Instanton gas approximation for the Hubbard model

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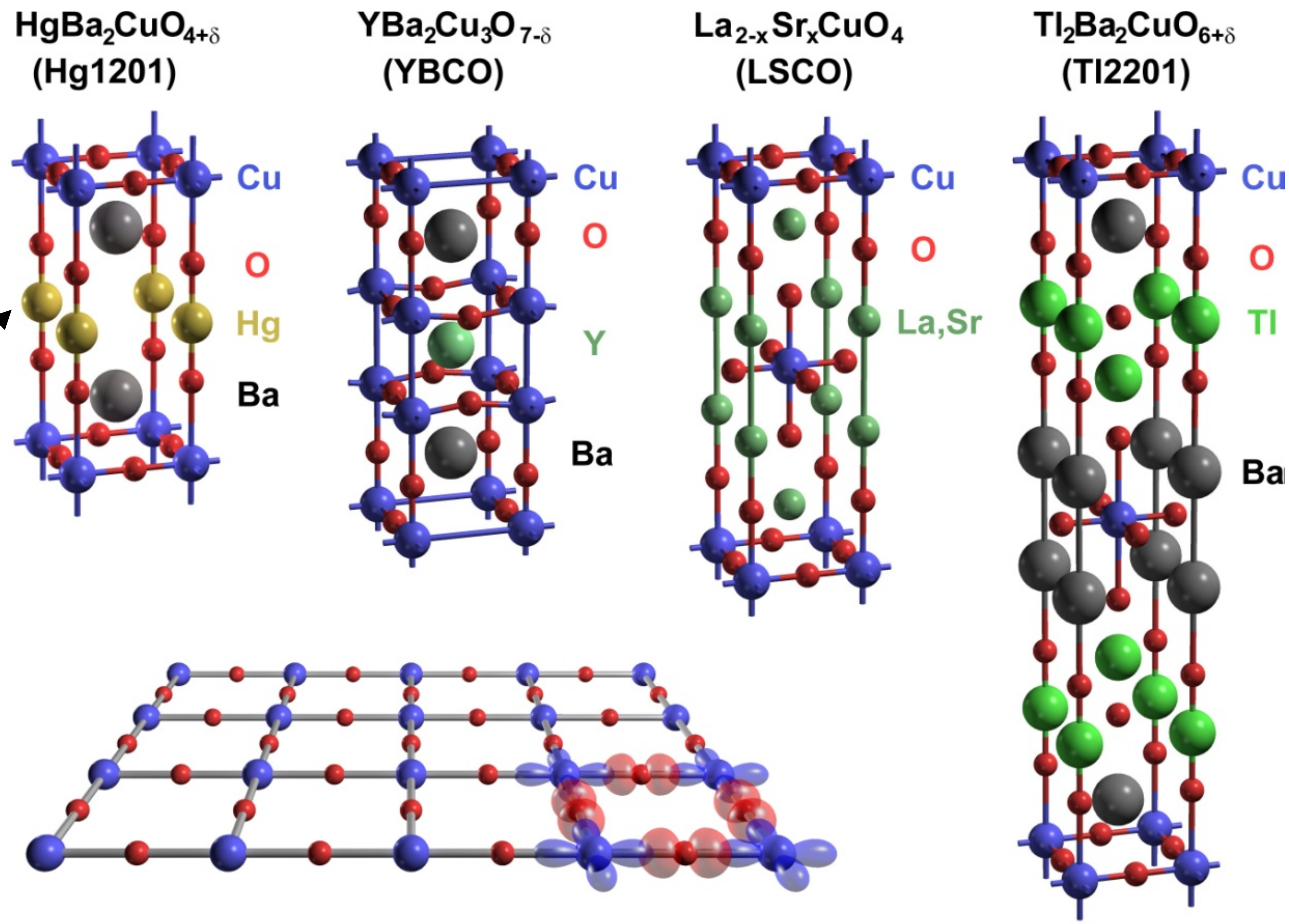
Partially available in arXiv:2207.06297

