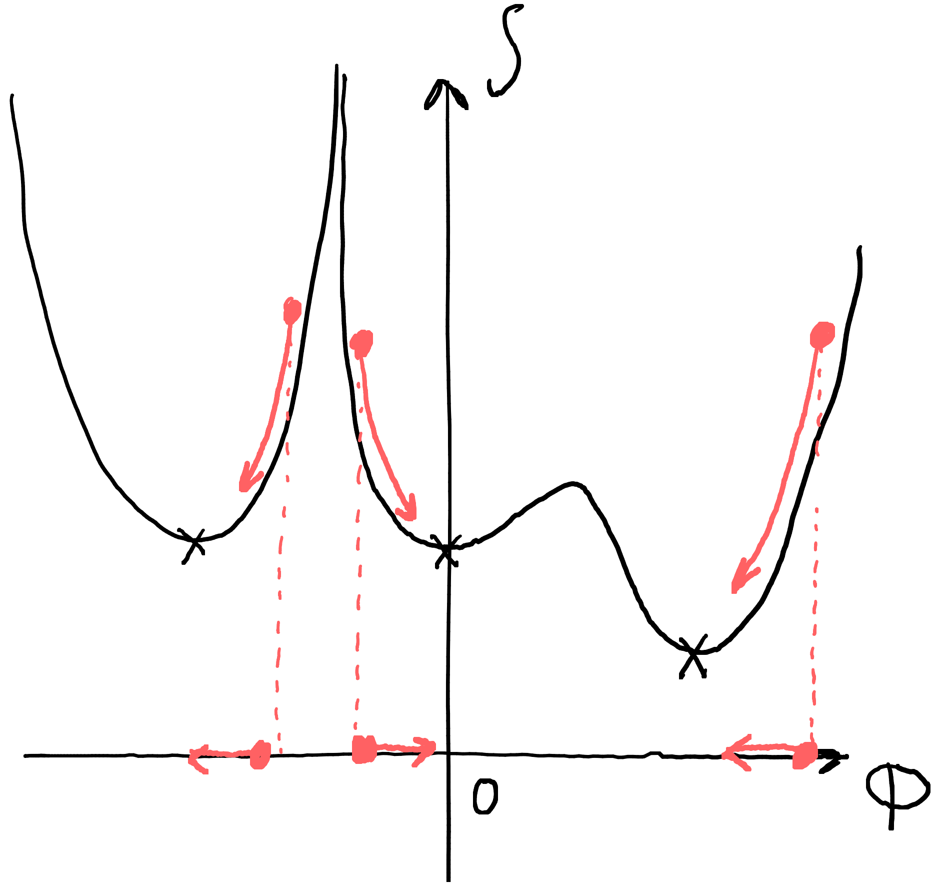
$$\begin{cases} \hat{c}_{x,\uparrow}, \hat{c}^\dagger_{x,\uparrow} \to \hat{a}_x, \hat{a}^\dagger_x, \\ \hat{c}_{x,\downarrow}, \hat{c}^\dagger_{x,\downarrow} \to \pm\hat{b}^\dagger_x, \pm\hat{b}_x \end{cases}$$

$$\hat{H} = -\kappa \sum_{\langle x,y\rangle} (\hat{a}^\dagger_x \hat{a}_y + \hat{b}^\dagger_x \hat{b}_y) + \frac{U}{2}\sum_x (\hat{n}_{x,el.} - \hat{n}_{x,h.})^2 + \mu\sum_x (\hat{n}_{x,el.} - \hat{n}_{x,h.})$$

$$e^{-\frac{\Delta\tau}{2}U\hat{q}^2_{\boldsymbol{x}}} \cong \int d\phi_{\boldsymbol{x}} e^{-\frac{\phi^2_{\boldsymbol{x}}}{2U\Delta\tau} + i\phi_{\boldsymbol{x}}\hat{q}_{\boldsymbol{x}}}$$

However, reasonable approximation to the thimbles weight can be only constructed for charge-coupled field

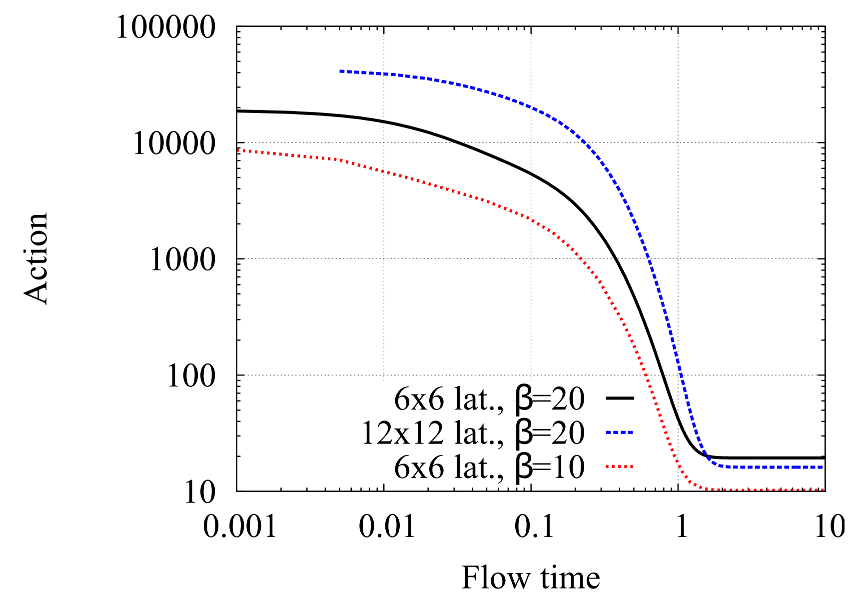
Recovering exact saddle points from Hybrid Monte Carlo data



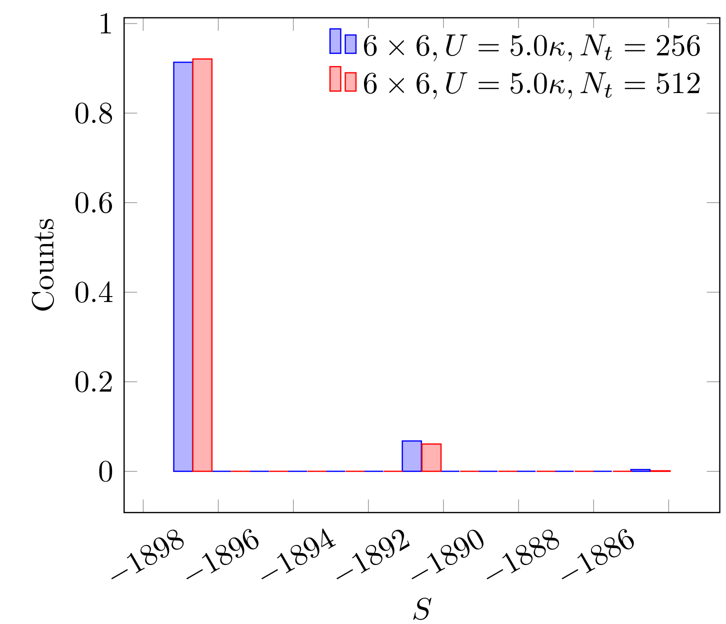
$$\mathcal{Z} = \int_{\mathbb{R}^N} \mathcal{D}\Phi \, e^{-S[\Phi]} = \sum_{\sigma} k_\sigma \mathcal{Z}_\sigma$$

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

History of the action:



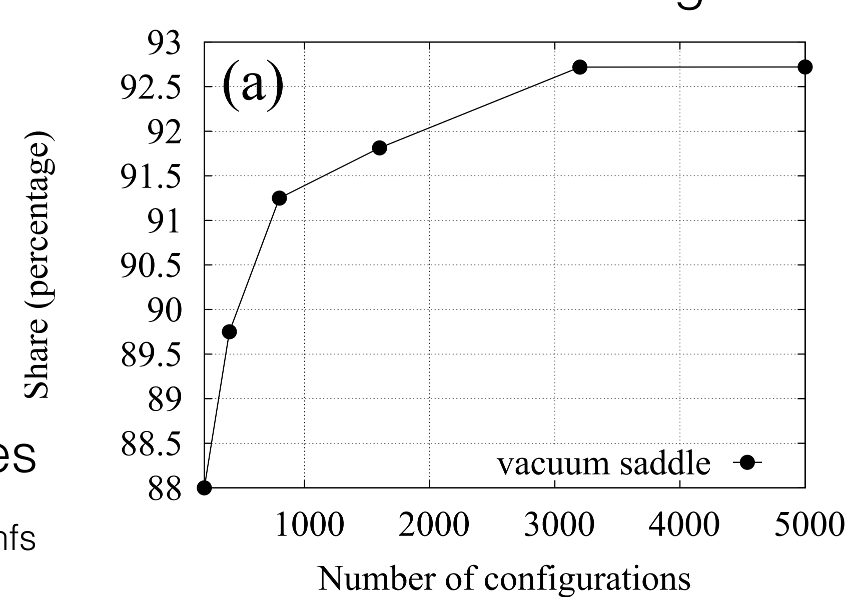
Histogram:

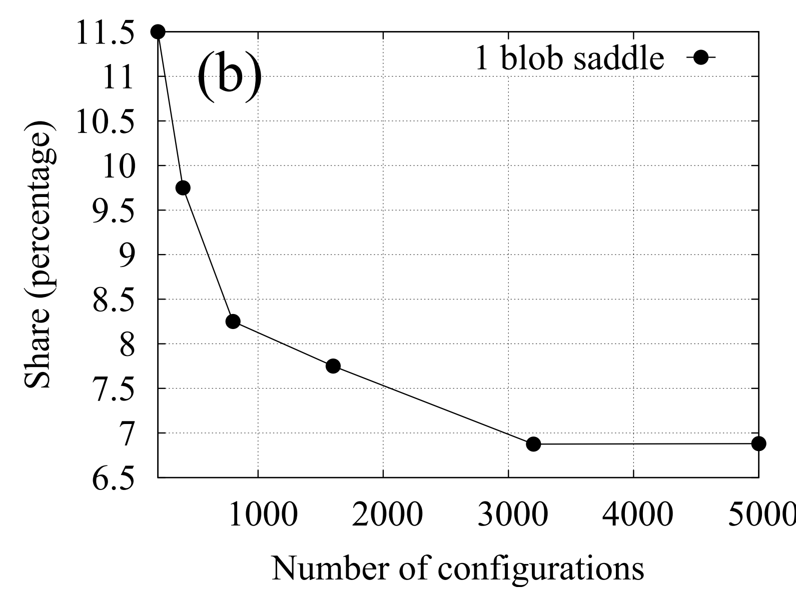


1) generation of lattice field configurations;
2) GF for each configuration;
3) Histogram for the final actions after GF shows

$$\frac{Z_\sigma}{Z}$$

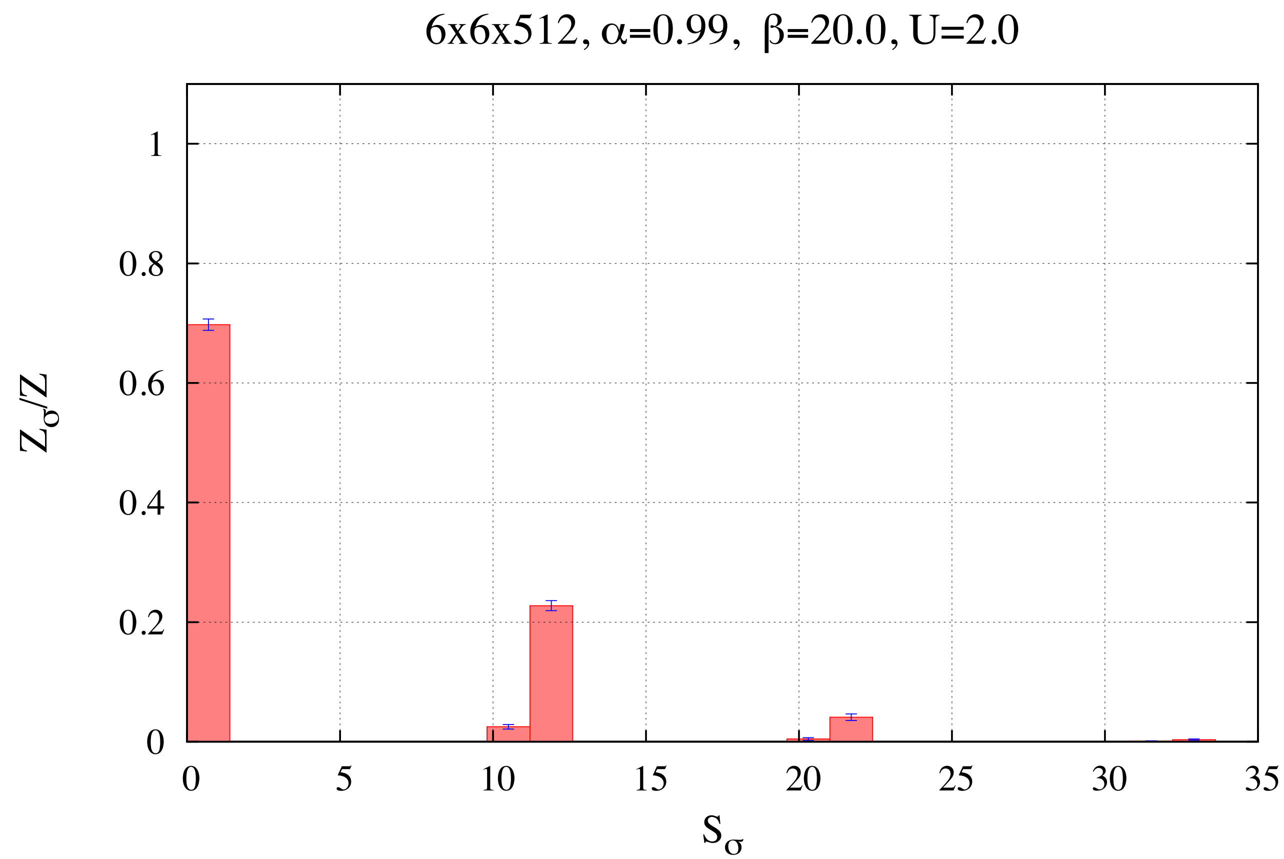
Stabilization of the histogram:

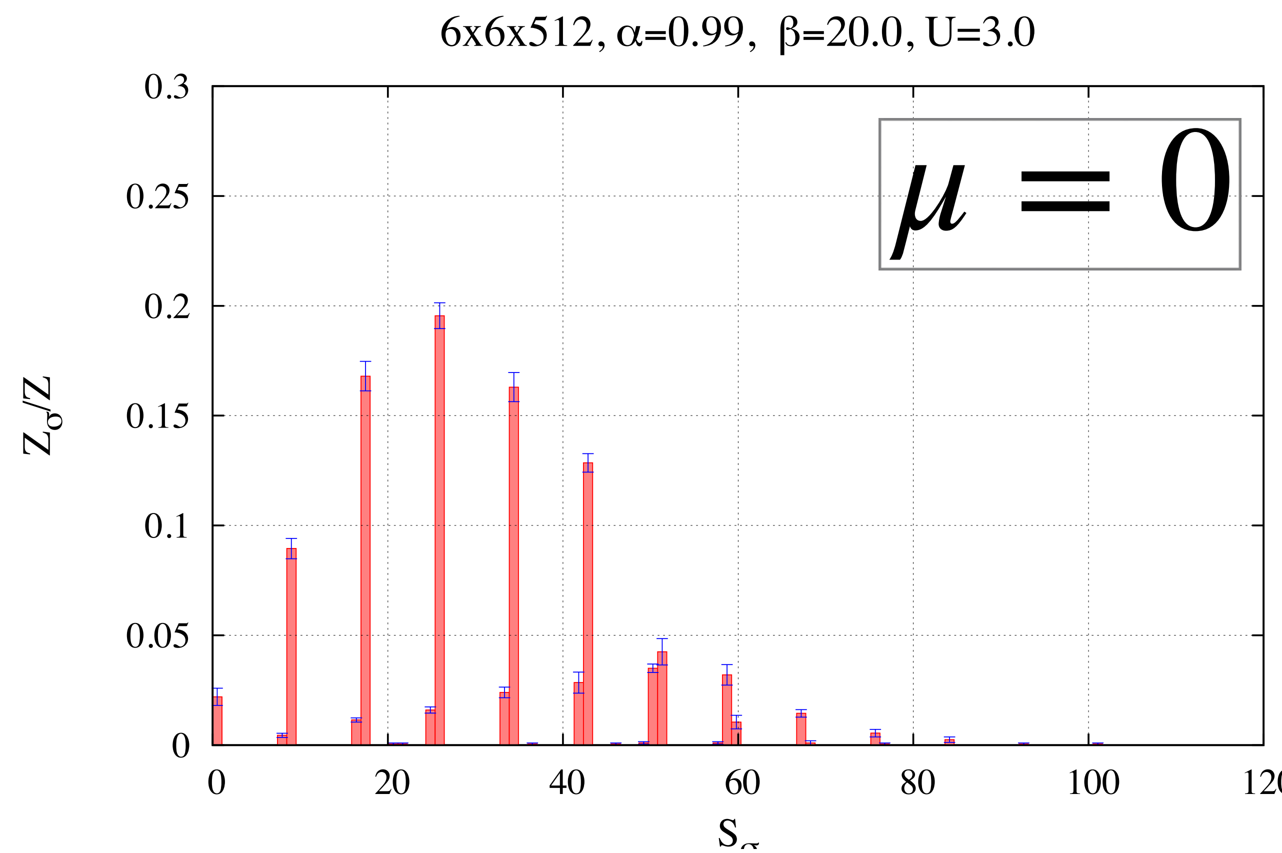


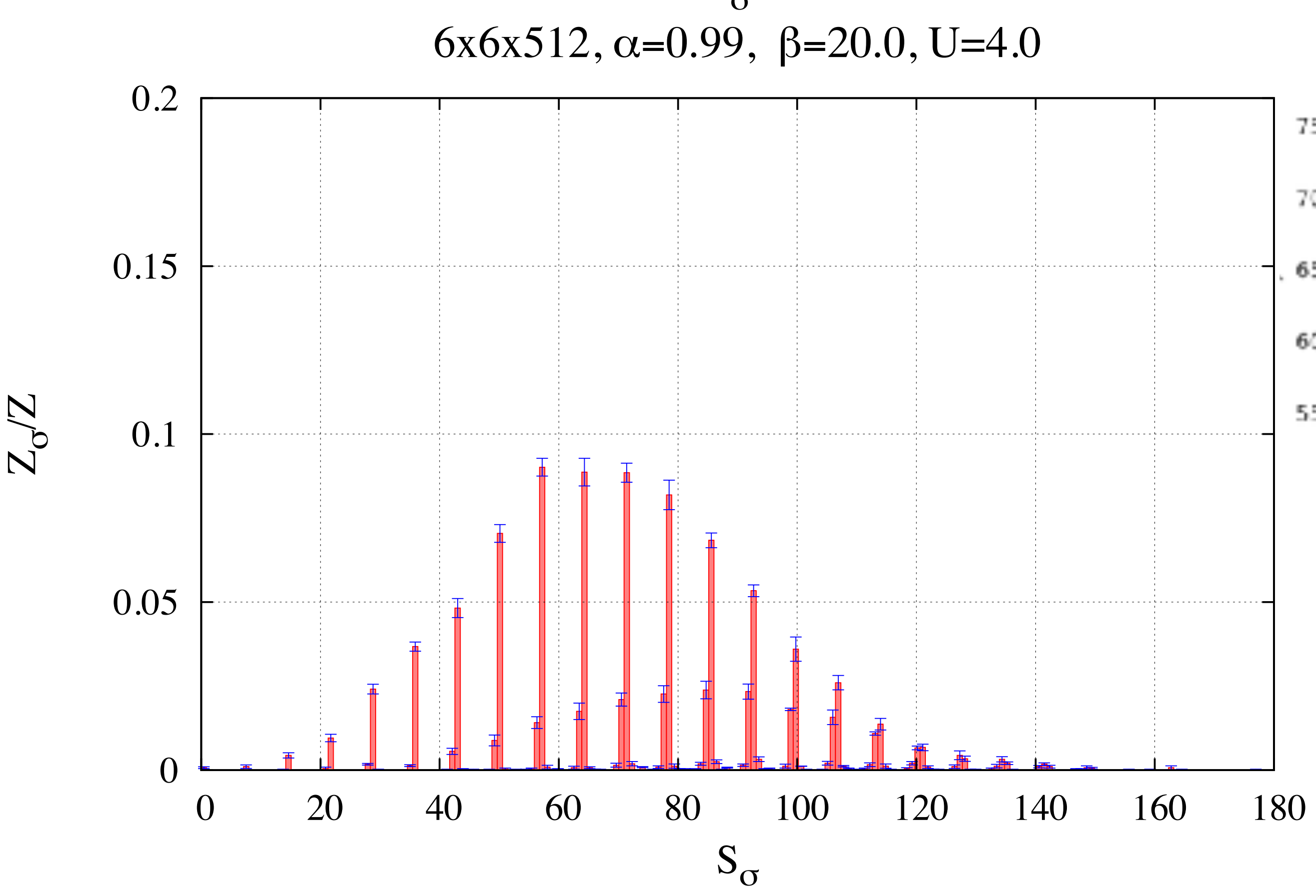


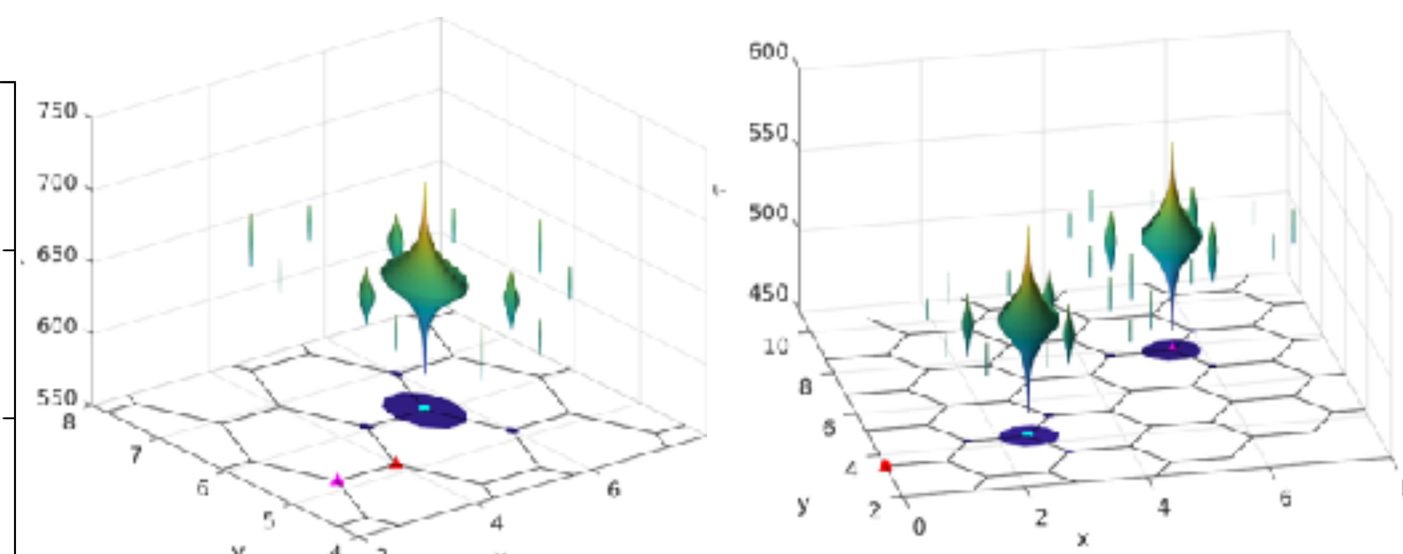
If HMC is ergodic, we can find all saddles with the share in partition function > $1/N_{\mathrm{confs}}$

Examples of saddles for the Hubbard model on hexagonal lattice









Building blocks for saddle point field configurations are localized both in space and Euclidean time: instantons and anti-instantons

Examples of saddles for the Hubbard model on hexagonal lattice: spin-coupled field (1)

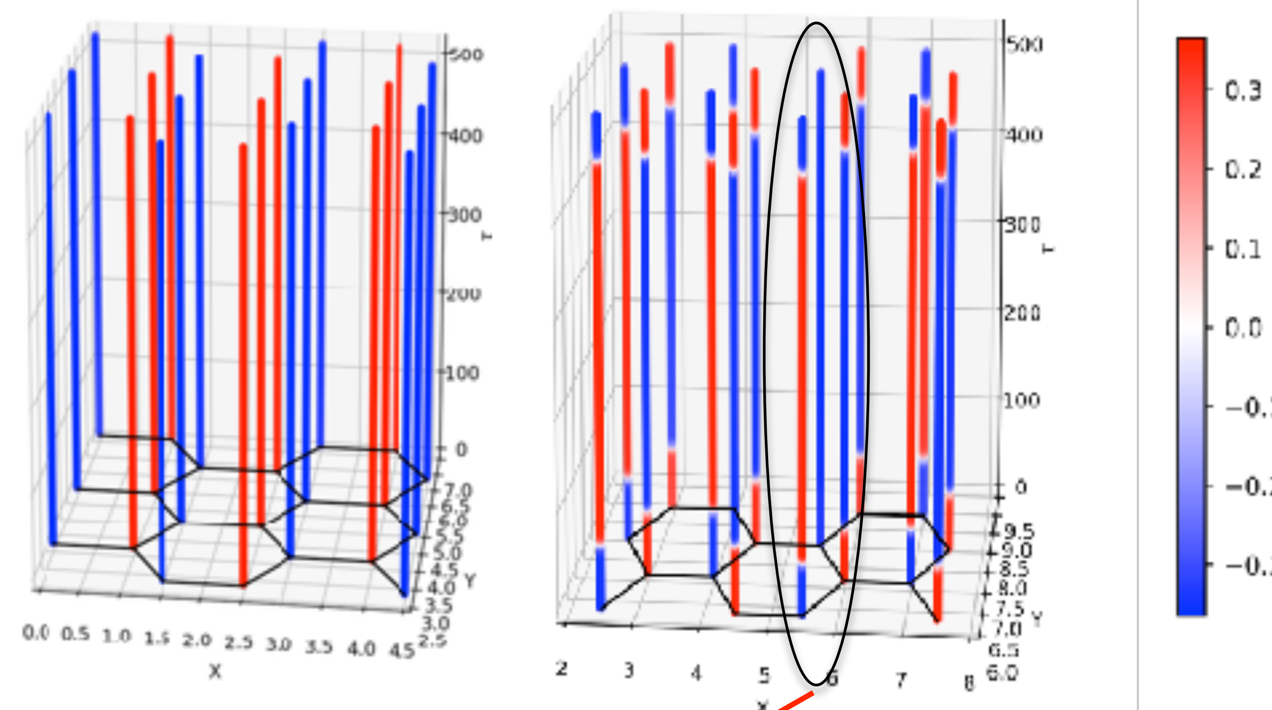
$$\frac{U}{2}(\hat{n}_{el.} - \hat{n}_{h.})^2 = \frac{\alpha U}{2}(\hat{n}_{el.} - \hat{n}_{h.})^2 - \frac{(1-\alpha)U}{2}(\hat{n}_{el.} + \hat{n}_{h.})^2 + (1-\alpha)U(\hat{n}_{el.} + \hat{n}_{h.})$$