Why Hubbard model? (1)

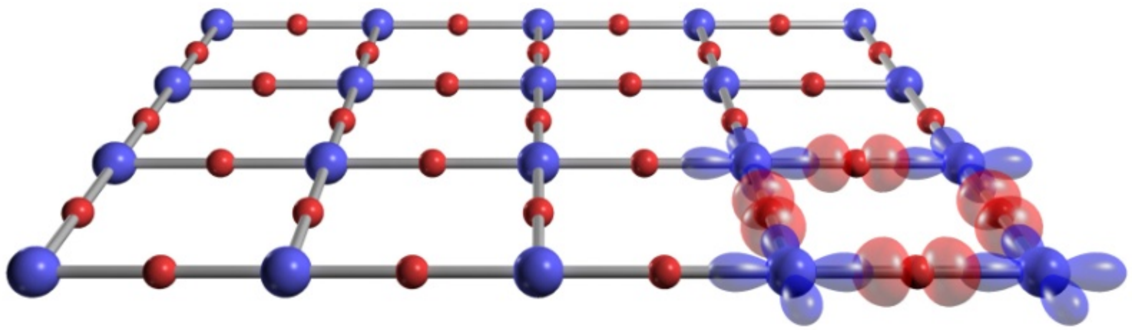
High Tc superconductivity in cuprates:

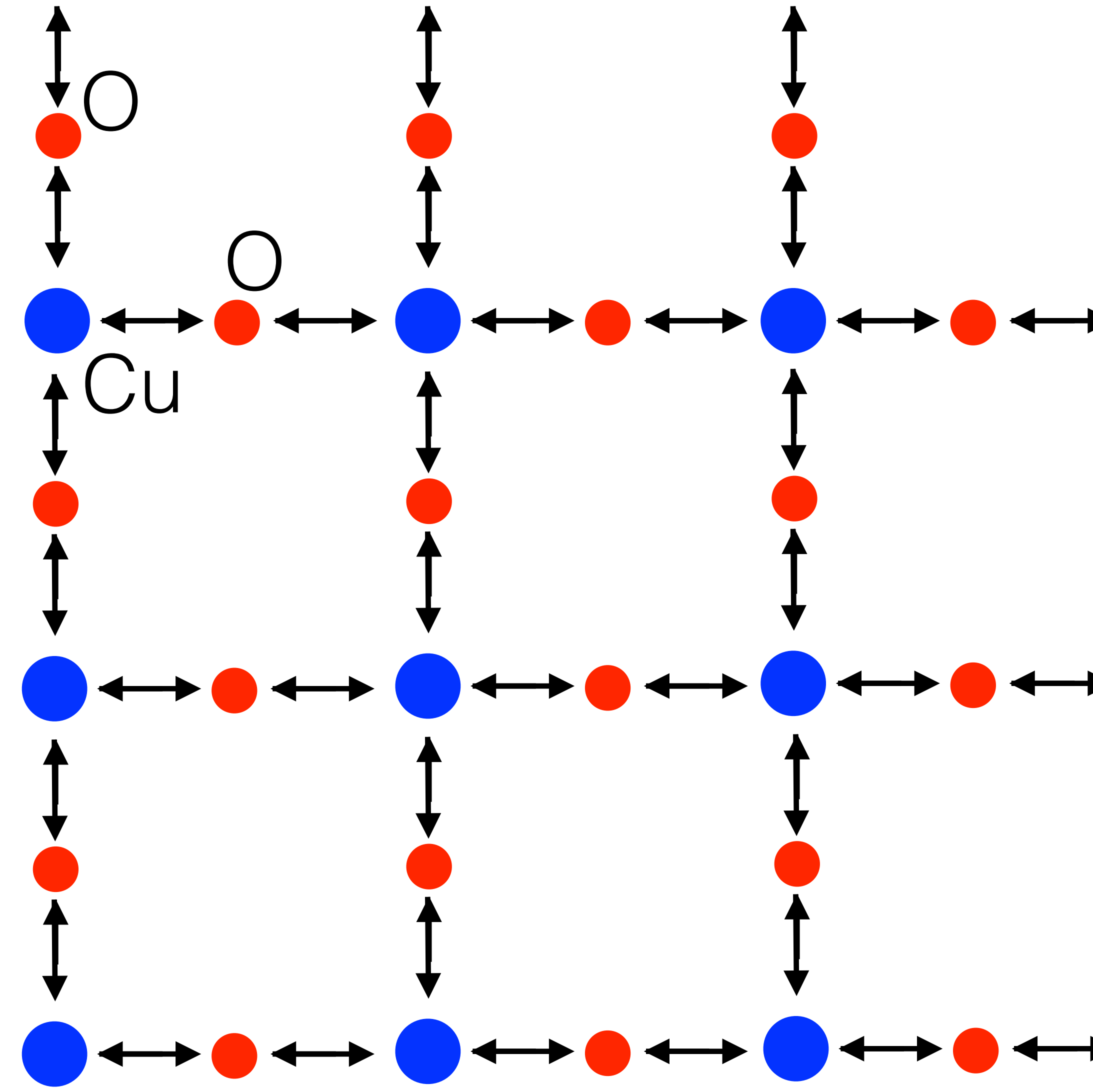
They all have CuO_2 layers alternated by charge reservoir layers