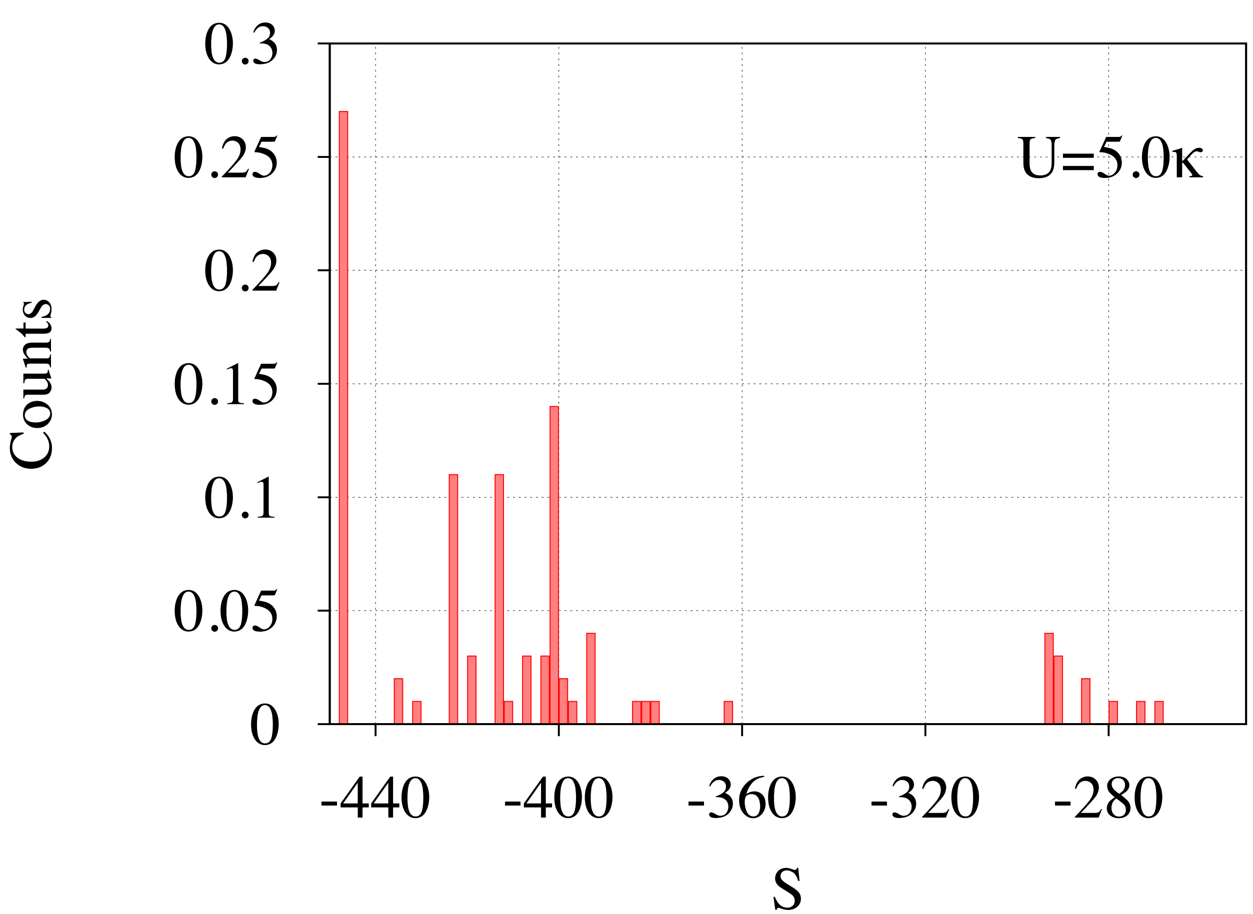
$$\mathcal{Z}_c = \int \mathcal{D}\phi_{x,\tau}\, \mathcal{D}\chi_{x,\tau}\, e^{-S_\alpha} \det M_{\text{el.}} \det M_{\text{h.}}$$

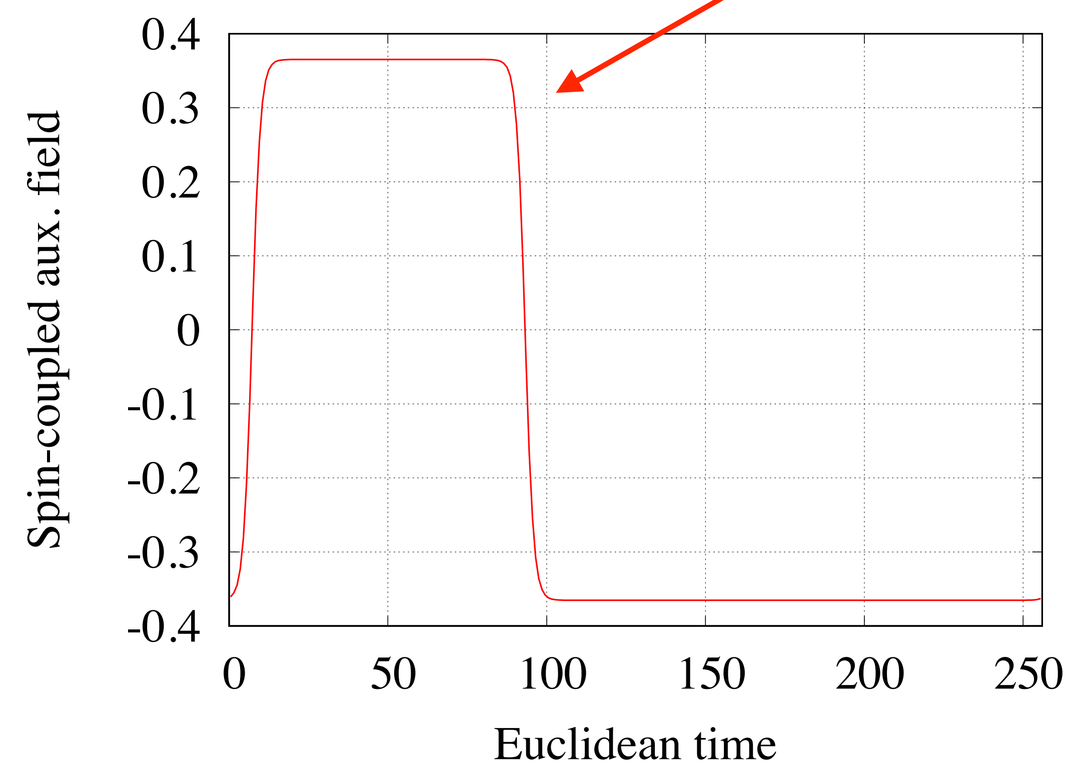
$$S_\alpha[\phi_{x,\tau}, \chi_{x,\tau}] = \sum_{x,\tau}\left[\frac{\phi^2_{x,\tau}}{2\alpha\delta U} + \frac{(\chi_{x,\tau} - (1-\alpha)\delta U)^2}{2(1-\alpha)\delta U}\right]$$

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

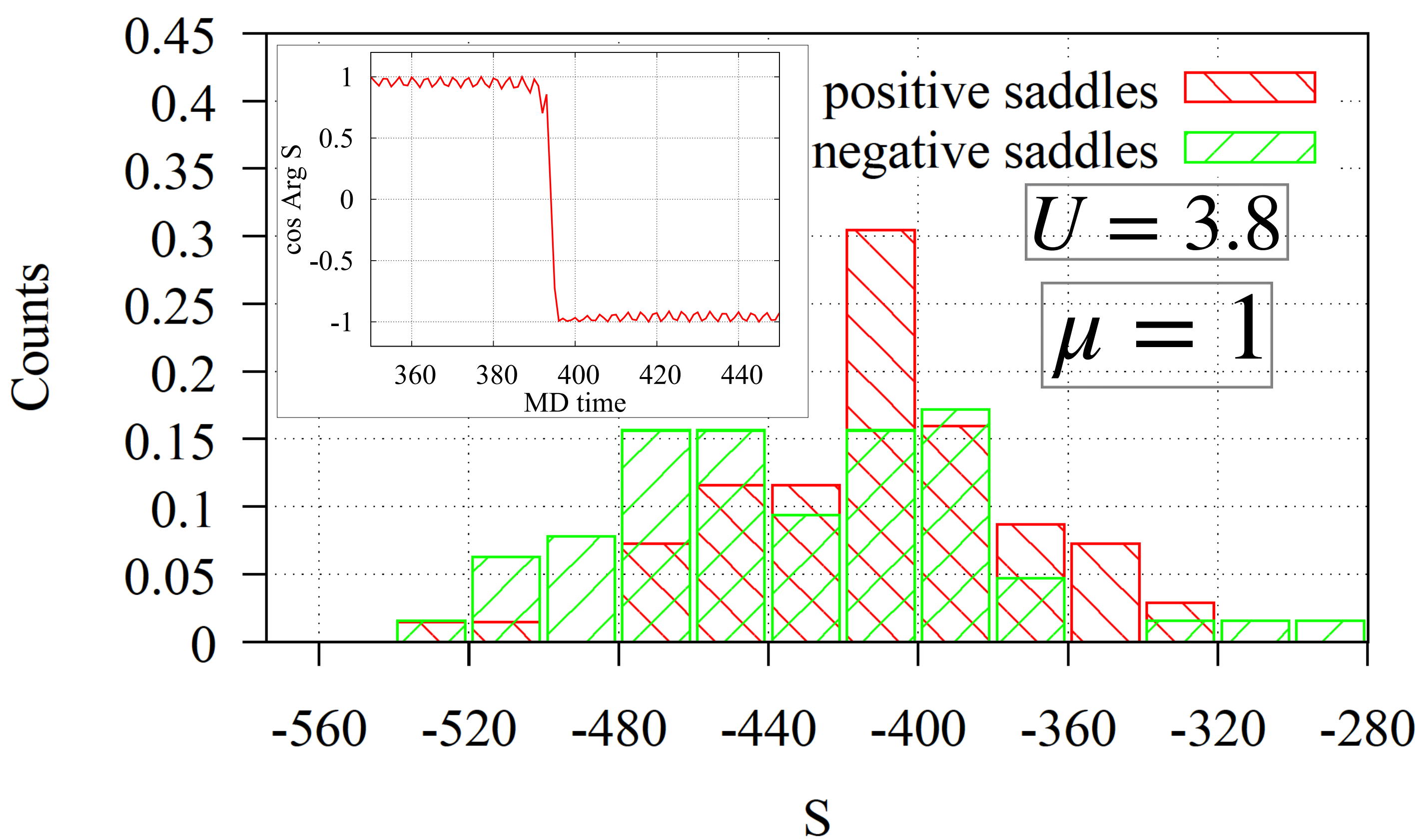
$\boxed{\mu = 0}$



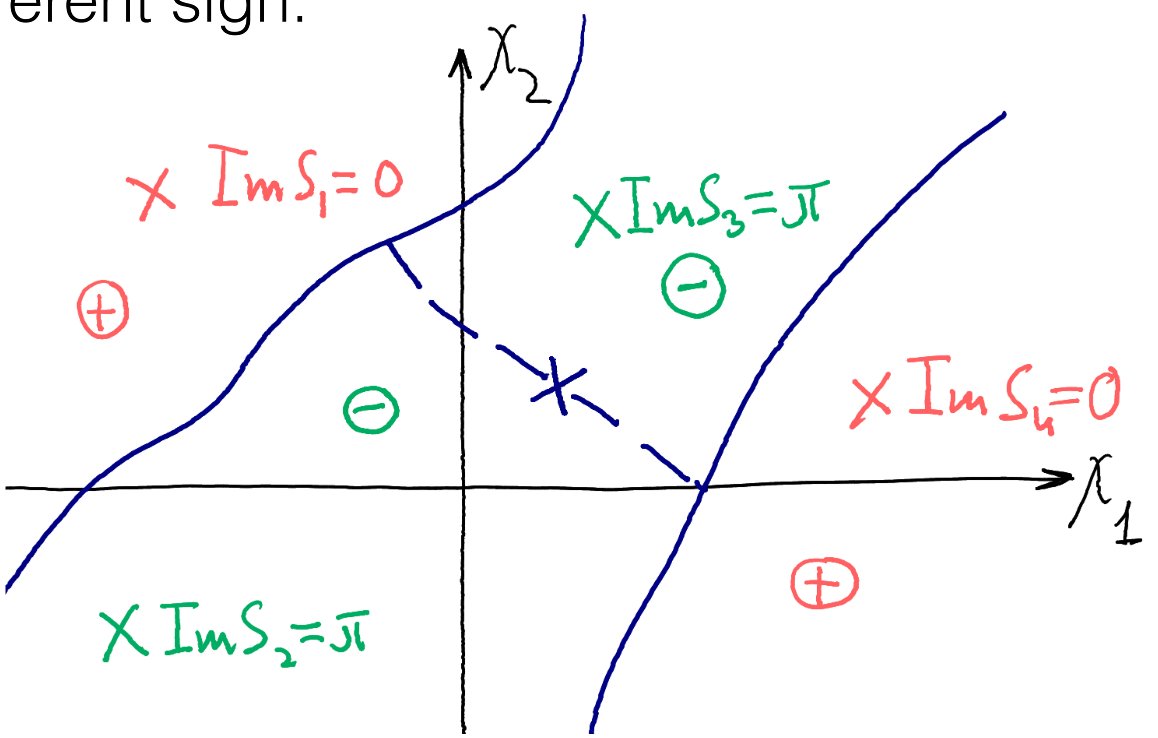


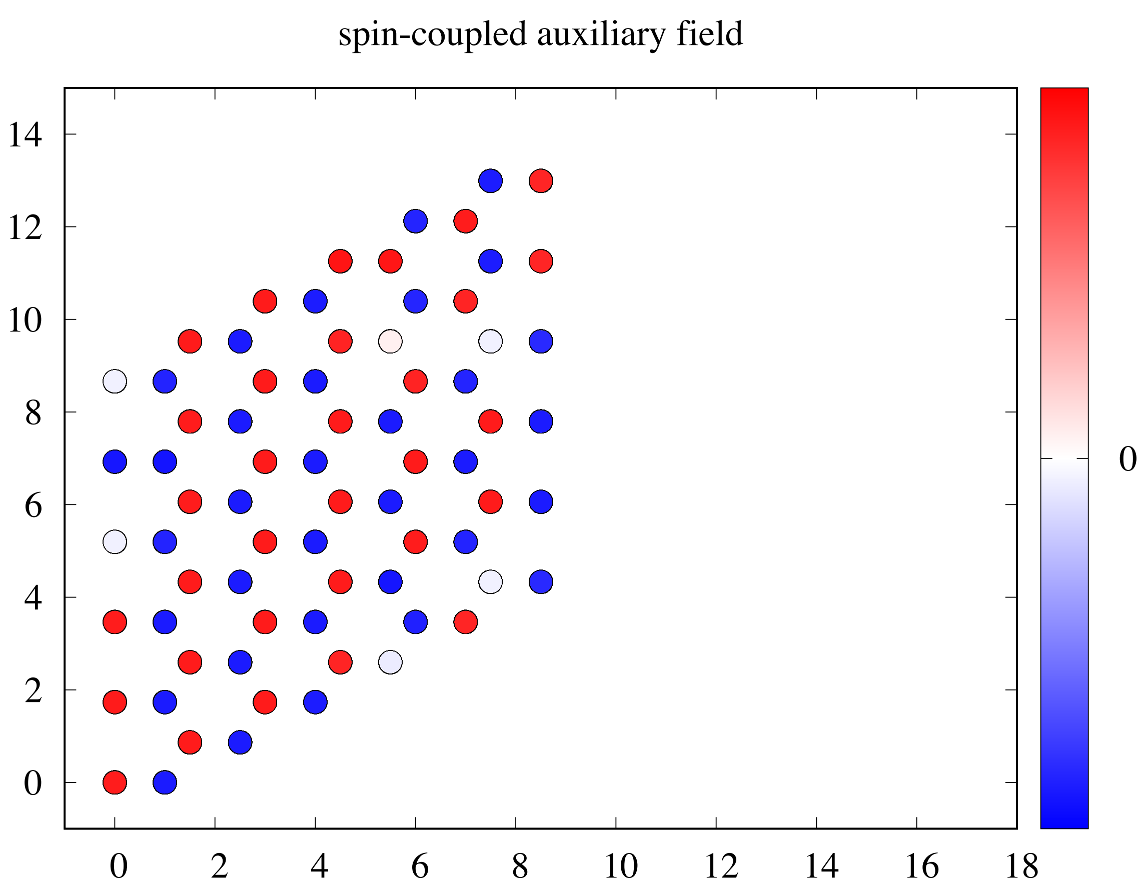


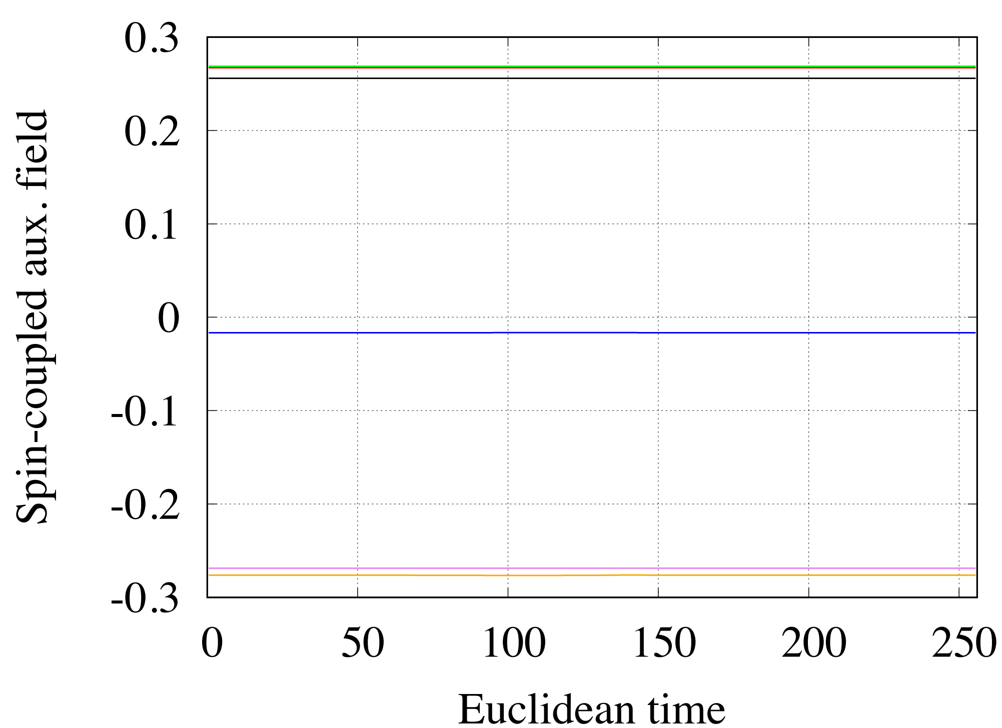
Examples of saddles for the Hubbard model on hexagonal lattice: spin-coupled field (2)



Saddle points are real but can have different sign:







Analytical solution for instantons (1)

$$S = \frac{\sum_{x,\tau} (\phi_{x,\tau})^2}{2U\Delta\tau} - \ln\det\left(M_{el.}M_{h.}\right)$$

$$\frac{\partial S}{\partial \phi_{x,\tau} x} = \frac{\phi_{x,\tau}}{\Delta\tau U} - \left(g^{2\tau}_{xx} i e^{i\phi_{x,\tau}} - \overline{g^{2\tau}_{xx}} i e^{-i\phi_{x,\tau}}\right) = 0 \xrightarrow{\Delta\tau \to 0} \phi_{x,\tau} = -U \,\mathrm{Im}\, g^{\tau}_{xx}$$

+Euclidean time evolution for equal-time GF

$$g^{(\tau+1)} = \{e^{-i\phi_{x,(\tau+1)}}\} e^{\Delta\tau h} g^{\tau} \{e^{i\phi_{x,(\tau+1)}}\} e^{-\Delta\tau h}$$

$$\begin{cases} \frac{d}{d\tau}\mathrm{Im}\, g_{xx}(\tau) = 6\kappa\, \mathrm{Im}\, g_{xy}(\tau) \\ \frac{d}{d\tau}\mathrm{Im}\, g_{xy}(\tau) = iU g_{xy}(\tau) \mathrm{Im}\, g_{xx}(\tau) + i\kappa\, \mathrm{Im}\, g_{xx}(\tau) \end{cases}$$

(locality of the solution is taken into account)

Nearest neighbors

At half-filling:

$$\mathrm{Im}\, g_{xx}(\tau) = d(\tau), \quad \mathrm{Re}\, g_{xx}(\tau) = 1/2, \quad g_{xy}(\tau) = a(\tau) + ib(\tau)$$

$$g_{<xy>}|_{vac.} = -1/G + R$$

$$G = U/\kappa$$

$$\begin{cases} a(\tau) = -1/G + R\cos\theta(\tau) \\ b(\tau) = R\sin\theta(\tau) \\ d(\tau) = \dot{\theta}(\tau)/G \end{cases}$$

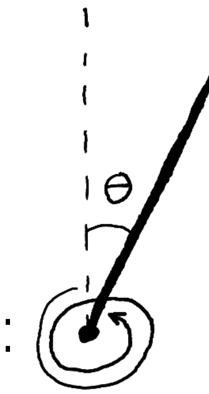
$$\boxed{\ddot{\theta}(s) = \sin\theta(s), s = \kappa\tau\sqrt{6GR}, s = 0...\kappa\beta\sqrt{6GR}}$$

Analytical solution for instantons (2)

Number of instantons and anti-instantons fixes the initial conditions

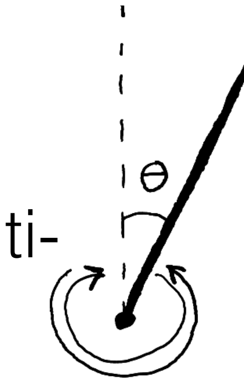
$$\frac{\dot{\theta}^2}{2} + \cos\theta = E_0 \qquad \beta / N_{inst.} = 2\int_0^{\pi} \frac{d\theta}{\sqrt{2(E_0 - \cos\theta)}}$$

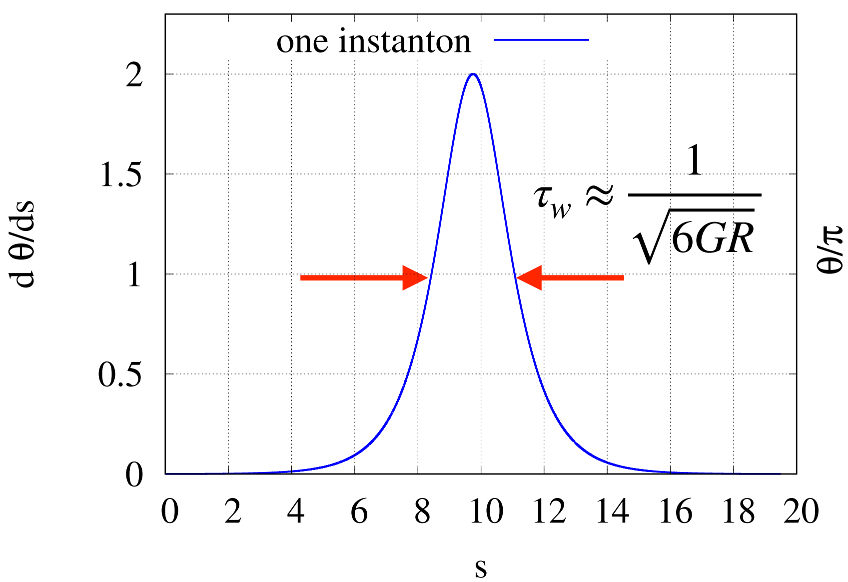
Two instantons:

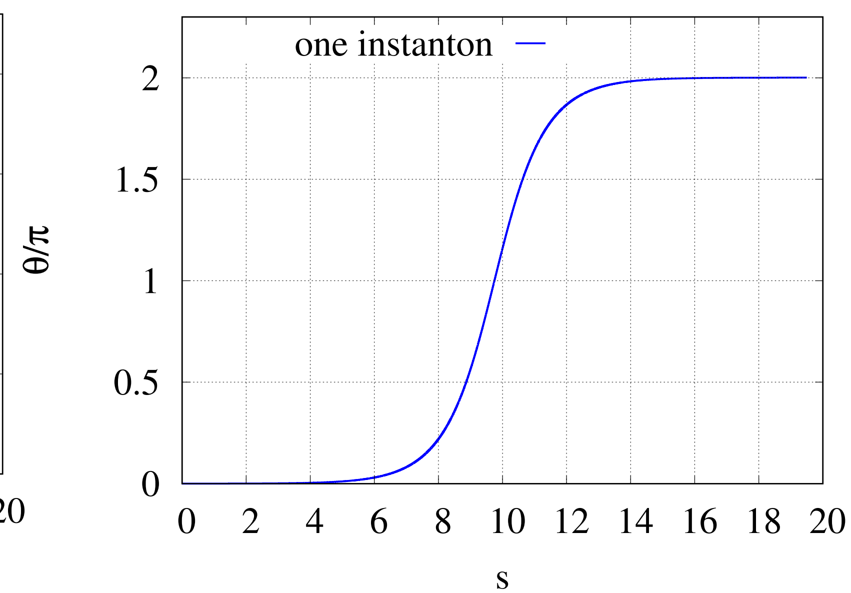


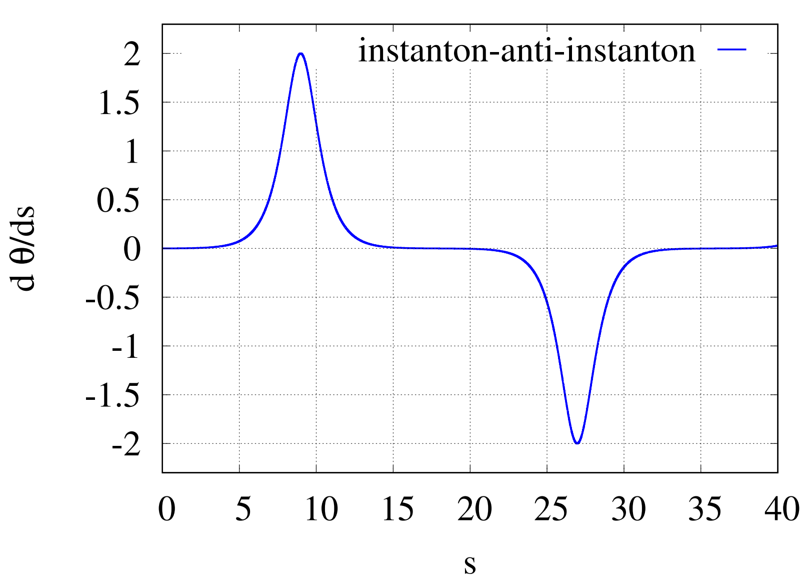
Analytical solution is possible in terms of elliptic integrals.

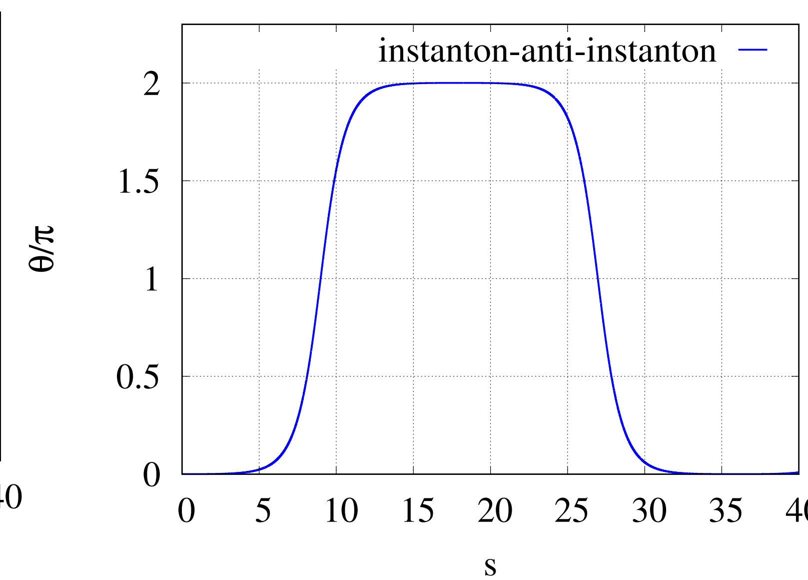
Instanton and anti-instanton:











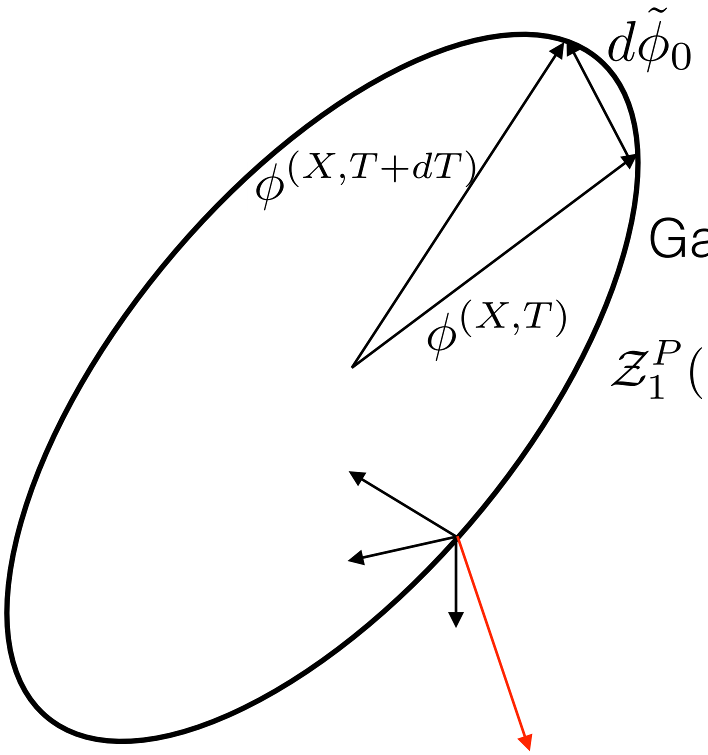
Reminder:

$$\boxed{\begin{gathered} \phi_x^\tau = -\,U\,\mathrm{Im}\,\bar{g}_{xx}^\tau \\ \mathrm{Im}\,g_{xx}(\tau) = d(\tau) \\ d(\tau) = \dot{\theta}(\tau)/G \end{gathered}}$$

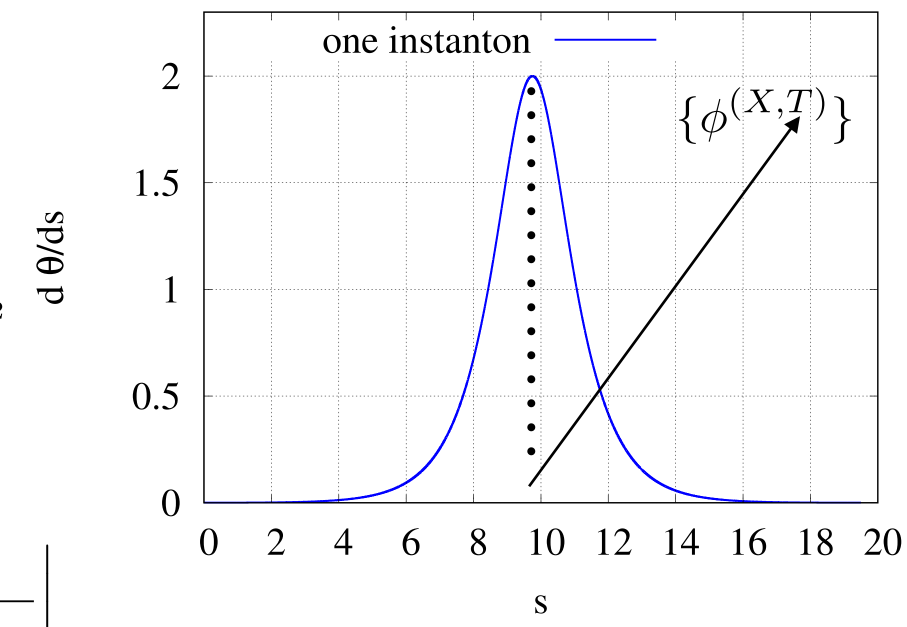
Winding number:

$$W = \frac{1}{2\pi}\int_0^{\beta} d\tau\,\theta(\tau)$$

Role of continuous symmetries



$$\mathcal{Z}_1 = 2N_S \mathcal{Z}_1^P(\{\phi^{(X,T)}\}) \int_{\mathcal{O}^{(1)}} d\tilde{\phi}_0$$



Gaussian approximation:

$$\mathcal{Z}_1^P(\{\phi^{(X,T)}\}) = \int \prod_{i=1}^{N_S N_\tau - 1} d\tilde{\phi}_i e^{-S^{(1)} - \frac{1}{2}\sum_{i=1}^{N_S N_\tau - 1} \lambda_i^{(1)} \tilde{\phi}_i^2}$$

All eigenvalues of Hessian except the zero mode:

$$\mathcal{H}^{(1)}_{(\boldsymbol{x},\tau_1),(\boldsymbol{y},\tau_2)} = \left.\frac{\partial^2 S(\phi)}{\partial \phi_{\boldsymbol{x},\tau_1} \partial \phi_{\boldsymbol{y},\tau_2}}\right|_{\phi=\phi^{(X,T)}}$$

$$\lambda_i^{(1)},\ i = 0 \ldots N_S - 1, \quad \lambda_0^{(1)} = 0$$

$$\det \mathcal{H}_\perp^{(1)} = \det\left(\mathcal{H}^{(1)} + \mathcal{P}^{(1)}\right) = \prod_{i=1}^{N_s N_\tau - 1} \lambda_i^{(1)}$$

$$\mathcal{Z}_1 = 2N_S \mathcal{Z}_1^P(\{\phi^{(X,T)}\}) L^{(1)} \longrightarrow L^{(1)} = \int_0^\beta dT \left\| \frac{\phi^{(X,T+dT)} - \phi^{(X,T)}}{dT} \right\|, \quad \frac{L^{(1)}}{\beta} = ||\Delta\phi^{(X,T)}|| = \sqrt{\sum_{\boldsymbol{x},\tau} \left(\frac{\phi^{(X,T)}_{\boldsymbol{x},\tau+1} - \phi^{(X,T)}_{\boldsymbol{x},\tau}}{\Delta\tau} \right)^2}$$

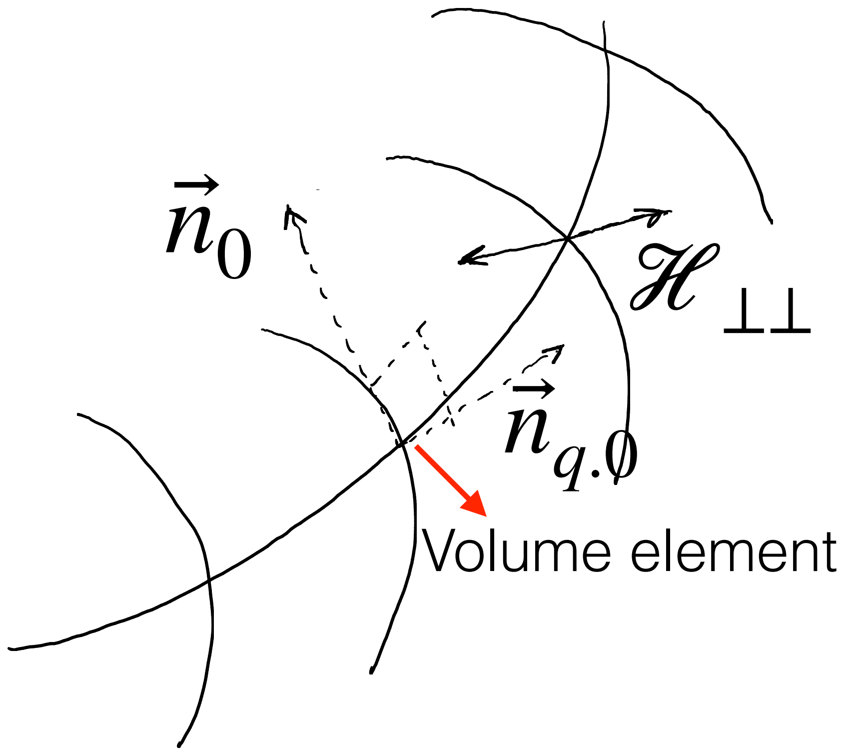
$$\mathcal{Z}_1 = 2N_S \beta e^{-S^{(1)}} ||\Delta\phi^{(X,T)}|| \sqrt{\frac{(2\pi)^{N_S N_\tau - 1}}{\prod_i' \lambda_i^{(1)}}}$$

$$\frac{\mathcal{Z}_1}{\mathcal{Z}_0} = 2N_S L^{(1)} e^{-\tilde{S}^{(1)}} \left(2\pi \frac{\det \mathcal{H}_\perp^{(1)}}{\det \mathcal{H}^{(0)}} \right)^{-1/2}$$

$$\tilde{S}^{(i)} = S^{(i)} - S_{vac.}$$

Many-instanton configurations

1) Variation of action depending on relative position of the instantons
2) Variation of the determinant of Hessian
3) Variation of the volume element along the directions defined by zero modes (obtained by triangulation inside multi-dimensional orbits)



Hessian for perpendicular directions:

$$\det \mathscr{H}_\perp^{(1)} = \det\left(\mathscr{H}^{(1)} + \mathscr{P}^{(1)}\right)$$

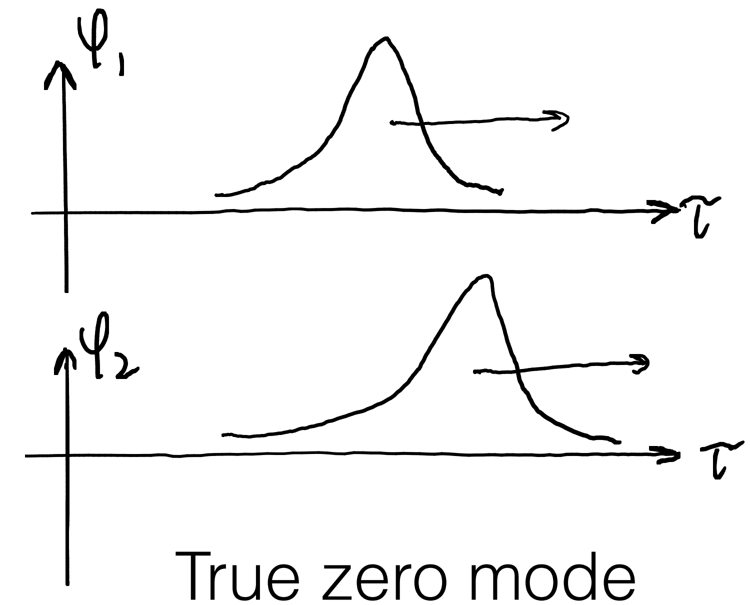
$$\mathscr{P}^{(1)} \sim |\,\partial_\tau \phi(\vec{x},\tau)\rangle\langle \partial_\tau \phi(\vec{x},\tau)\,|$$

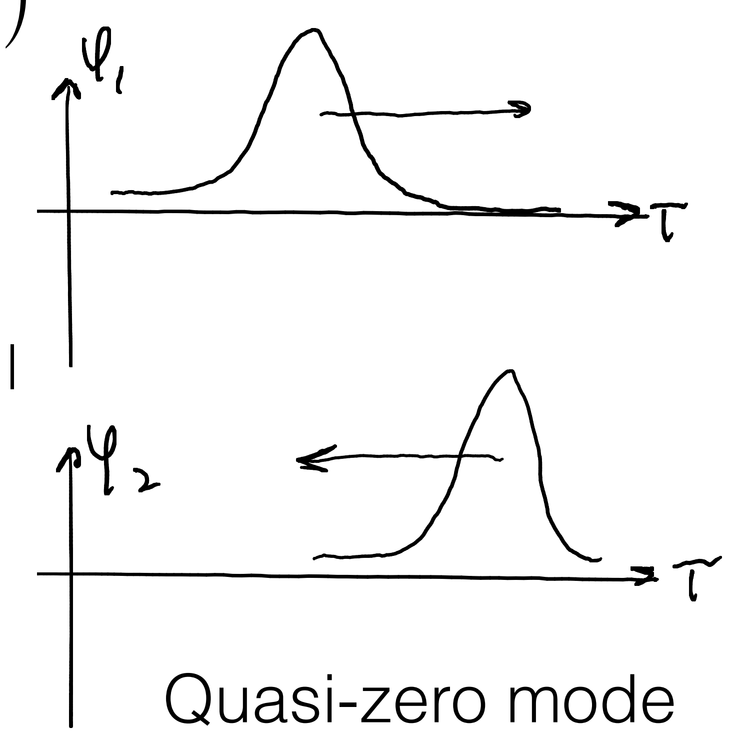
$$\frac{\det \mathscr{H}_\perp^{(1)}}{\det \mathscr{H}^{(0)}} = \det\left(\left(\mathscr{H}^{(1)} + \mathscr{P}^{(1)}\right)\left(\mathscr{H}^{(0)}\right)^{-1}\right)$$

$$\det \mathscr{H}_\perp^{(N)} \approx \det\left(\mathscr{H}^{(N)} + \sum_{q=1}^{N} \mathscr{P}_q^{(N)}\right)$$

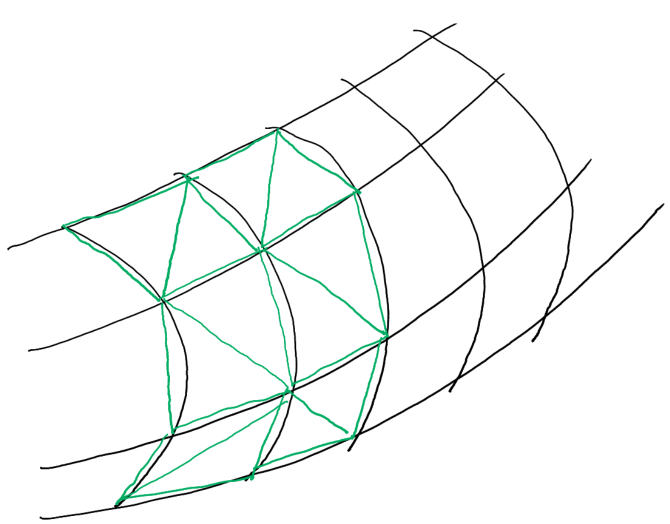
$$\mathscr{P}_q^{(N)} \sim |\,\partial_{\tau_q}\phi(\vec{x}_1\ldots\vec{x}_N,\tau_1\ldots\tau_N)\rangle\langle\partial_{\tau_q}\phi(\vec{x}_1\ldots\vec{x}_N,\tau_1\ldots\tau_N)\,|$$

$$\frac{\det \mathscr{H}_\perp^{(N)}}{\det \mathscr{H}^{(0)}} \approx \left[\det\left(\left(\mathscr{H}^{(1)} + \mathscr{P}^{(1)}\right)\left(\mathscr{H}^{(0)}\right)^{-1}\right)\right]^N$$

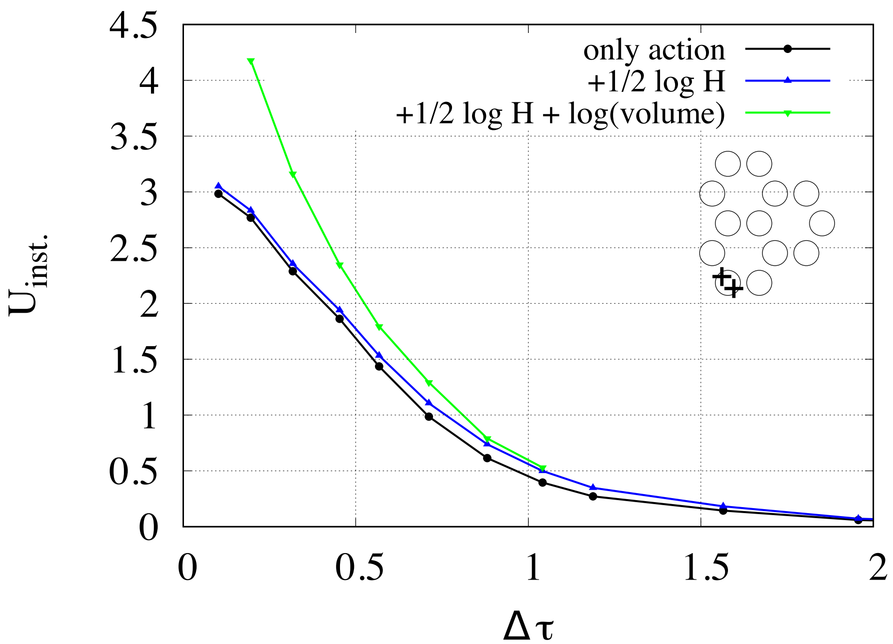


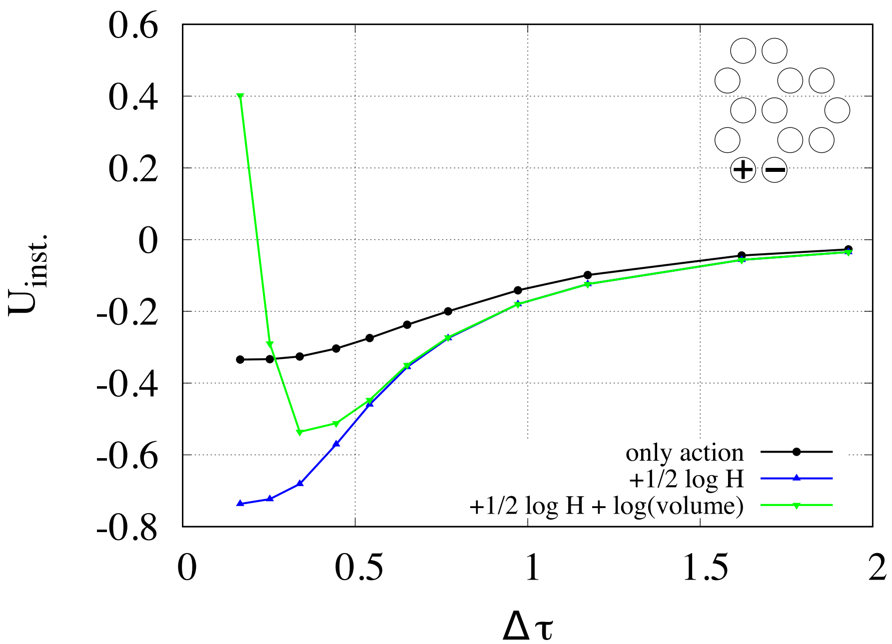


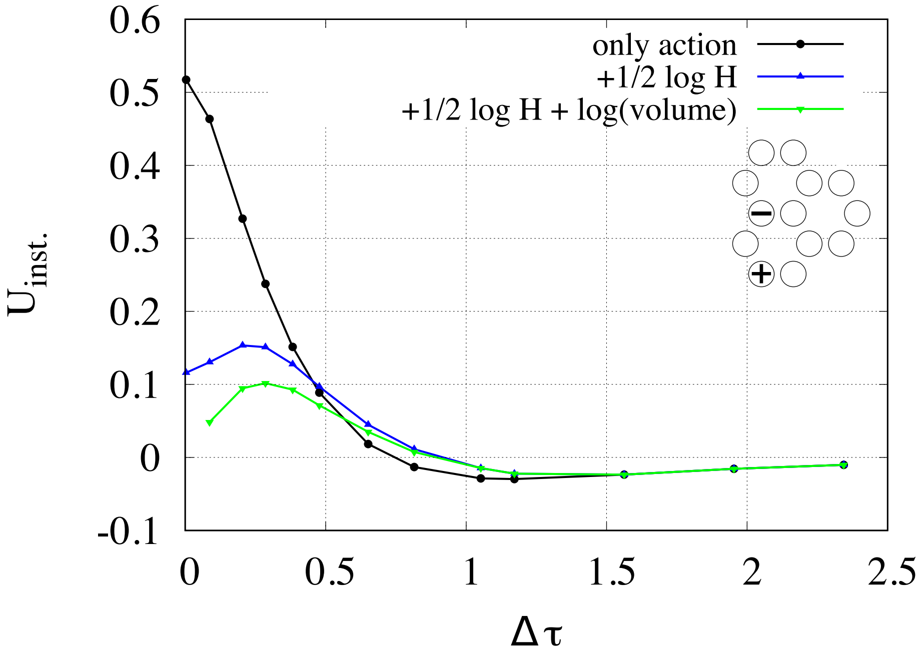
Triangulation of 2D surface

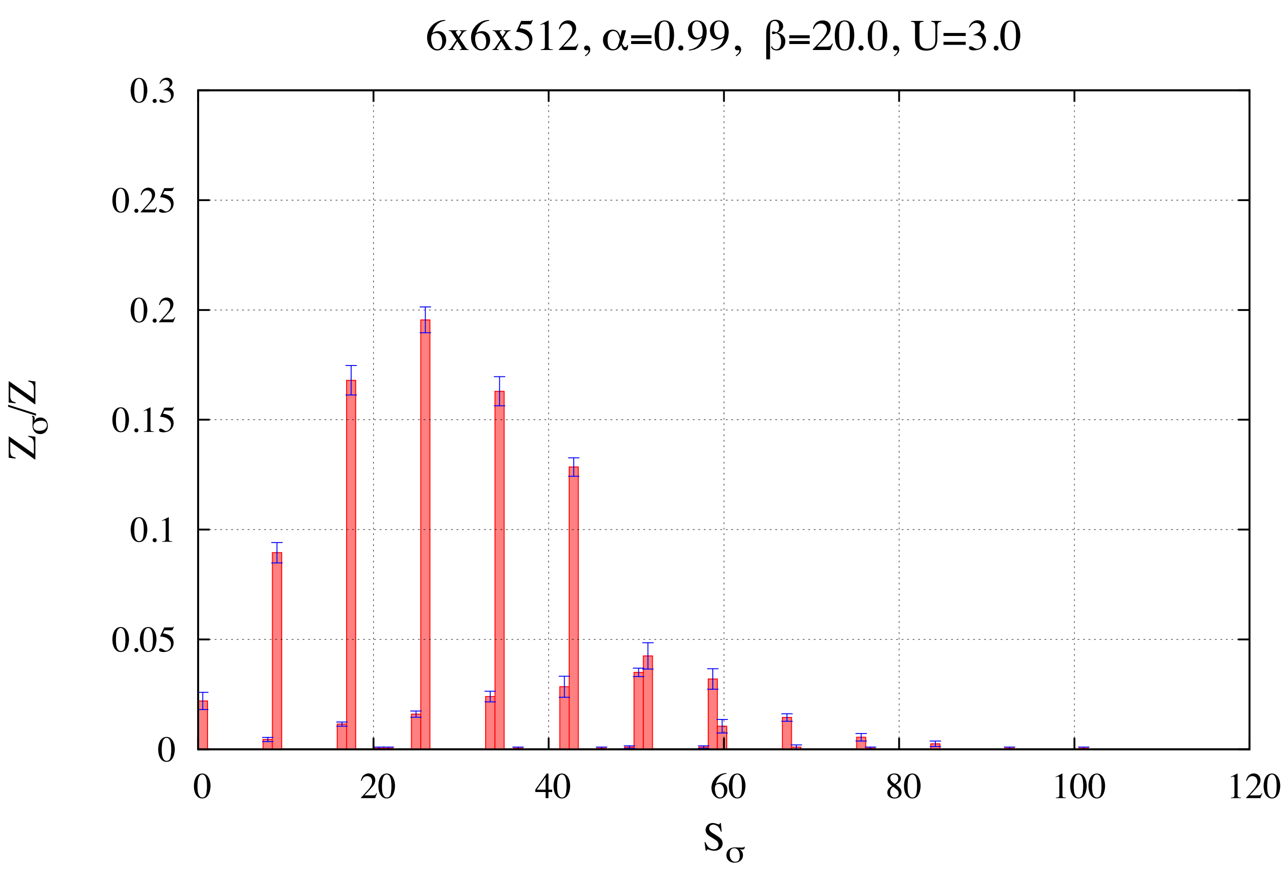


Examples of interaction curves

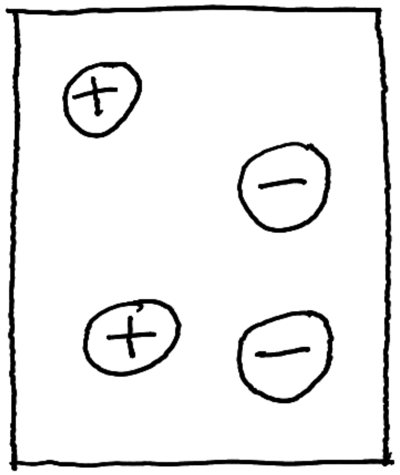




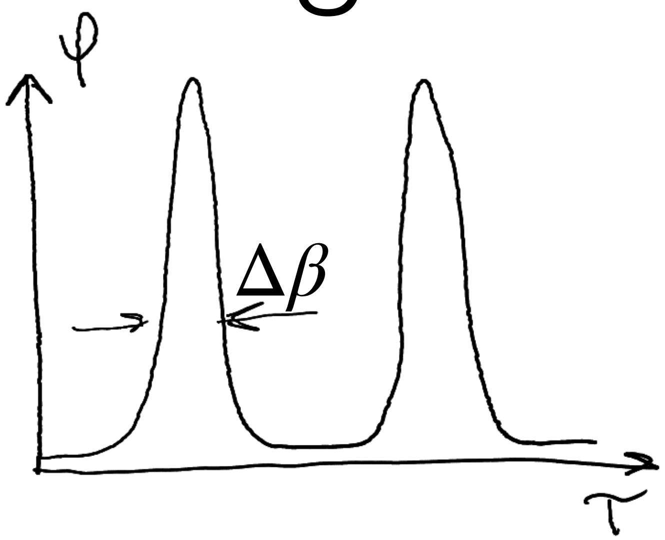




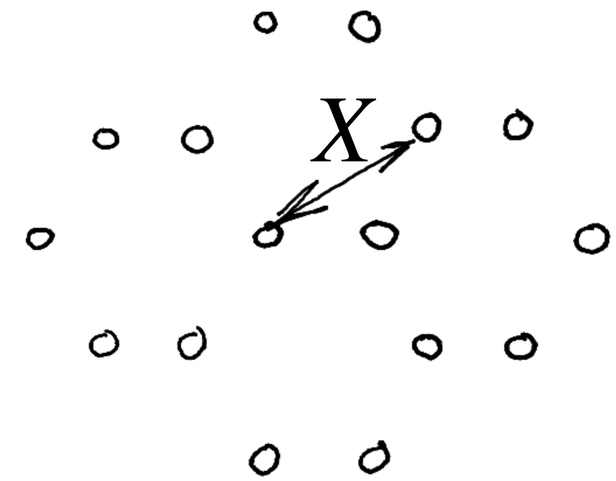
Analytical expression for the partition function for non-interacting instantons



All N-instanton saddle points with Gaussian fluctuations around them. No interaction. Two instantons can not occupy the same volume in 2+1D space-time.



Minimal distance in Euclidean time ~ instanton width



Minimal distance in space ~ lattice step

$$\frac{Z}{Z_0} = 1 + \sum_{K=1}^{K_{max}} \frac{1}{K!} (\beta N_s - \Delta\beta X) \ldots (\beta N_s - (K-1)\Delta\beta X) 2^{2K} \times e^{-S_1 K} \left\{ \left[\det\left(\mathscr{H}_\perp^{(1)} (\mathscr{H}^{(0)})^{-1} \right) \right]^{-1/2} \frac{L}{\sqrt{2\pi\beta}} \right\}^K$$

«vacuum» partition function: integral over vacuum thimble

instanton number

Equivalence of instantons

Combinatorial factors including sublattice and instanton - anti-instanton indexes

instanton action

Hessians and orbital length, using:

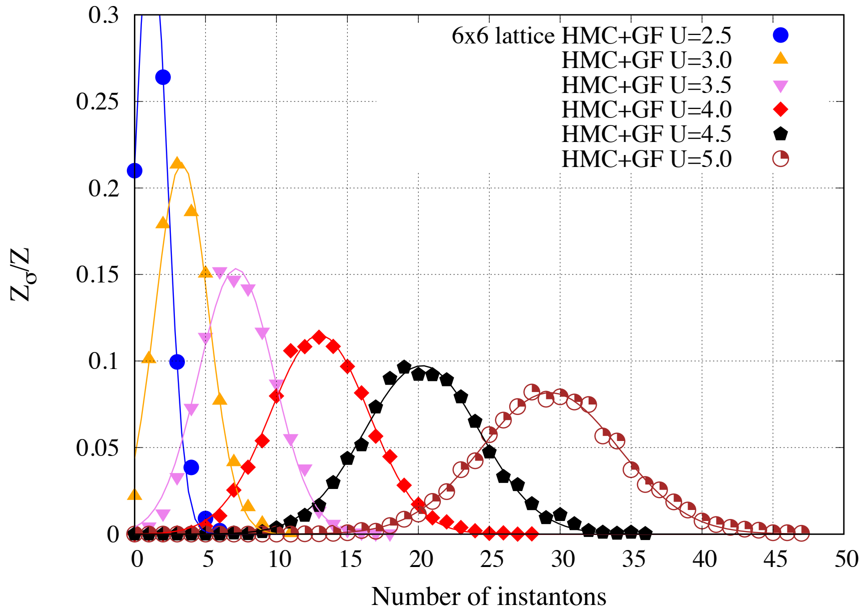
$$\frac{\det \mathscr{H}_\perp^{(N)}}{\det \mathscr{H}^{(0)}} \approx \left[\det\left(\left(\mathscr{H}^{(1)} + \mathscr{P}^{(1)} \right) \left(\mathscr{H}^{(0)} \right)^{-1} \right) \right]^N$$

If we sum up to completely filled lattice (all slots are taken):

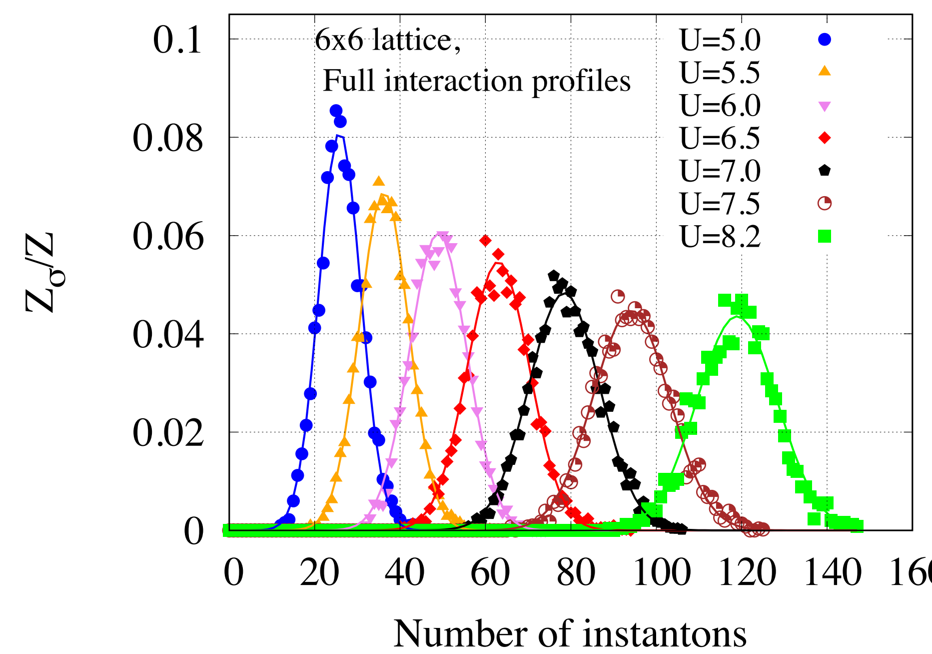
$$K_{max} = \frac{\beta}{\Delta\beta} \frac{N_s}{X}$$

Free energy density: $$\boxed{f = f_0 - \frac{1}{\Delta\beta X} \ln\left(1 + \frac{2 e^{-S_1} \Delta\beta X L}{\beta \sqrt{2\pi \det\left(\mathscr{H}_\perp^{(1)} (\mathscr{H}^{(0)})^{-1} \right)}} \right)}$$

Benchmark: distribution of instantons

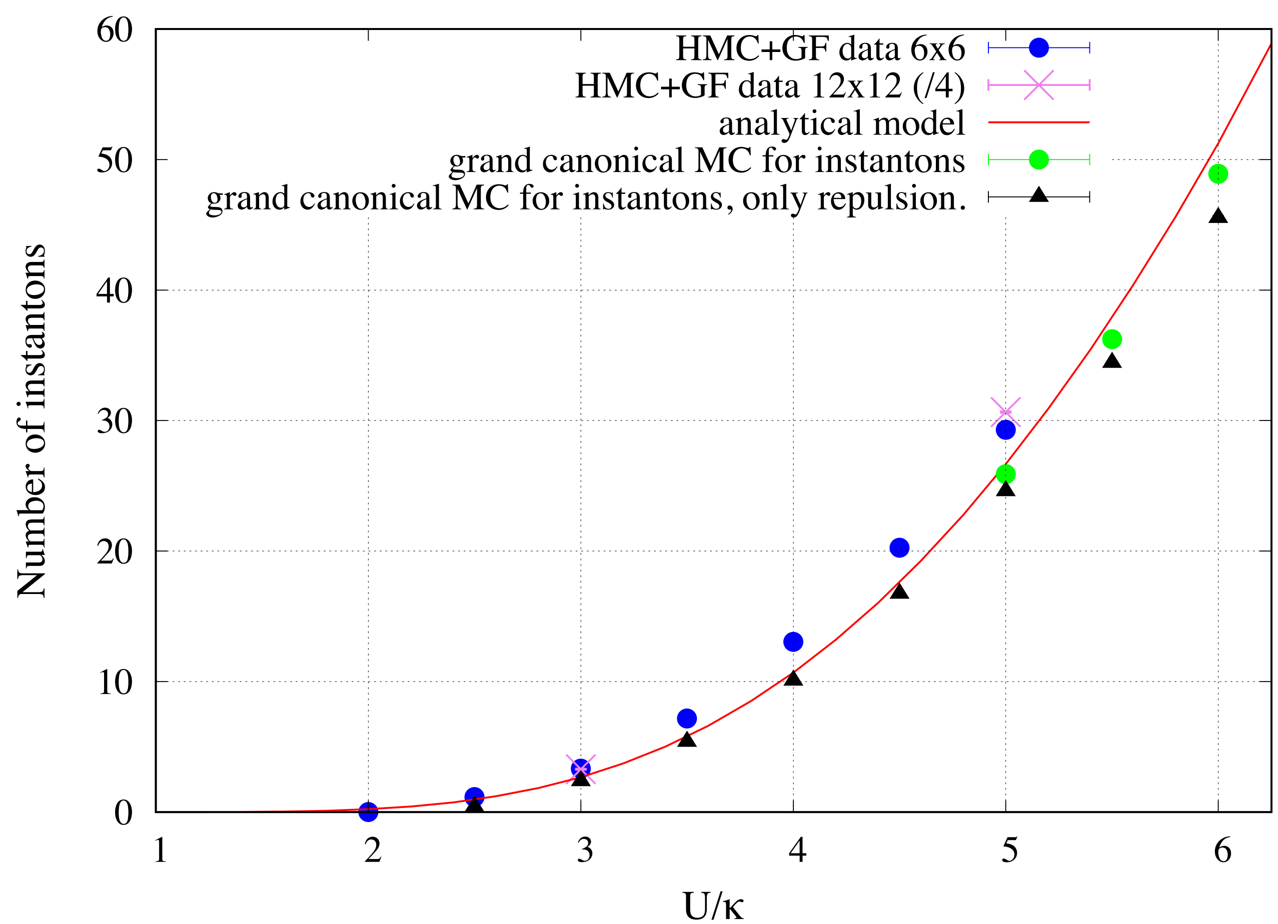


QMC data

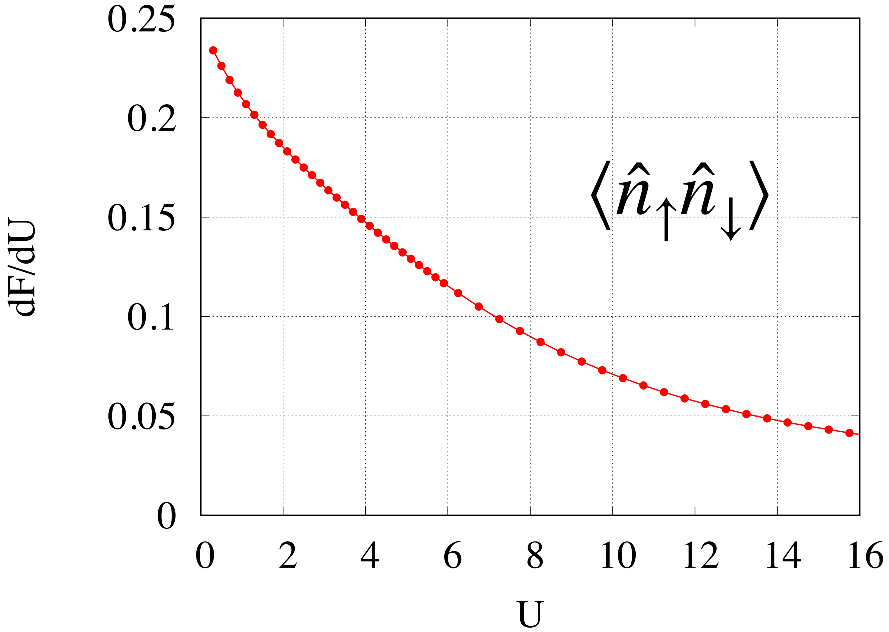


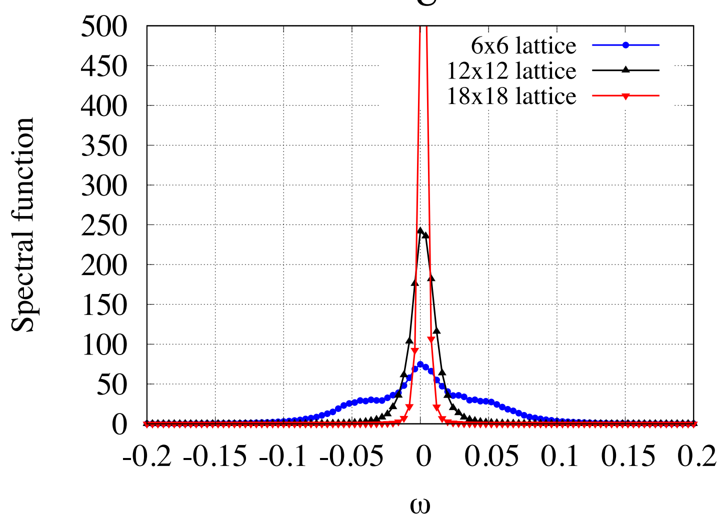
Grand canonical classical MC for instanton gas

Distribution for the number of instantons and its comparison vs analytical and classical MC predictions:

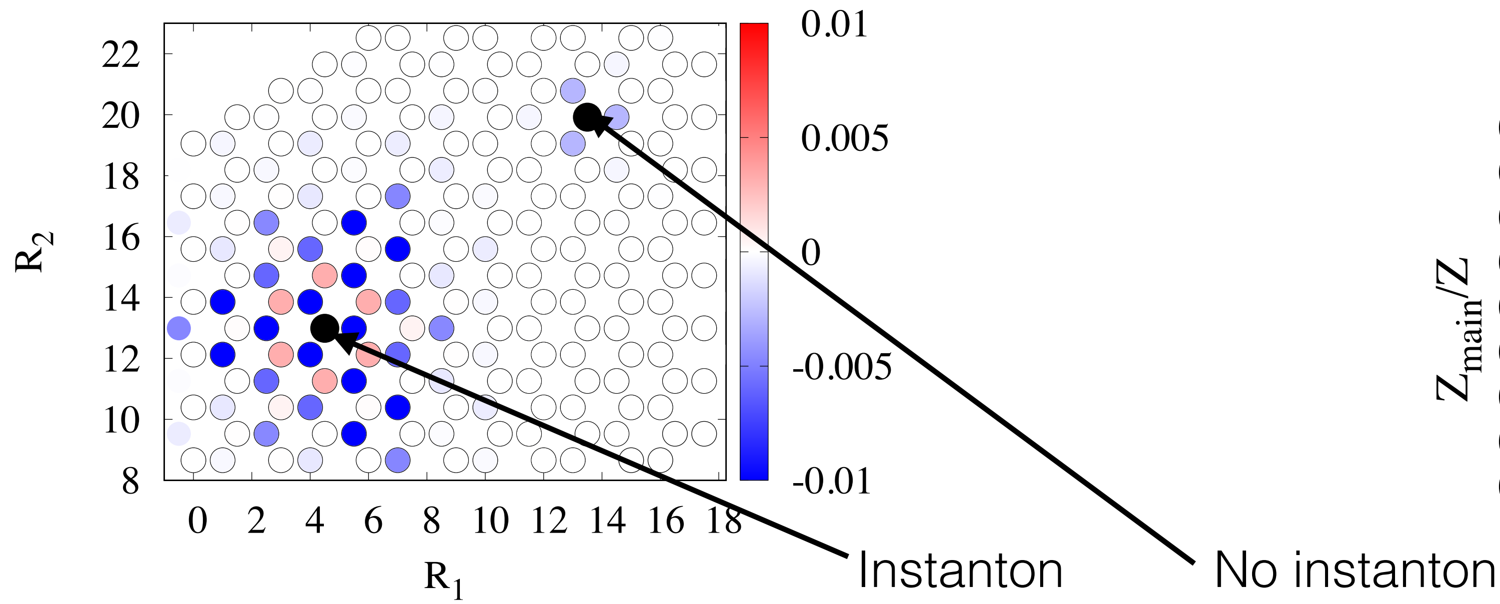


Spectral functions: comparison with QMC

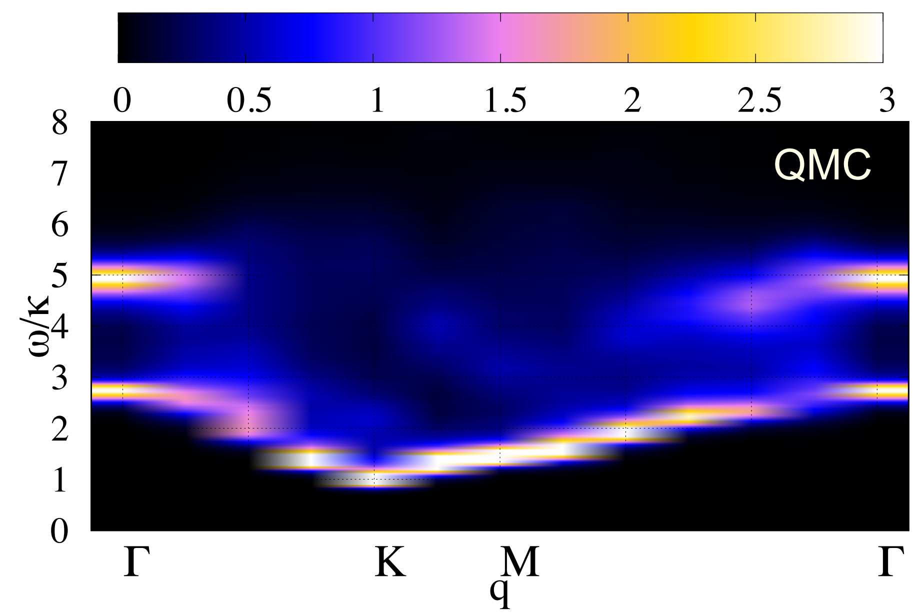


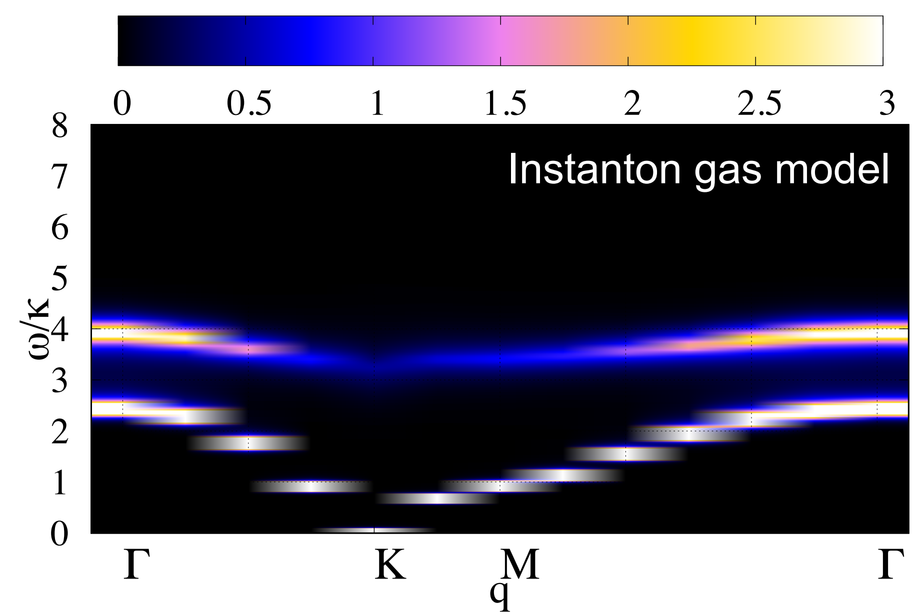


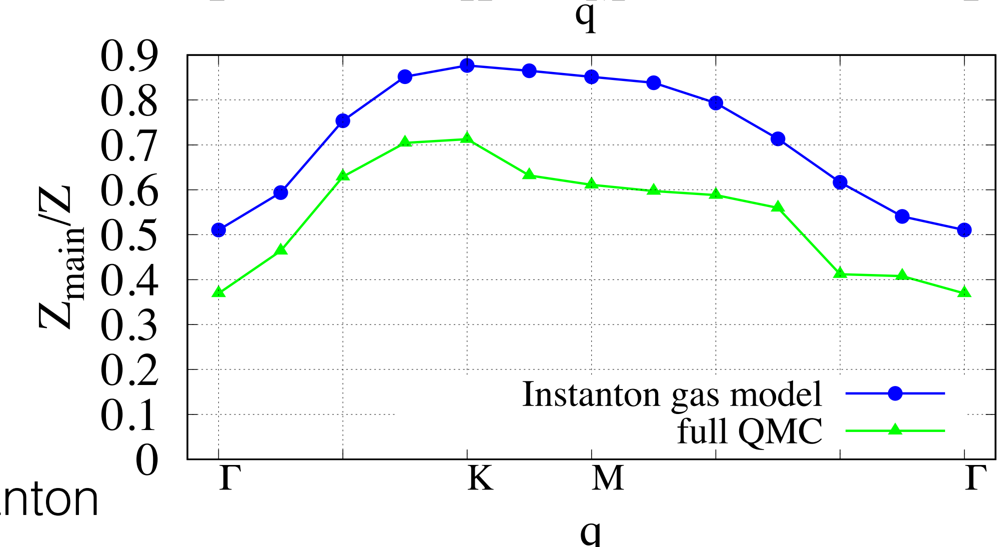
Broadening of the spectral function on smaller lattices: local AFM correlation.



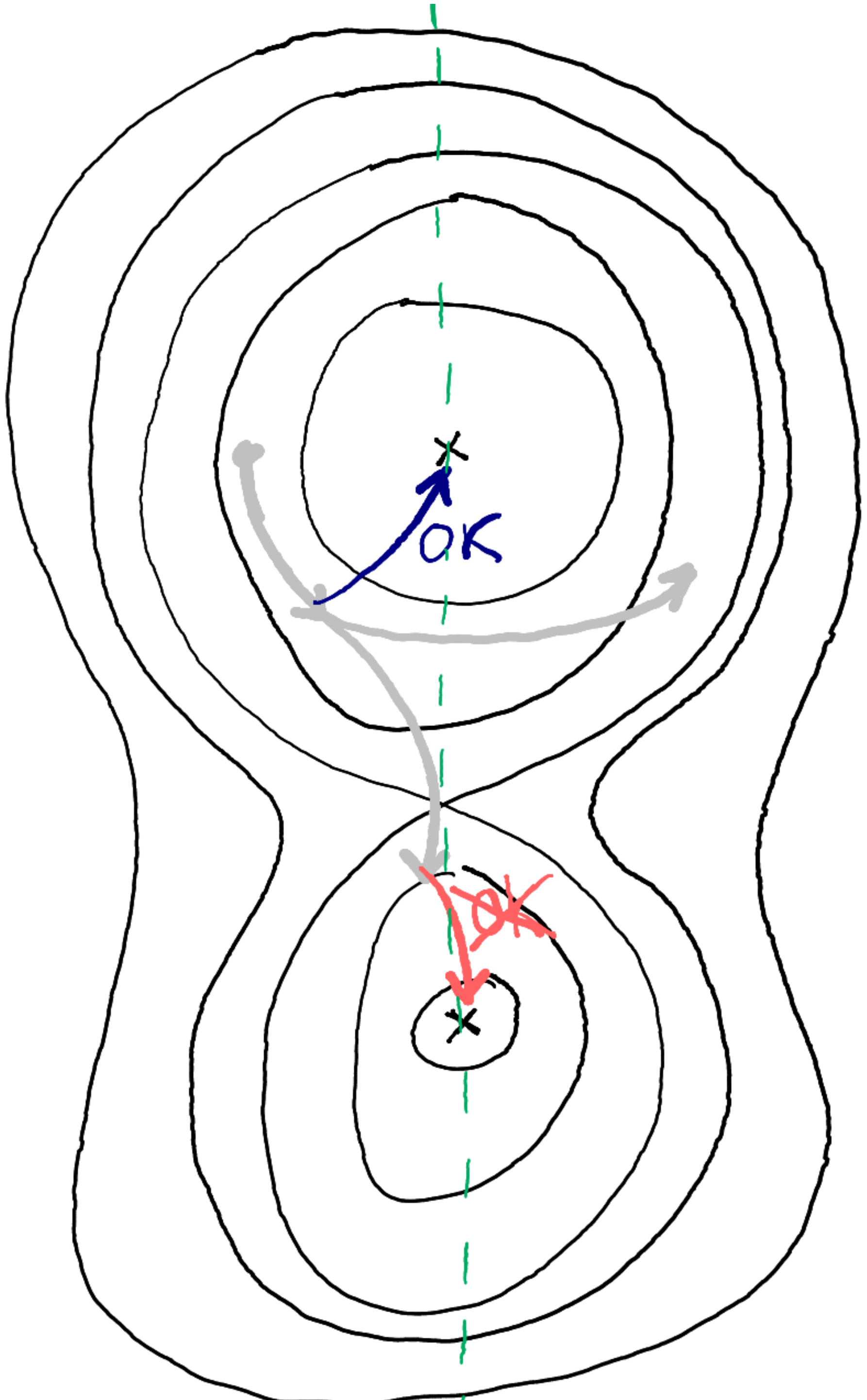
Spectral functions and relative spectral weight of the peaks in the whole BZ:

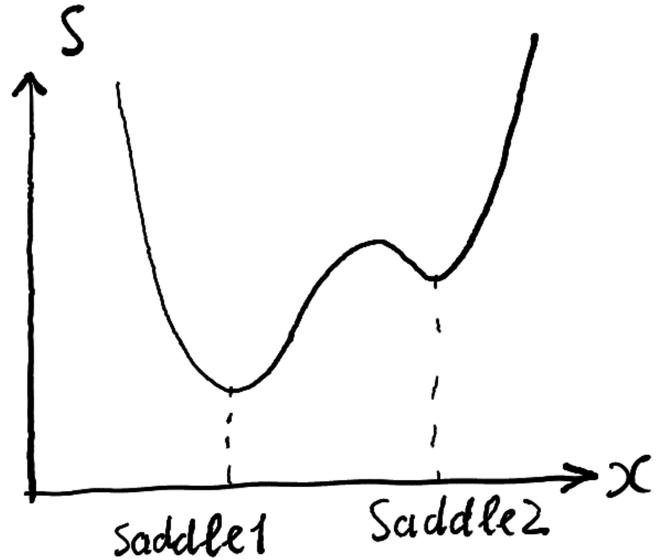






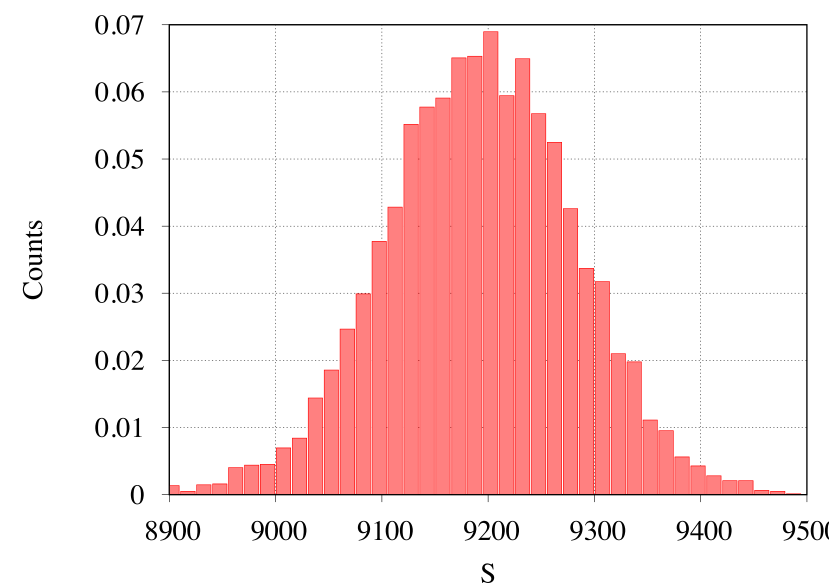
Full integral over one dominant thimble: algorithms



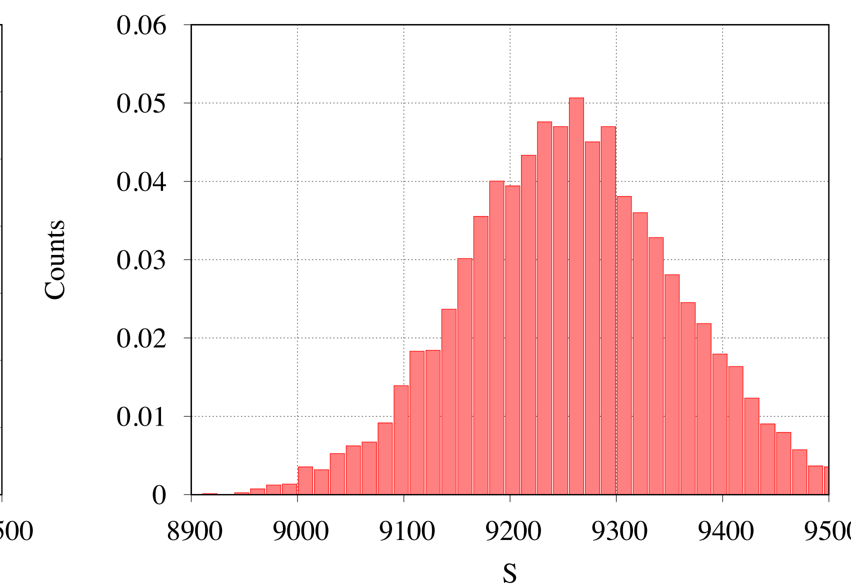


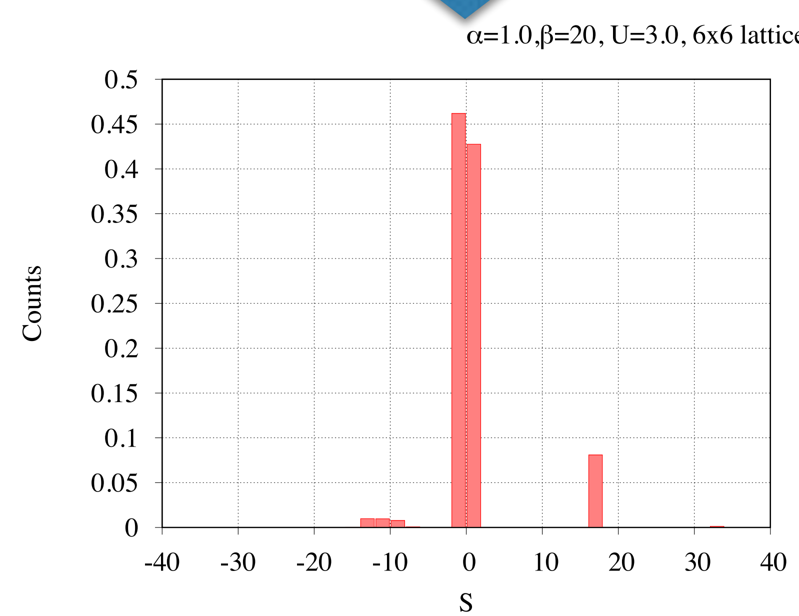
Check that we are still within the same thimble via GF after HMC update:

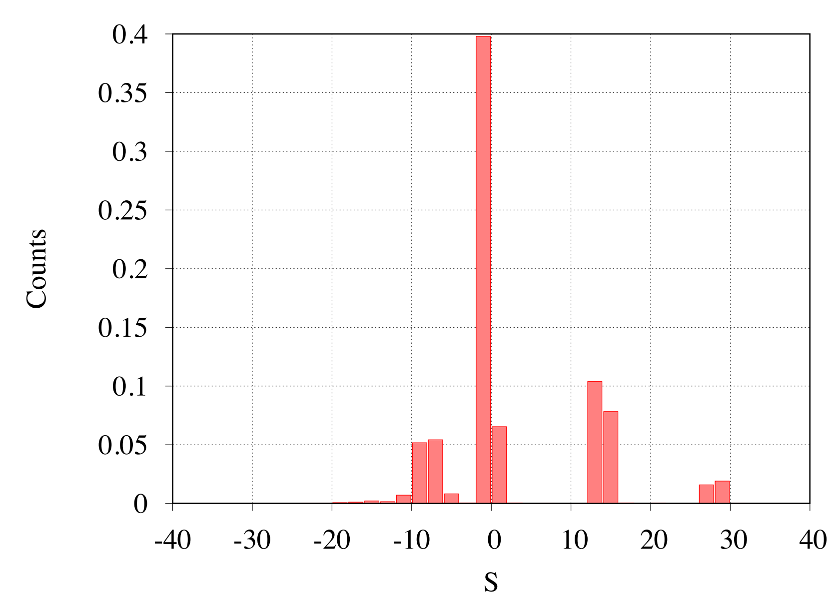
U=3.0



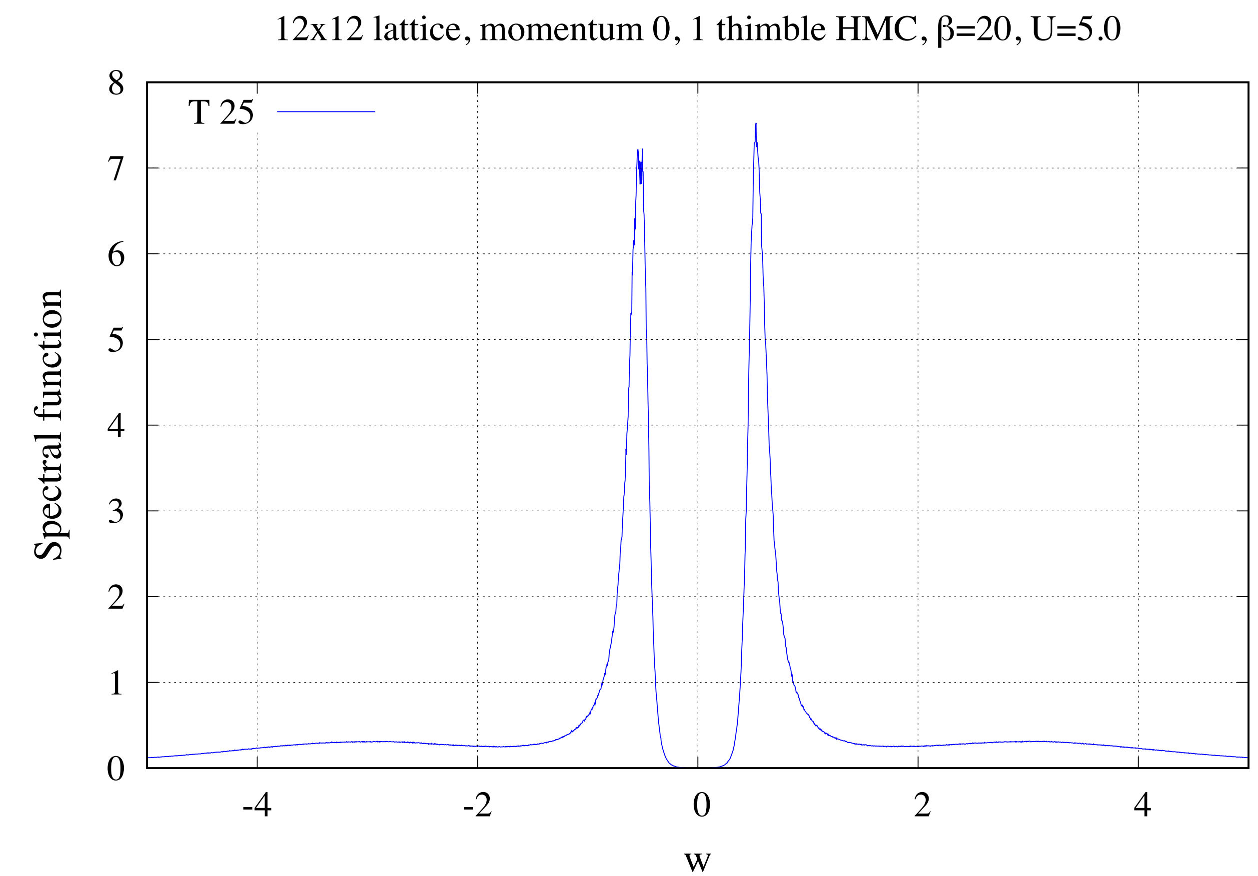
U=4.0

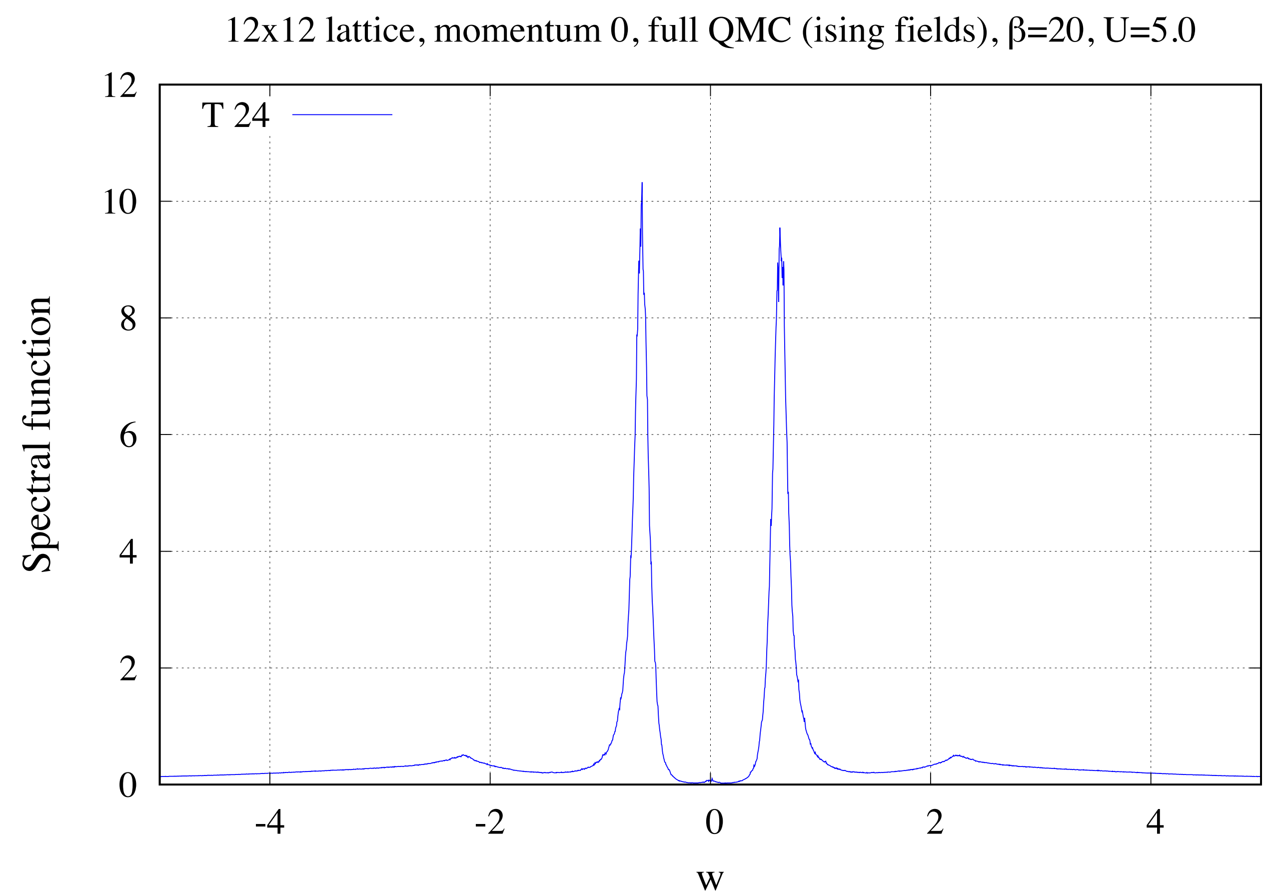




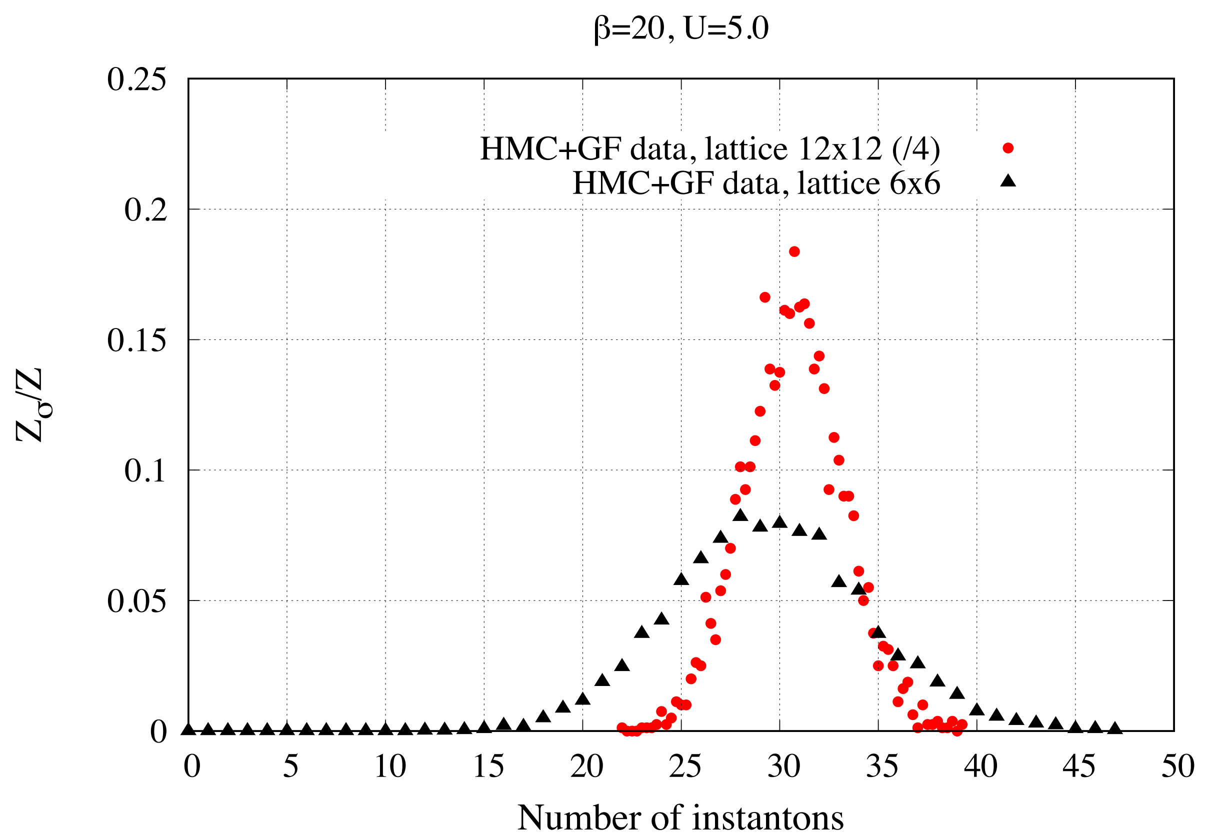


Full integral over the dominant thimble:results

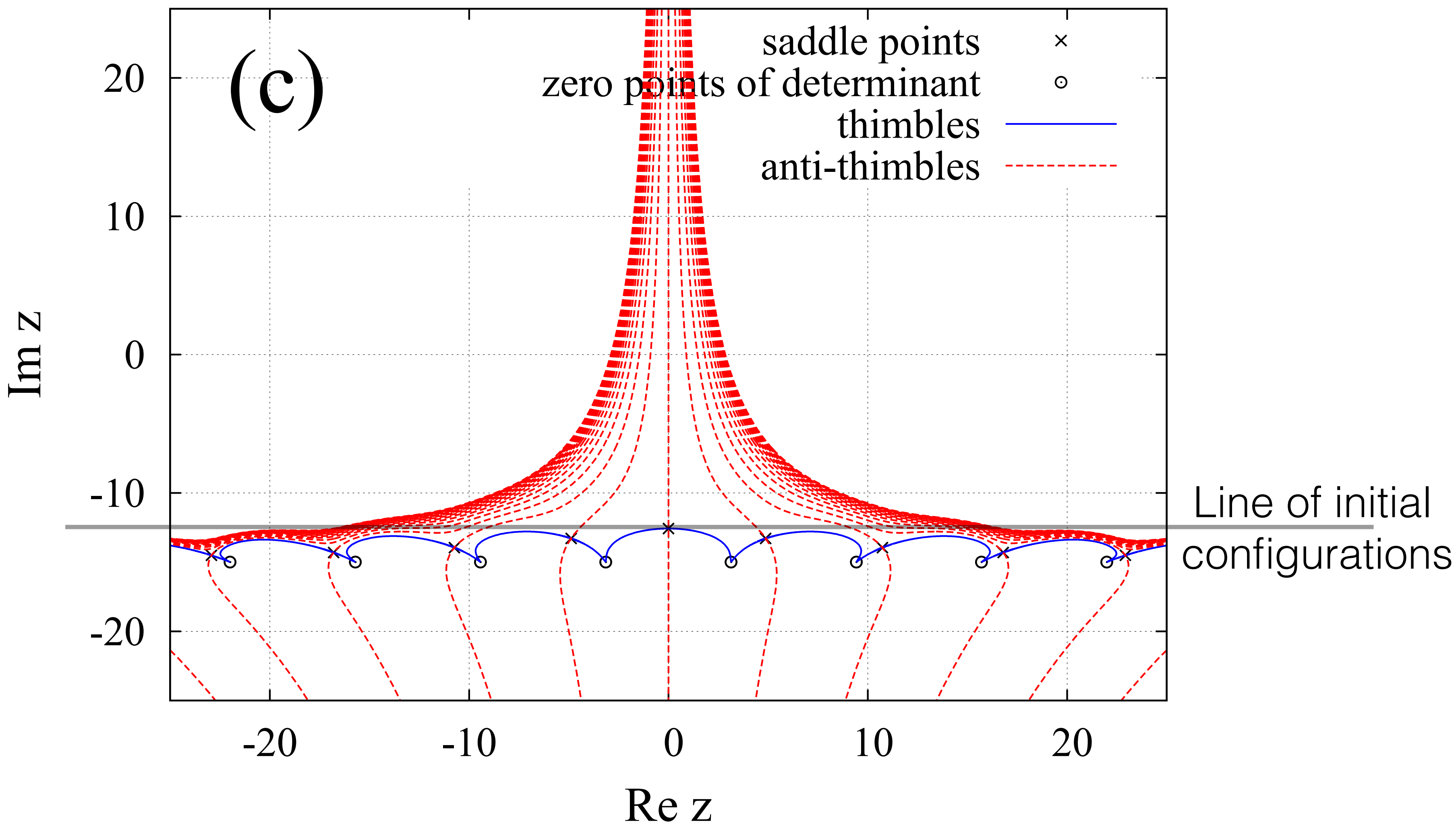




Integral over just one thimble attached to the «dominant» saddle randomly picked up from the peak of instanton number distribution:

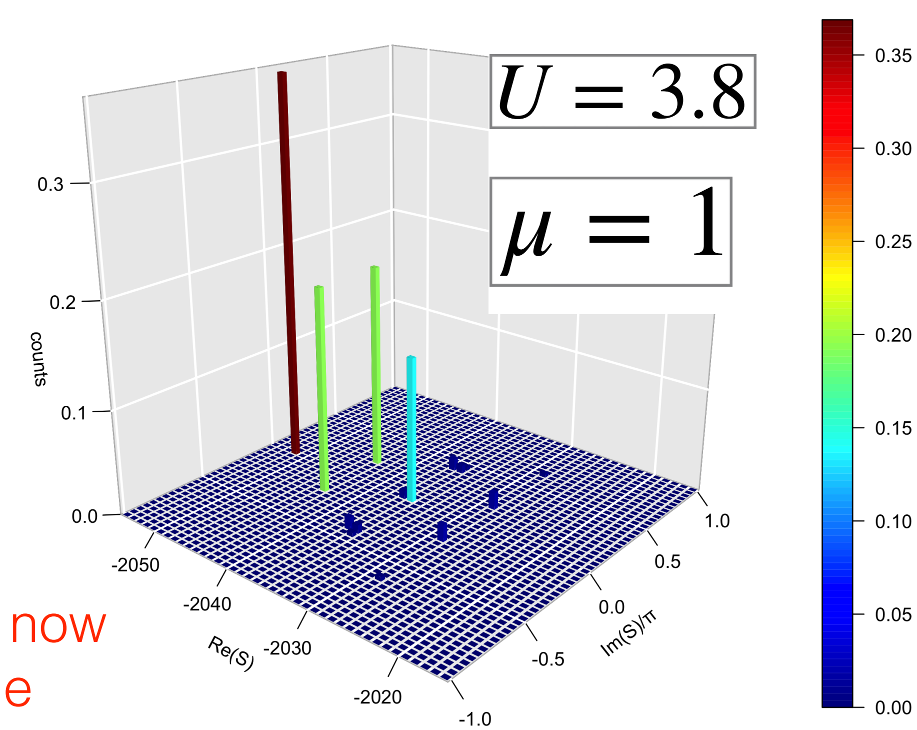


Complex instantons

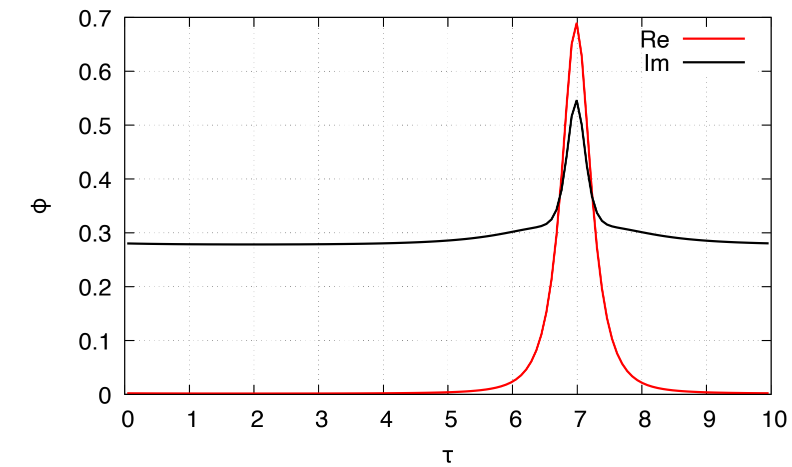


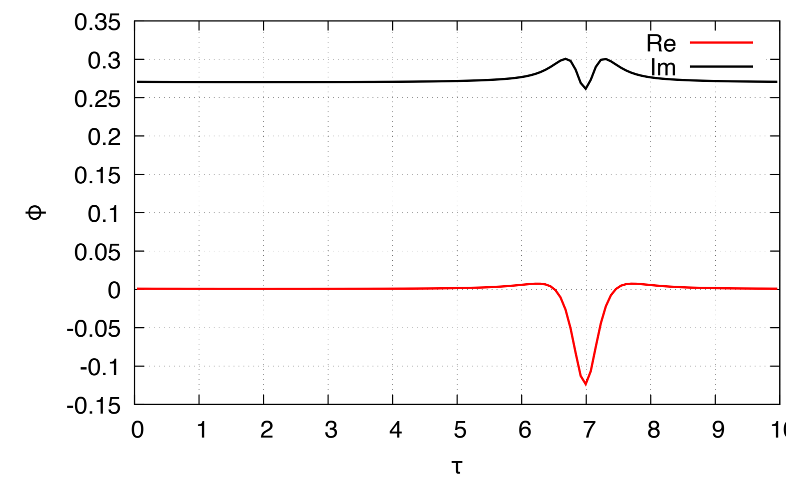
+ minimization of sum of squares of derivatives

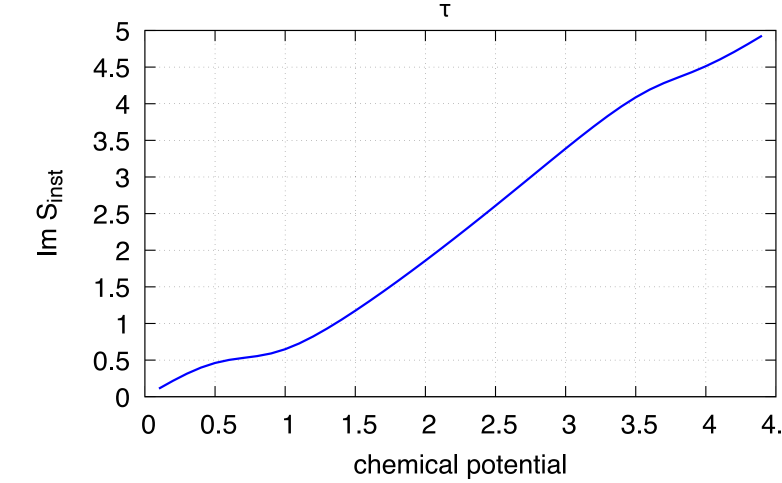
Distribution of actions:

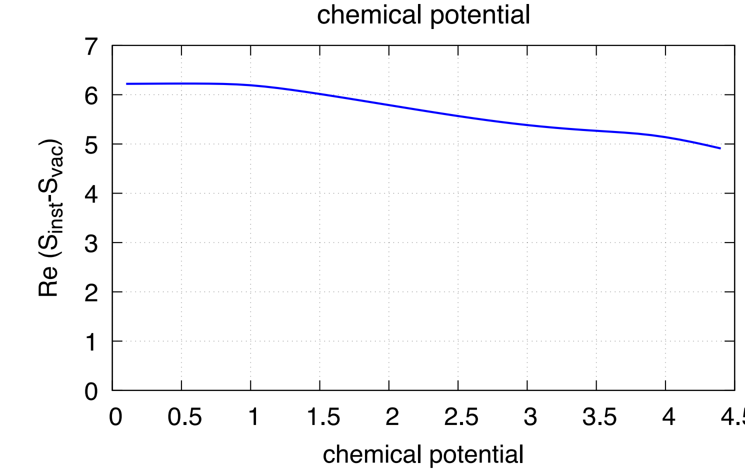


Actions remain equidistant, but now in complex plane







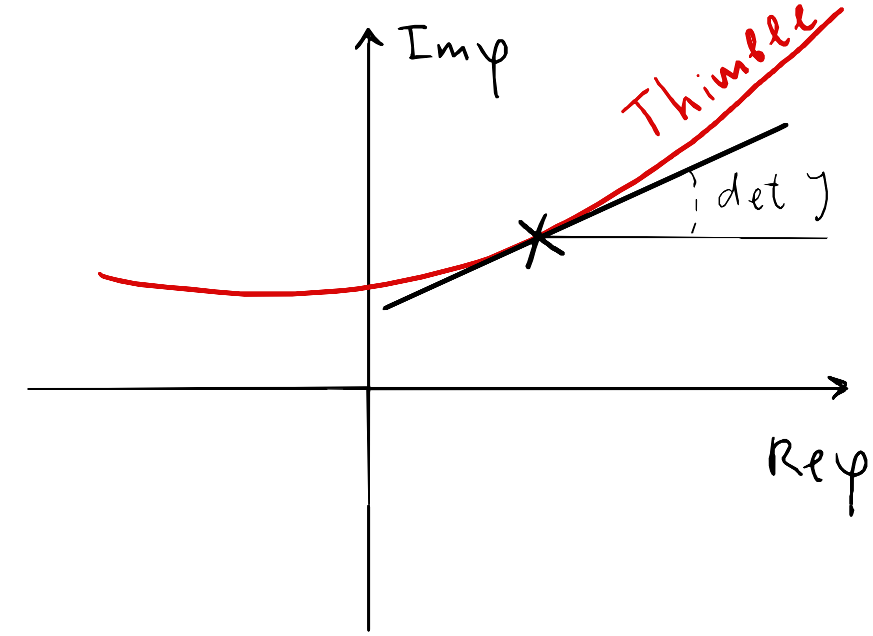


Jacobian

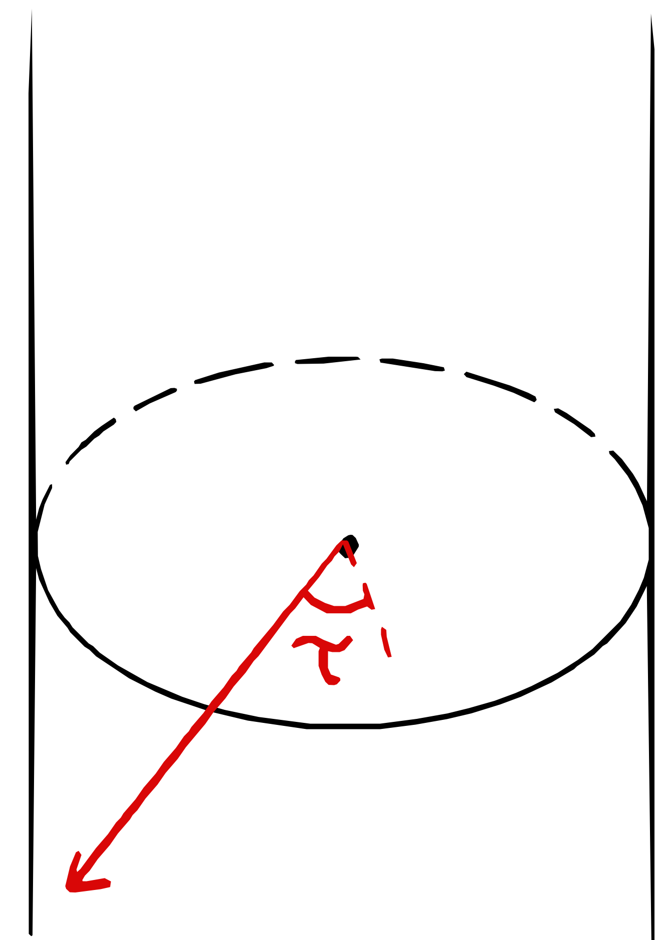
$$S \approx S_0 + \frac{1}{2}\sum_{i,j} \mathscr{H}_{ij}\Delta z_i \Delta z_j$$

$$\mathrm{Re}\, S \approx \mathrm{Re}\, S_0 + \frac{1}{2}\sum_{i} \lambda_i((\Delta\tilde{x})^2 - (\Delta\tilde{y})^2)$$

Double number of zero modes



$$z_{x,\tau} = z^{(0)}_{x,\tau}(T_0) + \sum_{j=1}^{N-1} (\mathrm{Re}\, V^j_{x,\tau} + i\, \mathrm{Im}\, V^j_{x,\tau}) T_j$$



Gaussian approximation for thimble weight:

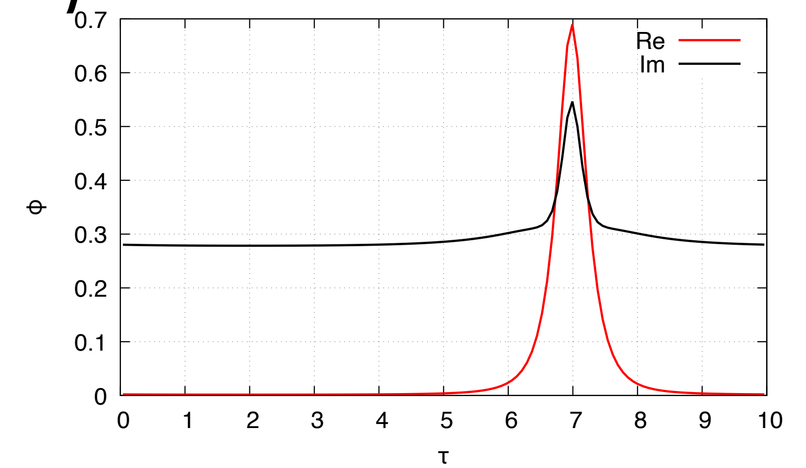
$$W = \int dT_0 \prod_{j=1}^{N-1} dT_j e^{-S(z^{(0)}_{x,\tau}(T_0))} e^{-\frac{1}{2}\sum_{j=1}^{N-1}\lambda_j T_j^2} \left\| \frac{\partial z_{x,\tau}}{\partial T_j} \right\|$$

$$\left\| \frac{\partial z_{x,\tau}}{\partial T_j} \right\| = \left\| \begin{matrix} \frac{\partial z^{(0)}_{1,1}}{\partial T_0} & V^1_{1,1} & \dots & V^{N-1}_{1,1} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial z^{(0)}_{N_s,N_\tau}}{\partial T_0} & V^1_{N_s,N_\tau} & \dots & V^{N-1}_{N_s,N_\tau} \end{matrix} \right\|$$

Finding directions for 1-instanton saddle

Linear functional to fix the center of the configuration:

$$F_T[\phi_{x,\tau}]\,|_{T=C[\phi_{x,\tau}]} = 0 \qquad F_T[\phi_{x,\tau}] = \sum_{x,\tau} \sin\frac{2\pi}{\beta}(\Delta\tau t - T)\mathrm{Re}\,\phi_{x,\tau}$$



Zero modes:

$$W^{(i)}_{x,\tau}, i = 1{,}2$$

Other modes:

$$V^{(i)}_{x,\tau}, i = 1\ldots N-1$$

Combination of zero modes keeping the center constant:

$$F_{C[\phi_{x,\tau}]}[\phi_{x,\tau} + W^{(1)}_{x,\tau}C_1 + W^{(2)}_{x,\tau}C_2] = 0$$

$$C_1 F_{C[\phi_{x,\tau}]}[W^{(1)}_{x,\tau}] + C_2 F_{C[\phi_{x,\tau}]}[W^{(2)}_{x,\tau}] = 0$$

$M_{x,\tau}$ - shifts the center

$N_{x,\tau}$ - does not shift the center

Final optimization:

$$\tilde{M}_{x,\tau} = M_{x,\tau} cos\theta + N_{x,\tau} sin\theta$$

Maximization:

$$\left(\tilde{M}_{x,\tau} \cdot \frac{\Delta\phi_{x,\tau}}{\Delta\tau}\right) \qquad \frac{\Delta\phi_{x,\tau}}{\Delta\tau} = \frac{\phi_{x,\tau+1} - \phi_{x,\tau-1}}{\Delta 2\tau}$$

Finding directions for 2-instanton saddle

4 zero modes: $W^{(i)}_{x,\tau}, i = 1...4$

2 functionals, one fixes the center, another the time distance between instantons:

$$F_T[\phi_{x,\tau}] = 0 \qquad G_D^{C[\phi_{x,\tau}]}[\phi_{x,\tau}] = 0 \qquad G_D^T = \sum_{\tau,x} \mathrm{Re}\, \phi_{x,\tau} K^{T,D}_{x,\tau}$$

$$K^{T,D}_{x,\tau} = \frac{\phi^{(1)}_{x-X_1,\tau-T-D/2+1} - \phi^{(1)}_{x-X_1,\tau-T-D/2-1}}{\Delta 2\tau} + \frac{\phi^{(1)}_{x-X_2,\tau-T+D/2+1} - \phi^{(1)}_{x-X_2,\tau-T+D/2-1}}{\Delta 2\tau}$$

2-dim subspace where center and distance change and 2-dim subspace where they are constant:

$$\begin{cases} F_{C[\phi_{x,\tau}]}[\phi_{x,\tau} + \sum_i W^{(i)}_{x,\tau} C_i] = 0 \\ G^{D[\phi_{x,\tau}]}_{C[\phi_{x,\tau}]}[\phi_{x,\tau} + \sum_i W^{(i)}_{x,\tau} C_i] = 0 \end{cases} \longrightarrow \qquad N^1_{x,\tau}\ N^2_{x,\tau} \qquad M^1_{x,\tau}\ M^2_{x,\tau}$$

One mode shifts center, another shifts distance:

$$F_{C[\phi_{x,\tau}]}[\phi_{x,\tau} + \sum_i M^{(i)}_{x,\tau} B_i] = 0 \longrightarrow \qquad M^{(1,1)}_{x,\tau} \quad M^{(2,1)}_{x,\tau}$$

Optimization I:

$$\left(\tilde{M}^{(1,1)}_{x,\tau} \cdot \frac{\Delta \phi_{x,\tau}}{\Delta \tau} \right) \qquad \tilde{M}^{(1,1)}_{x,\tau} = M^{(1,1)}_{x,\tau} cos\theta_1 + \left(N^{(1)}_{x,\tau} \sin \xi_1 + N^{(2)}_{x,\tau} \cos \xi_1 \right) sin\theta_1$$

Optimization II:

$$\left(\tilde{M}^{(2,1)}_{x,\tau} \cdot \frac{\phi^{D+1}_{x,\tau} - \phi^{D-1}_{x,\tau}}{2\Delta\tau} \right) \text{+condition:} \perp \tilde{M}^{(1,1)}_{x,\tau} \qquad \tilde{M}^{(2,1)}_{x,\tau} = M^{(2,1)}_{x,\tau} cos\theta_2 + \left(N^{(1)}_{x,\tau} \cos \xi_1 - N^{(2)}_{x,\tau} \sin \xi_1 \right) sin\theta_2$$

$$\theta_1, \xi_1 \ll 1$$

Finding directions in general case

$M^i_{x,\tau}$ $\quad N^i_{x,\tau}$ $\quad i = 1 ... N_{inst.}$ $\qquad N_{inst}$ collective coordinates

Found from:

$$\begin{cases} F^1_{C_1}[\phi_{x,\tau} + \sum_{i=1}^{N_{inst}} W^{(i)}_{x,\tau} C_i] = 0 \\ F^2_{C_1,C_2}[\phi_{x,\tau} + \sum_{i=1}^{N_{inst}} W^{(i)}_{x,\tau} C_i] = 0 \\ \vdots \\ F^{N_{inst.}}_{C_1 ... C_{N_{inst}}}[\phi_{x,\tau} + \sum_{i=1}^{N_{inst}} W^{(i)}_{x,\tau} C_i] = 0 \end{cases}$$

Zero mode changing the 1st collective coordinate:

$$F^1_{C_1}[\phi_{x,\tau} + \sum_{i=1}^{N_{inst}} M^{(i)}_{x,\tau} B_i] = 0 \longrightarrow M^{(1,1)}_{x,\tau} \qquad M^{(1,k)}_{x,\tau}, k = 2 ... N_{inst}$$

Zero mode changing the 2nd collective coordinate:

$$F^2_{C_1,C_2}[\phi_{x,\tau} + \sum_{k=2}^{N_{inst}} M^{(1,k)}_{x,\tau} B_k] = 0 \longrightarrow M^{(2,1)}_{x,\tau} \qquad M^{(2,k)}_{x,\tau}, k = 2 ... N_{inst} - 1$$

…and so on

Optimizations: $\left(\tilde{M}^{(1,1)}_{x,\tau} \cdot D^{(1)}\right)$ $\qquad \tilde{M}^{(1,1)}_{x,\tau} = M^{(1,1)}_{x,\tau} cos\theta_1 + \mathcal{N}_1 sin\theta_1$

$\left(\tilde{M}^{(2,1)}_{x,\tau} \cdot D^{(2)}\right)$ $\qquad \tilde{M}^{(2,1)}_{x,\tau} = M^{(2,1)}_{x,\tau} cos\theta_2 + \mathcal{N}_2 sin\theta_2$ $\qquad \mathcal{N}_2 \perp \tilde{M}^{(1,1)}_{x,\tau}$

…and so on

General properties of complex N-instanton saddles

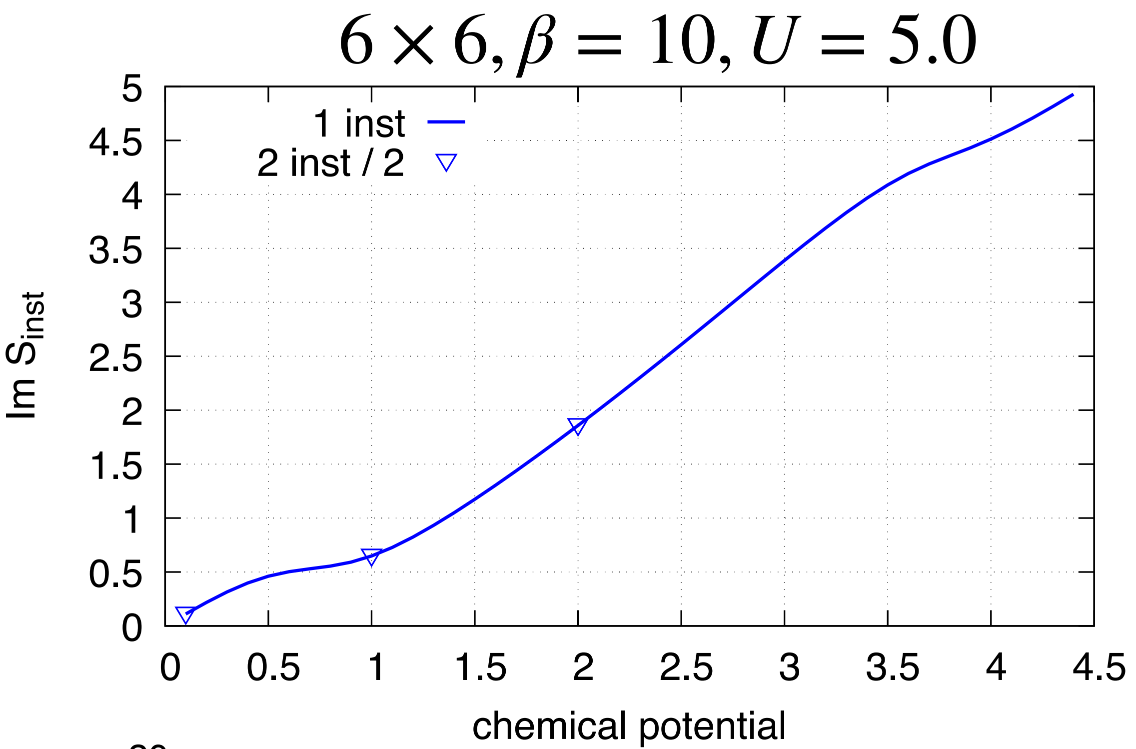
$$N_{inst} = N_+ + N_-$$

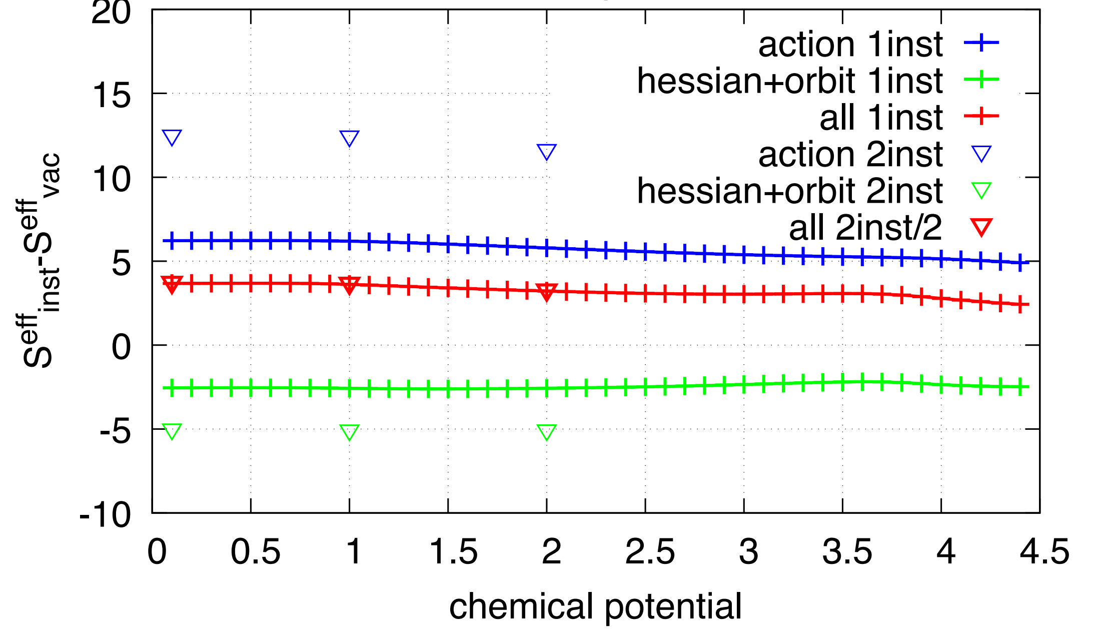
$$\frac{\det \mathscr{H}_\perp^{(N_+,N_-)}}{\det \mathscr{H}^{(0)}} \approx \left[\det\left(\left(\mathscr{H}^{(1)} + \mathscr{P}^{(1)}\right)\left(\mathscr{H}^{(0)}\right)^{-1}\right)\right]^N$$

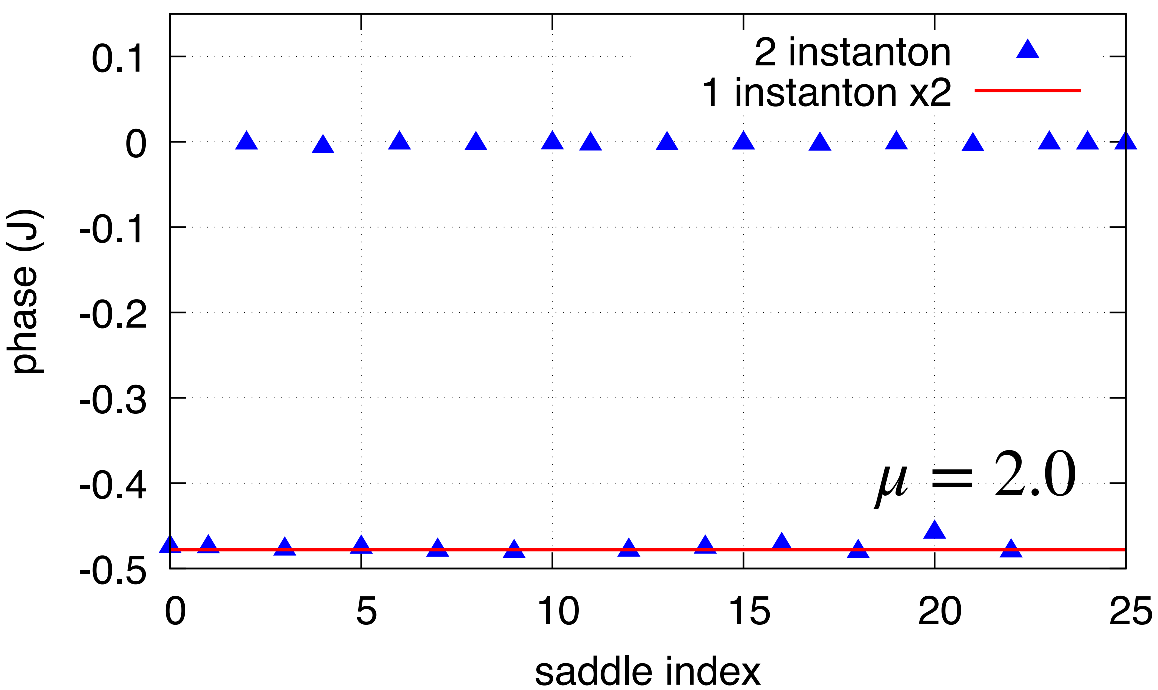
$$S_{N_+,N_-} = S_0 + \mathrm{Re}\, S_1(N_+ + N_-) + i\, \mathrm{Im}\, S_1(N_+ - N_-)$$

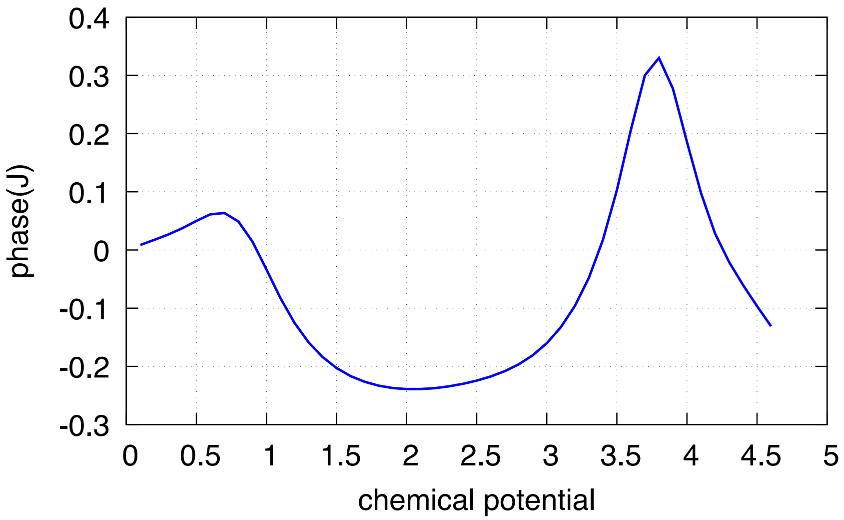
$$J_{N_+,N_-} = J_1^{N_+} \bar{J}_1^{N_-}$$

$$S^{eff} = \mathrm{Re}\, S_1 + \frac{1}{2} \ln \det \mathscr{H}_\perp - \ln |J|$$

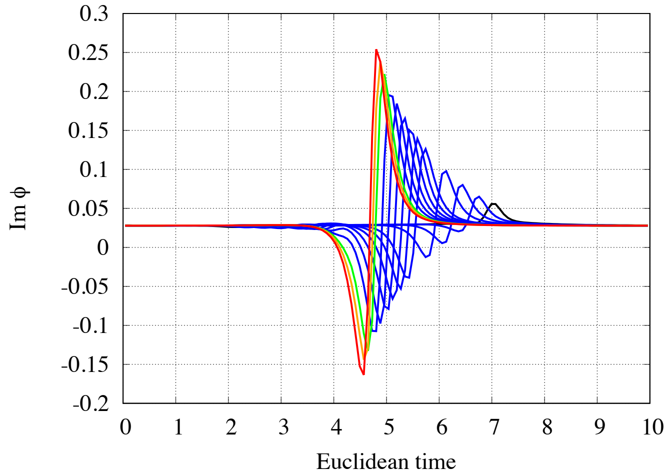


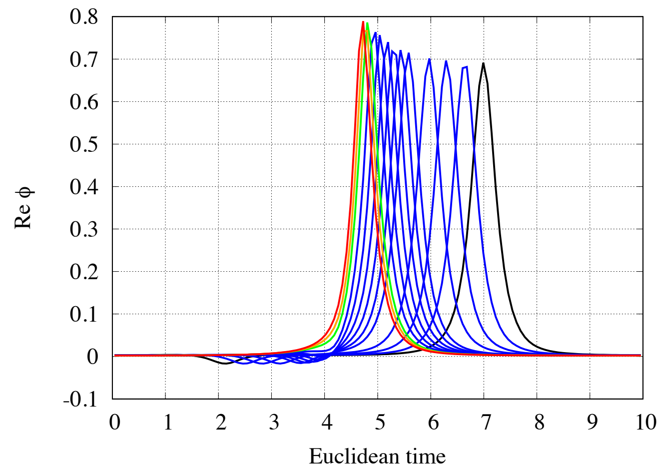


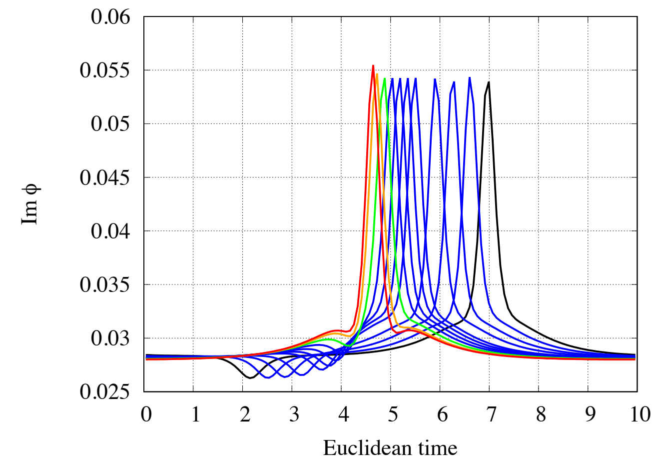


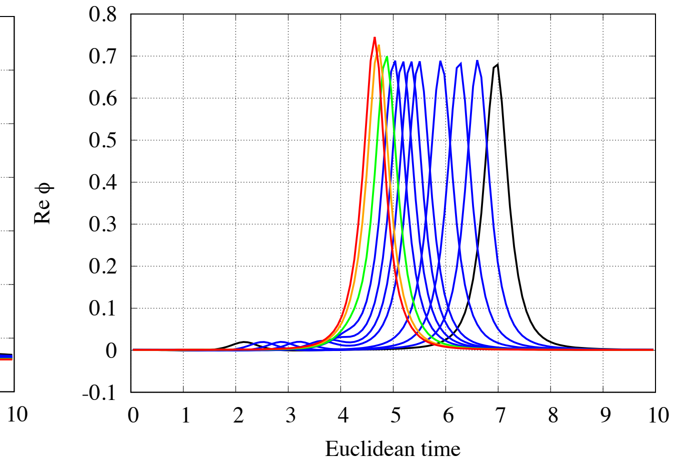


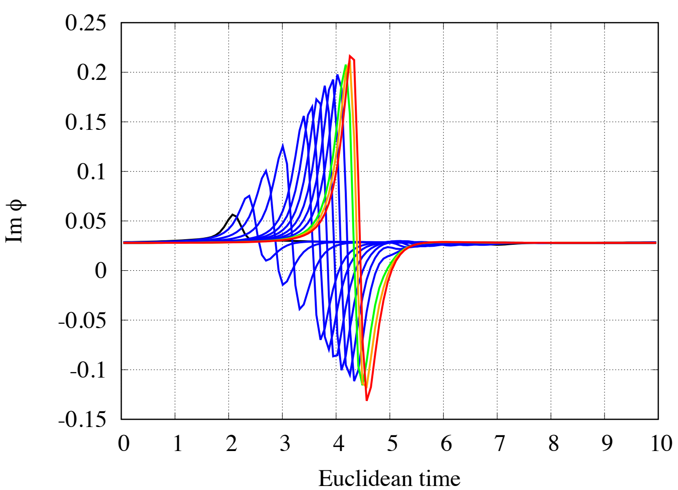
Interaction of complex instantons

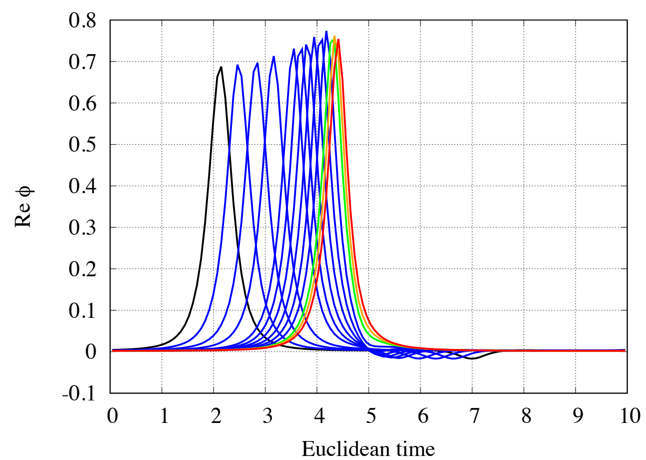


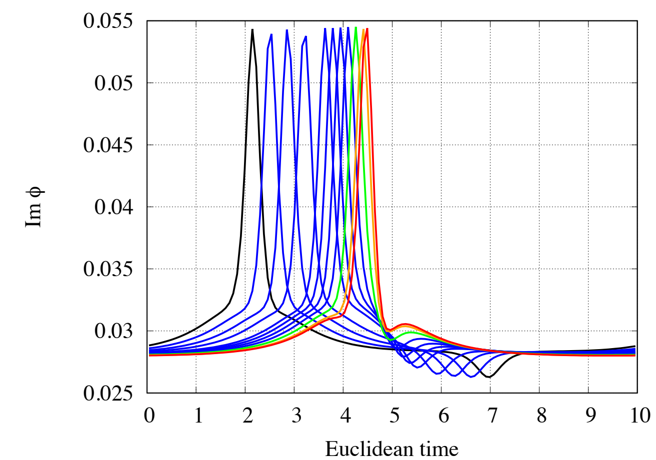


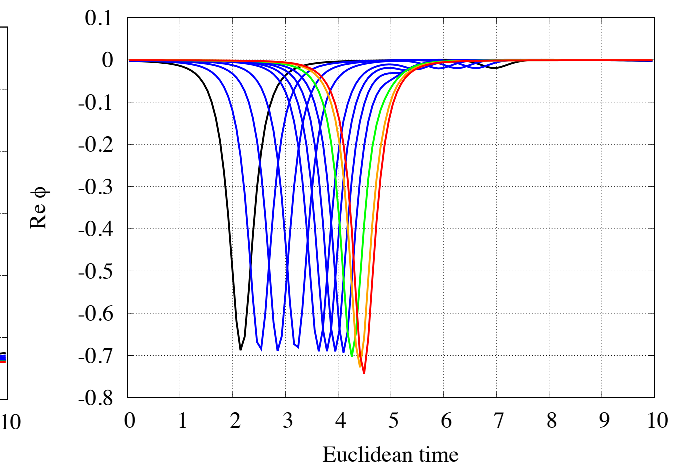


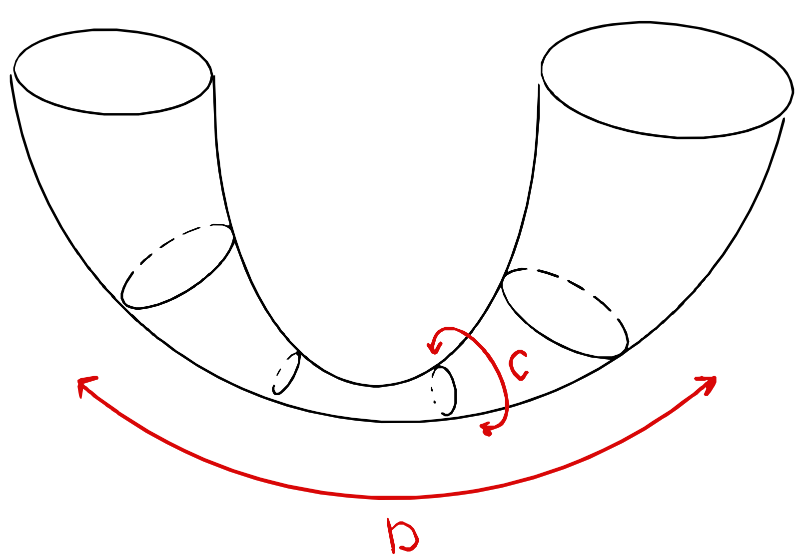


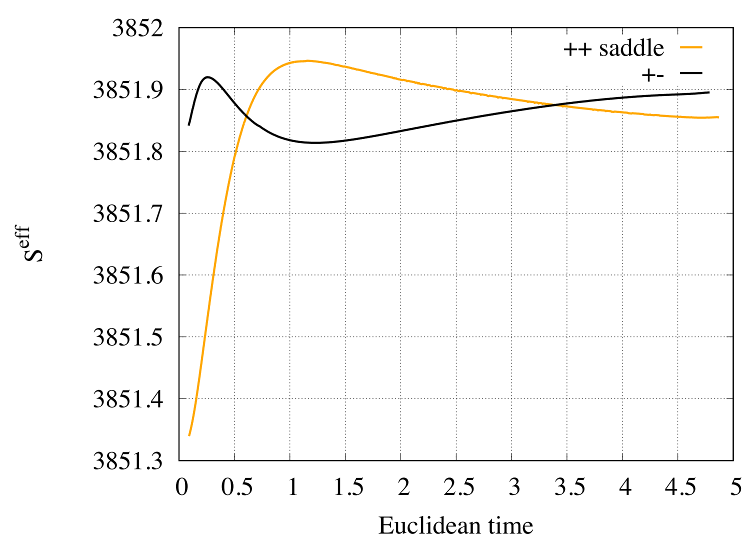


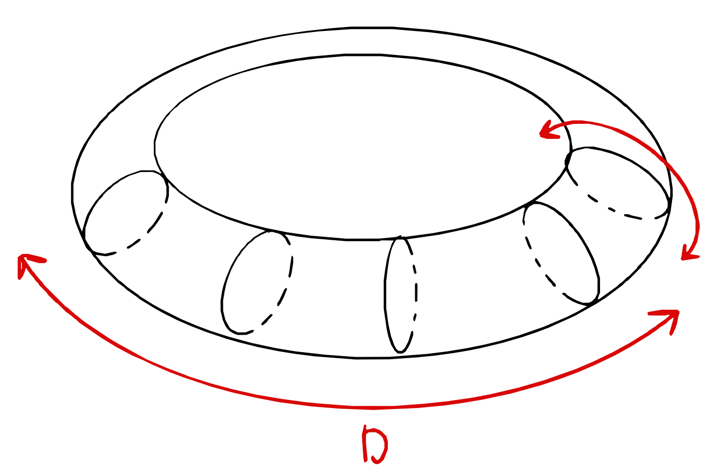










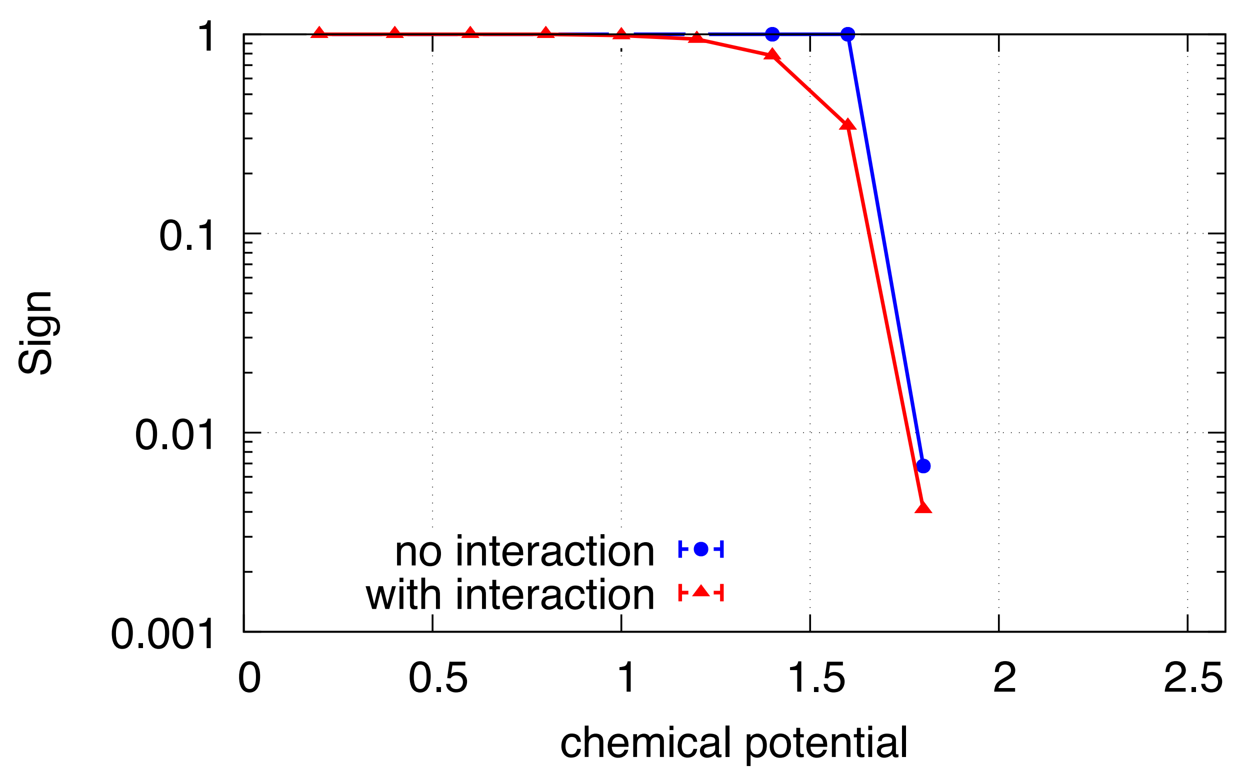


Gas of weakly interacting complex instantons

$$\frac{Z}{Z_0} = 1 + \sum_{K=1}^{K_{max}} \frac{1}{K!}(\beta N_s - \Delta\beta X)\dots(\beta N_s - (K-1)\Delta\beta X)2^{2K} \times e^{-S_1 K} \left\{ \left[\det\left(\mathscr{H}_\perp^{(1)} (\mathscr{H}^{(0)})^{-1} \right) \right]^{-1/2} \frac{L}{\sqrt{2\pi\beta}} \right\}^K$$

$$1 + \sum_{K_+=1, K_-=1}^{K_{max}} \frac{1}{K!}(\beta N_s - \Delta\beta X)\dots(\beta N_s - (K-1)\Delta\beta X)2^{K} \times e^{-\mathrm{Re}\, S_1 K} e^{-i\,\mathrm{Im}(S_1 + \Phi_J)(K_+ - K_-)} \left\{ \left[\det\left(\mathscr{H}_\perp^{(1)} (\mathscr{H}^{(0)})^{-1} \right) \right]^{-1/2} \frac{L}{\sqrt{2\pi\beta}} \right\}^K$$

$$\boxed{f = f_0 - \frac{1}{\Delta\beta X} \ln\left(1 + \frac{2e^{-\mathrm{Re}\, S_1} \cos(\mathrm{Im}\, S_1 + \Phi_J)\Delta\beta X L}{\beta\sqrt{2\pi \det\left(\mathscr{H}_\perp^{(1)} (\mathscr{H}^{(0)})^{-1} \right)}} \right)}$$



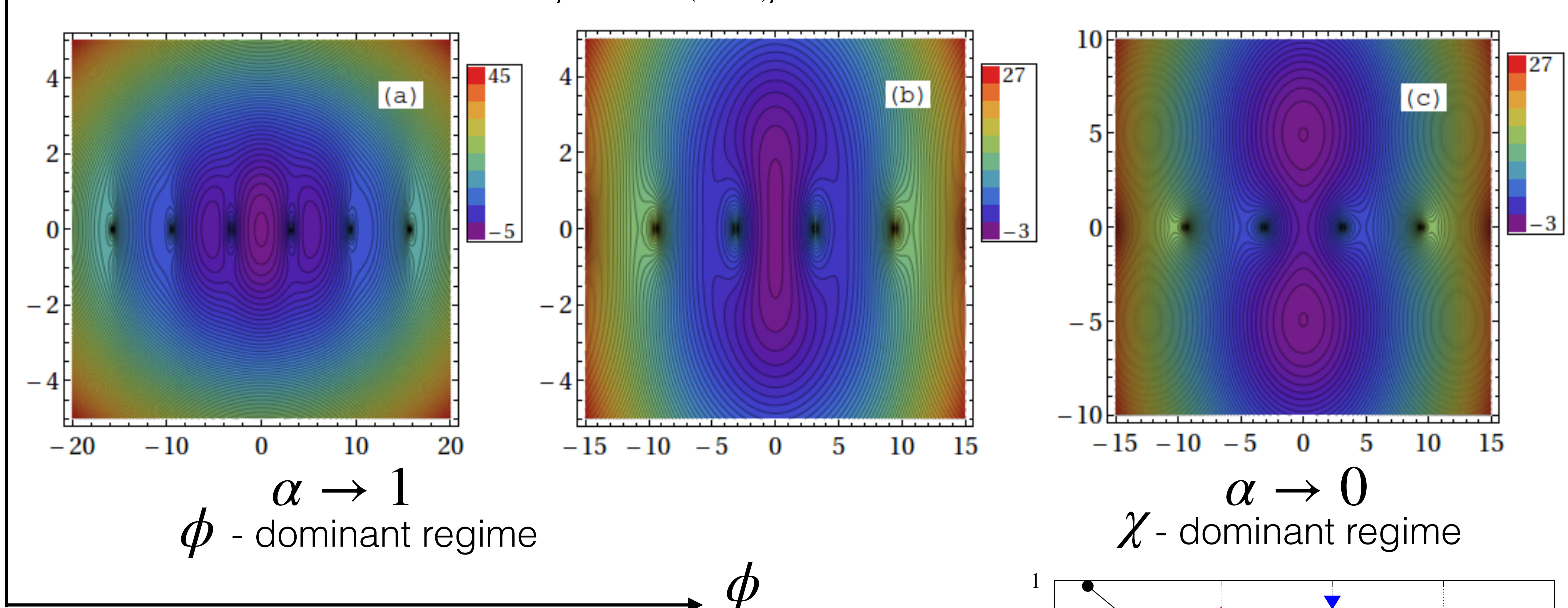
!

$6 \times 6, \beta = 5, U = 5.0$

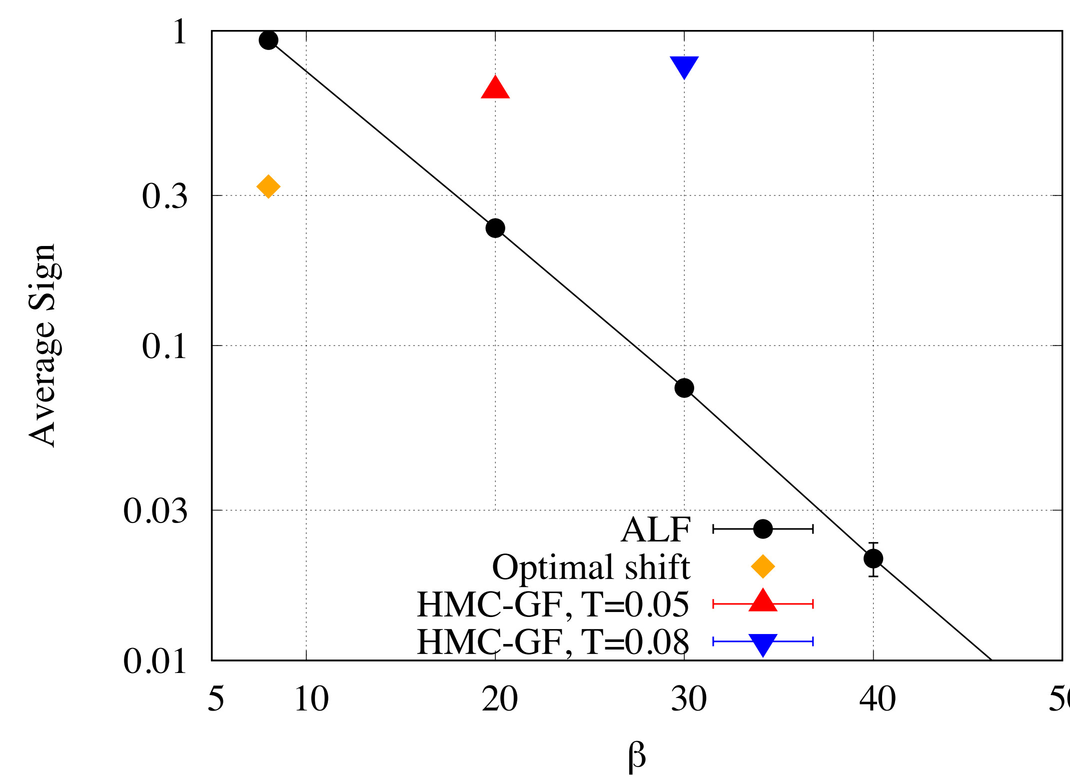
Single thimble regime combining two fields

χ

$$S(x) = \frac{\phi^2}{2\alpha\beta U} + \frac{(\chi - (1-\alpha)\beta U)^2}{2(1-\alpha)\beta U} - \ln\left((1+e^{i\phi-\chi})(1+e^{-i\phi-\chi})\right)$$



	$\langle \hat{K} \rangle$	$\langle \hat{S}_x^{(1)} \hat{S}_y^{(1)} \rangle$
ED	19.5781	-0.14624
BSS-QMC	19.587±0.002	-0.1466±0.0008
HMC, $\alpha = 1.0$	19.65±0.31	-0.112±0.0069
HMC, $\alpha = 0.8$	19.52±0.17	-0.142±0.0062



Resummation

$$Z = \sum_{k_-,k_+} C_{k_-,k_+} e^{-i(k_+-k_-)\mathrm{Im}\, S^{eff}} e^{-(k_++k_-)\mathrm{Re}\, S^{eff}}$$

Observable: $$\langle O \rangle = \frac{\sum_{\mathcal{J}} \int_{\mathcal{J}} dz e^{-S} O(z)}{\sum_{\mathcal{J}} \int_{\mathcal{J}} dz e^{-S}} = \frac{\sum_{\mathcal{J}} \langle O \rangle_{\mathcal{J}} W_{\mathcal{J}}}{\sum_{\mathcal{J}} W_{\mathcal{J}}}$$

$$\langle O \rangle_{\mathcal{J}} = \frac{\int_{\mathcal{J}} dz e^{-S} O(z)}{\int_{\mathcal{J}} dz e^{-S}} = O(k_+, k_-) \approx O_0 + O_1^+(k_+ + k_-) + O_1^-(k_+ - k_-) + O_2^{++}(k_+ + k_-)^2 \ldots$$

$W_{\mathcal{J}}$ - from instanton gas

$$\langle O \rangle = \frac{\sum_{k_-,k_+} C_{k_-,k_+} e^{-i(k_+-k_-)\mathrm{Im}\, S^{eff}} e^{-(k_++k_-)\mathrm{Re}\, S^{eff}} [O_0 + O_1^+(k_+ + k_-) + O_1^-(k_+ - k_-) + O_2^{++}(k_+ + k_-)^2 \ldots .]}{\sum_{k_-,k_+} C_{k_-,k_+} e^{-i(k_+-k_-)\mathrm{Im}\, S^{eff}} e^{-(k_++k_-)\mathrm{Re}\, S^{eff}}}$$

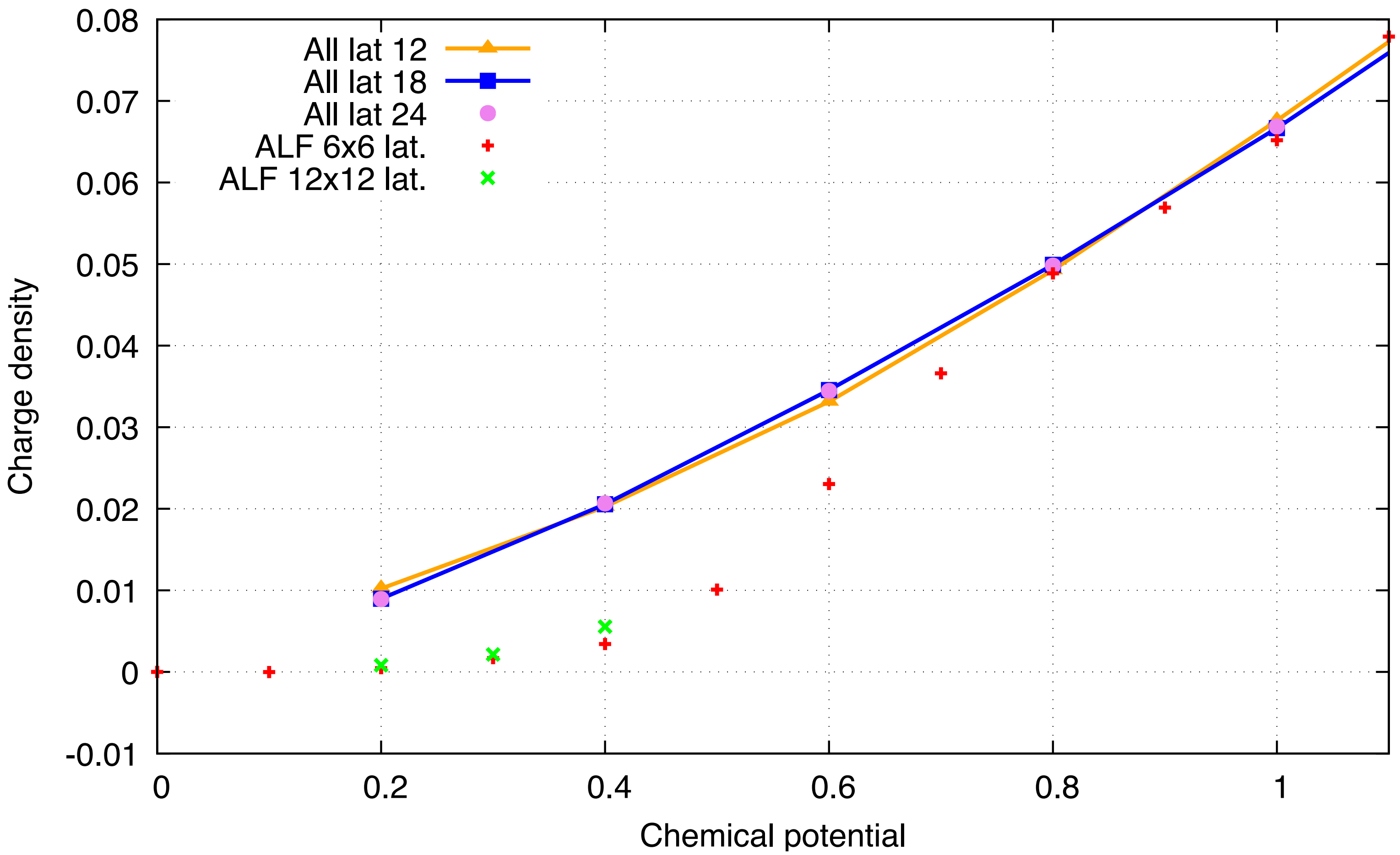
$$\langle O \rangle = O_0 + O_1^+ \langle k_+ + k_- \rangle + O_1^- \langle k_+ - k_- \rangle + O_2^{++} \langle (k_+ + k_-)^2 \rangle + \ldots$$

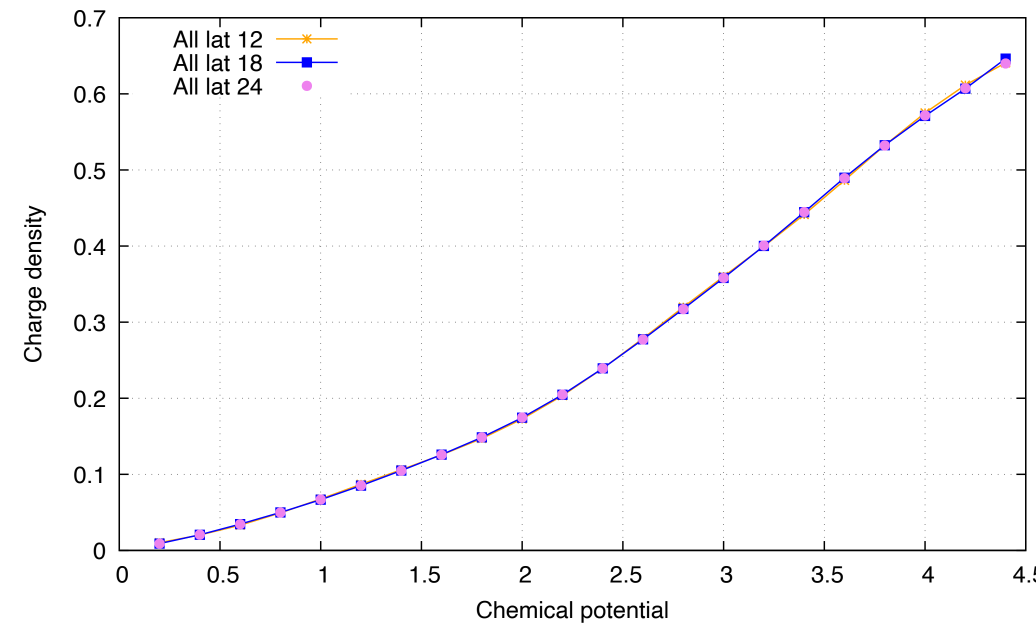
$$\langle k_+ + k_- \rangle = -\frac{\partial \ln Z}{\partial\, \mathrm{Re}\, S^{eff}}; \quad \langle k_+ - k_- \rangle = i \frac{\partial \ln Z}{\partial\, \mathrm{Im}\, S^{eff}}; \ldots$$

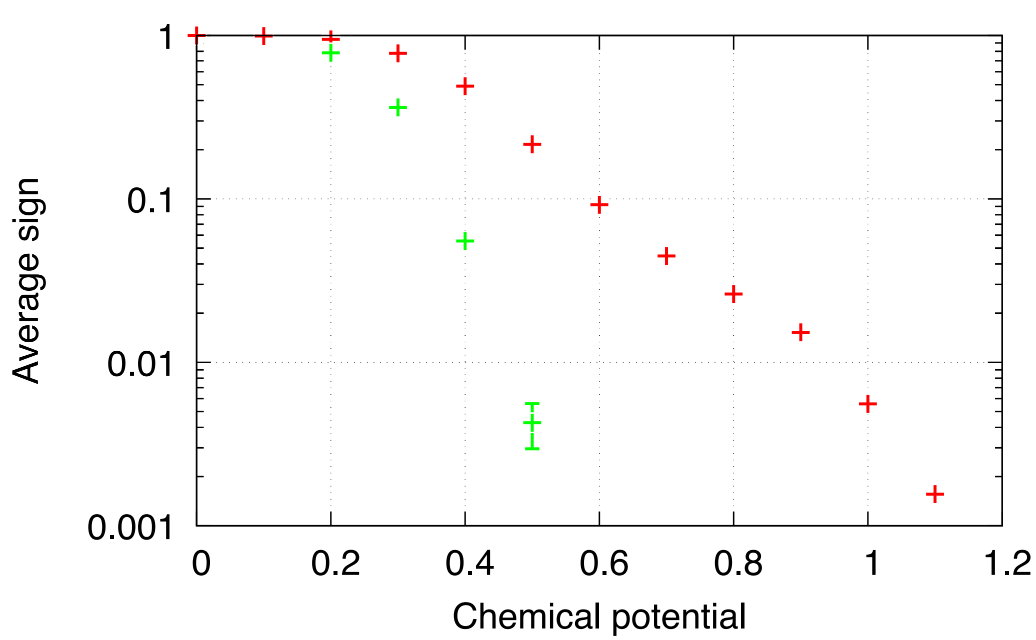
Resummation - charge density away of half-filling

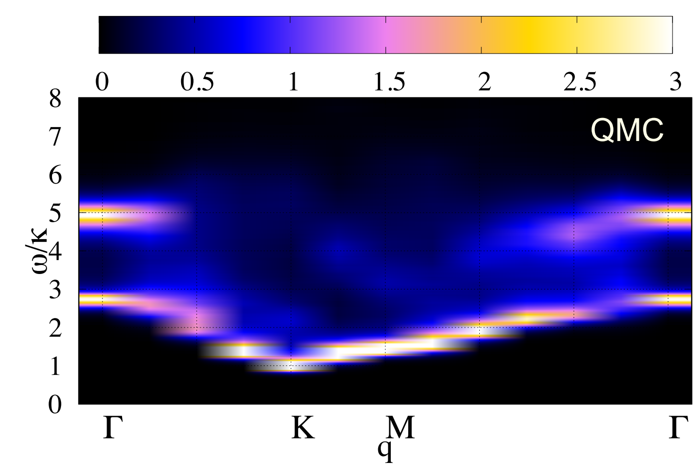
$$\phi_{x,\tau} = -U \,\mathrm{Im}\, g^{\tau}_{xx}$$

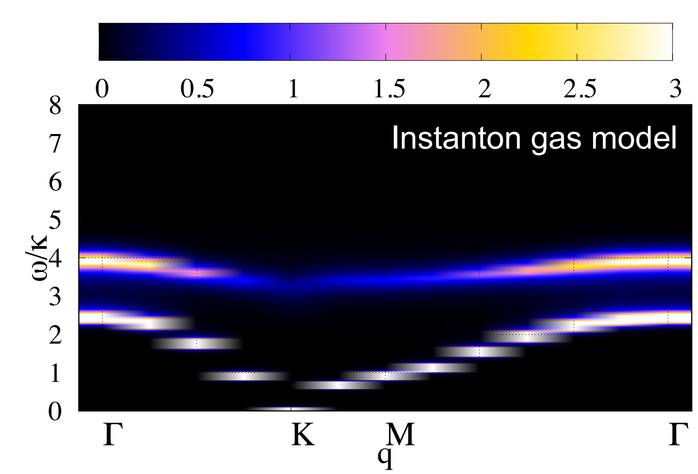
$$\langle O \rangle = O_0 + O_1^{+}\langle k_+ + k_- \rangle + O_1^{-}\langle k_+ - k_- \rangle$$



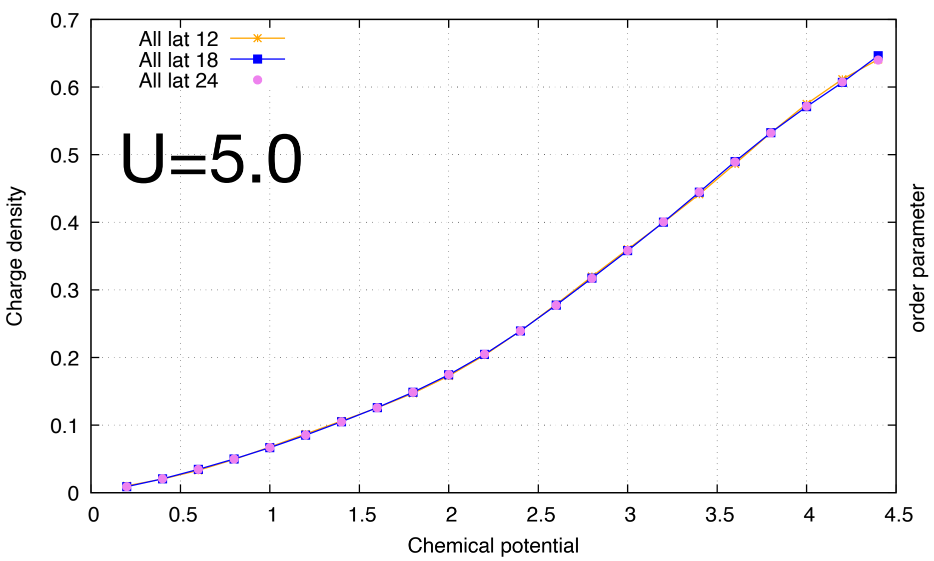


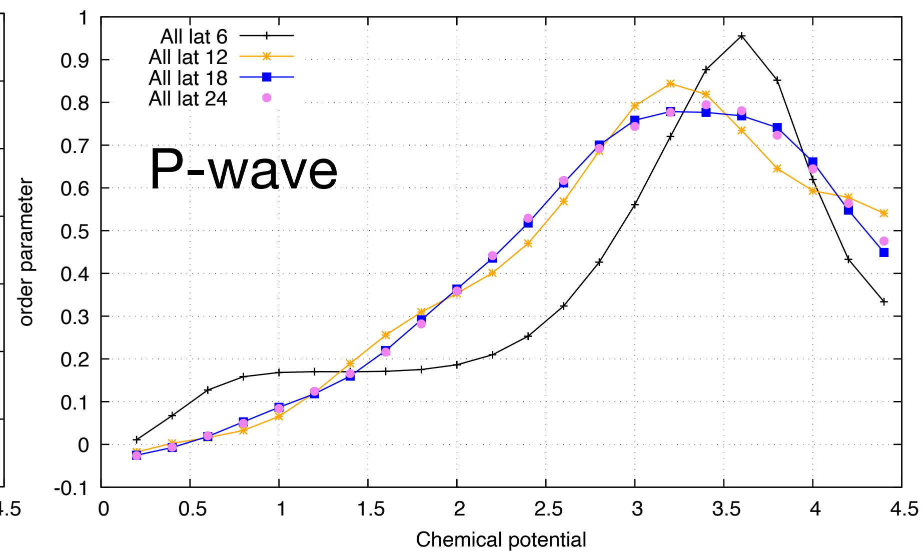


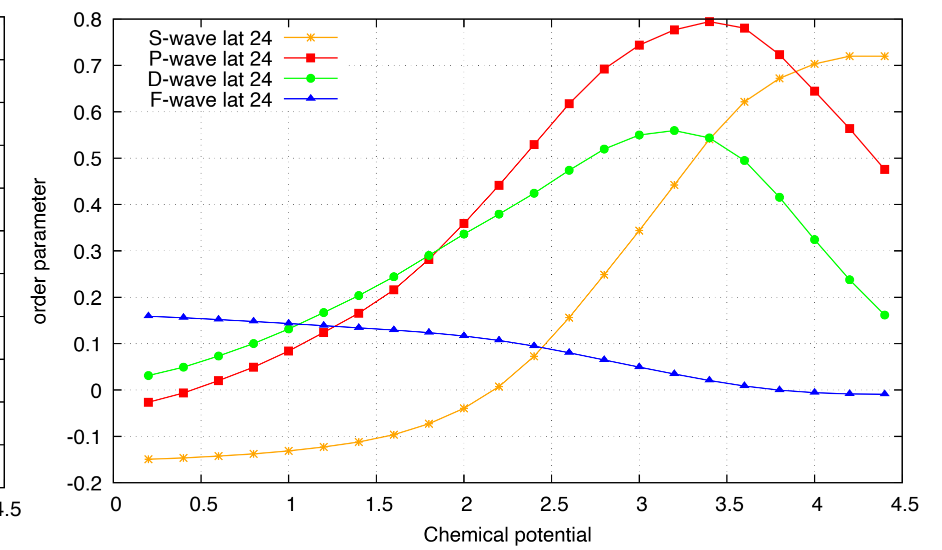




Resummation - non-local correlation







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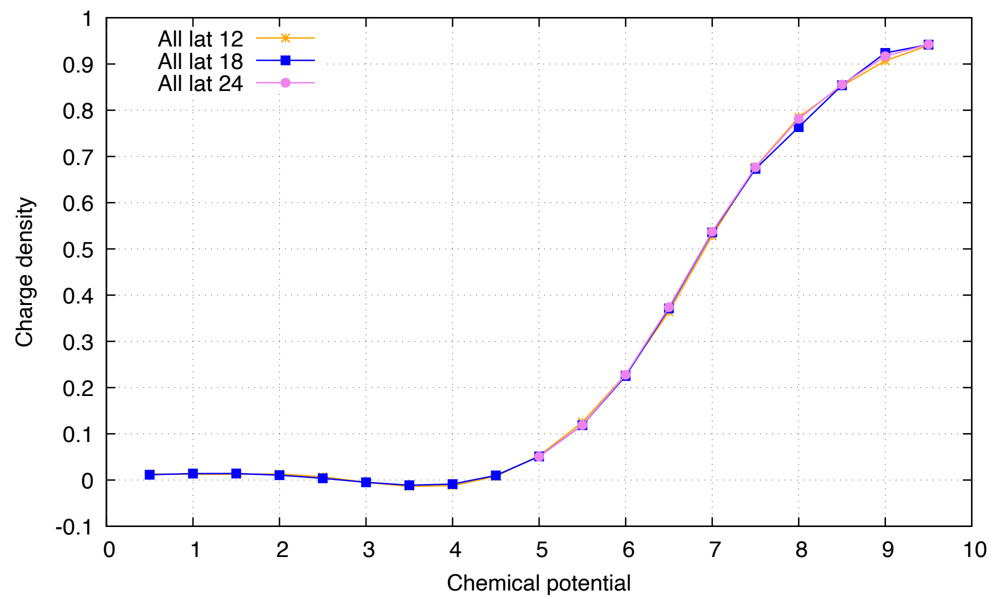
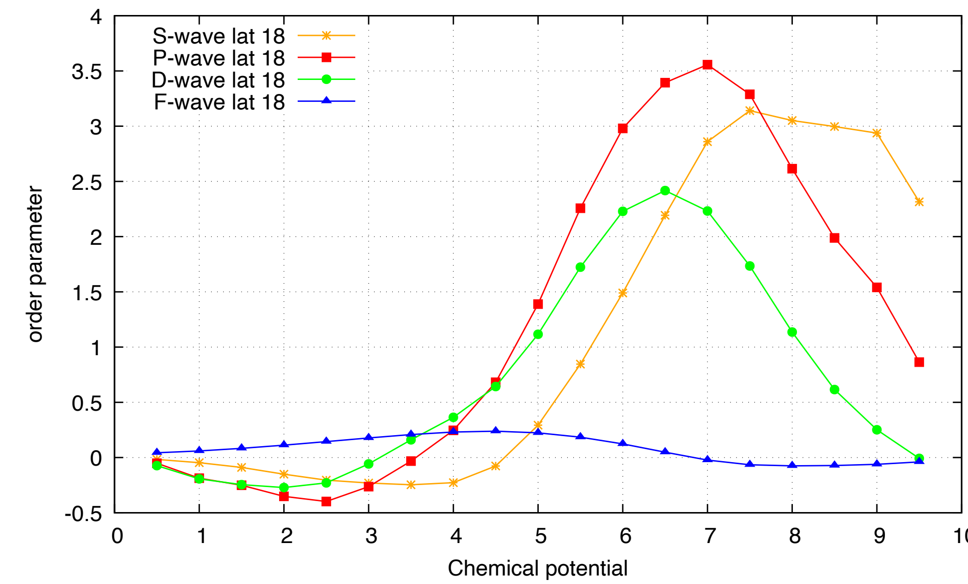


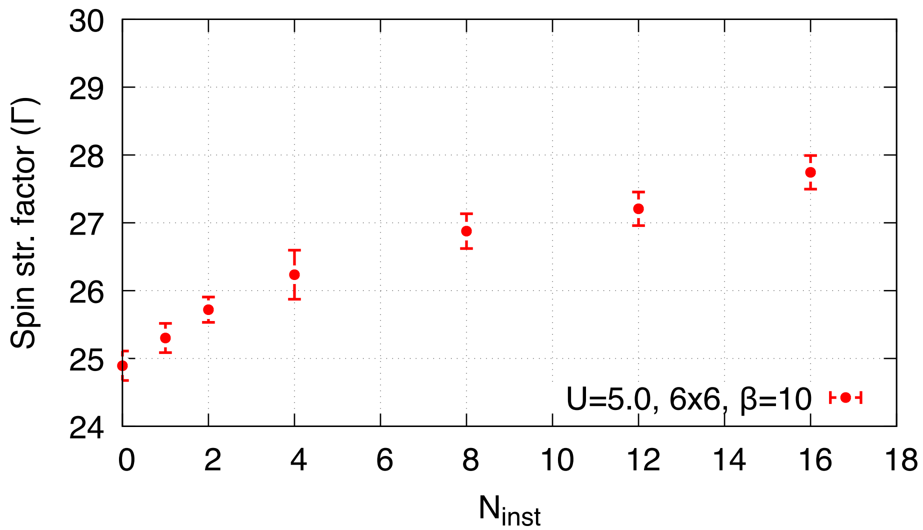


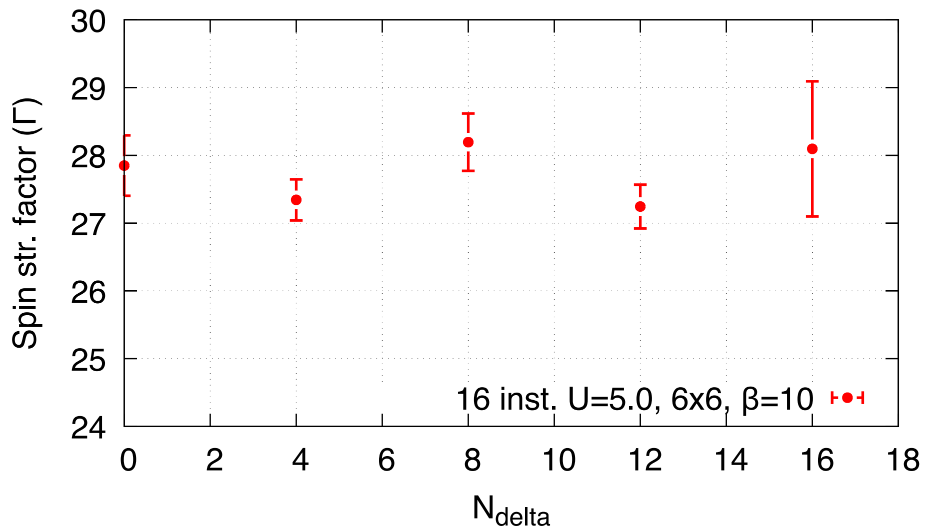
$$\langle O\rangle = O_0 + O_1^+\langle k_+ + k_-\rangle + O_1^-\langle k_+ - k_-\rangle$$

Taken from saddle point field configurations

Further perspectives

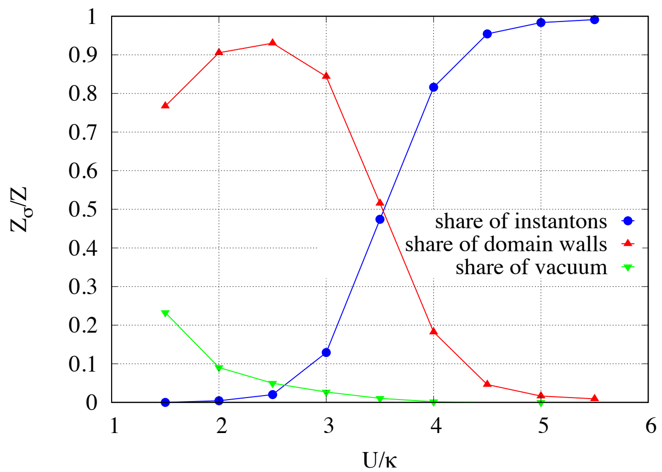
1) better approximation for the thimble integral

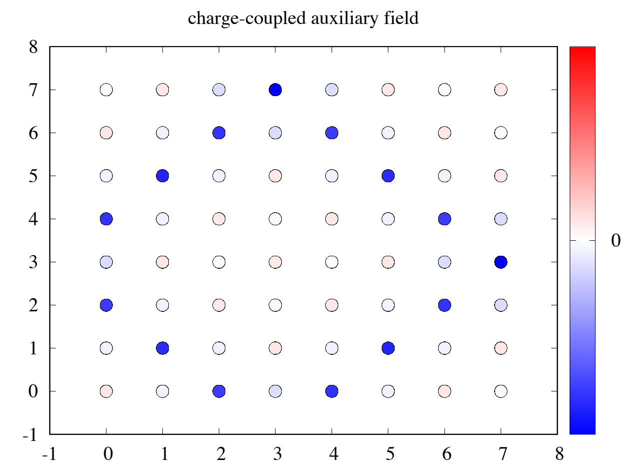




$$\langle O \rangle = O_0 + O_1^+ \langle k_+ + k_- \rangle + O_1^- \langle k_+ - k_- \rangle + O_2^{++} \langle (k_+ + k_-)^2 \rangle + \ldots$$

2) Square lattice Hubbard model





Square lattice Hubbard model features not only localized instantons but also domain walls as saddles points

3) Connections to CPQMC

$$|E_0\rangle \approx \sum_X \int \prod_{i=1}^{k_+ + k_-} dT_i \; W(X,T) \; \prod_\tau e^{-\hat{H}_{tb.}\Delta\tau} e^{i \sum_x z(X,T) \hat{q}_x} |\Omega\rangle$$

Weights and profiles taken from instanton gas model