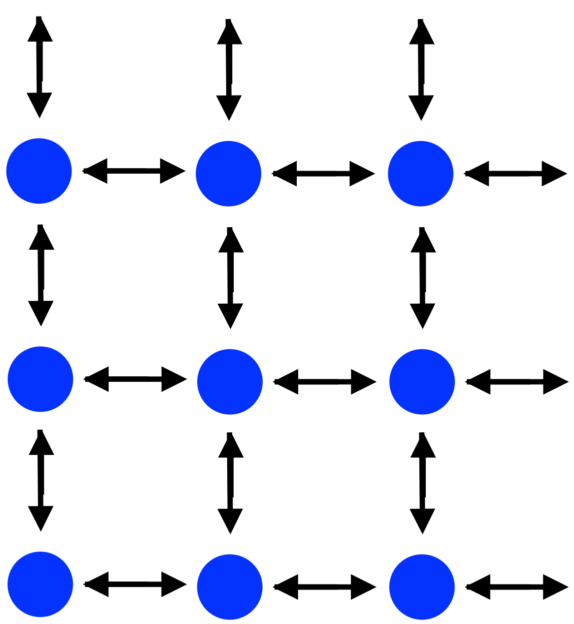
N. Barišić et al, Proceedings of the National Academy of Sciences 110(30)

Why Hubbard model? (2)





Single band Hubbard model



Three-band Hubbard model

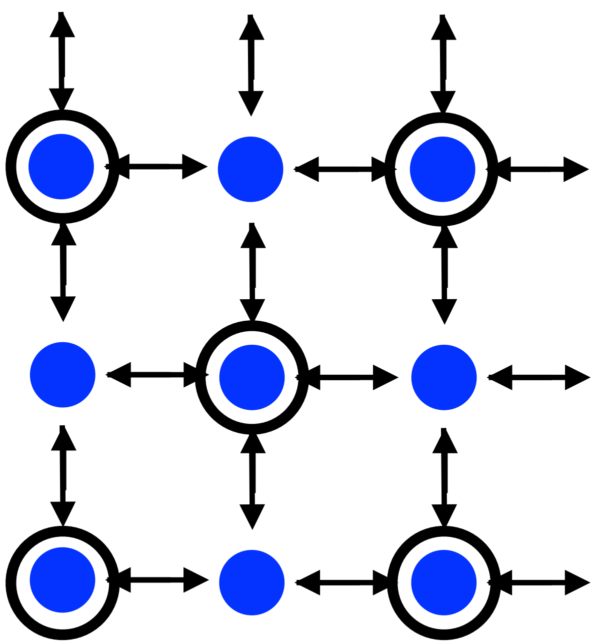
Charge reservoir layers are taken into account through the chemical potential

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

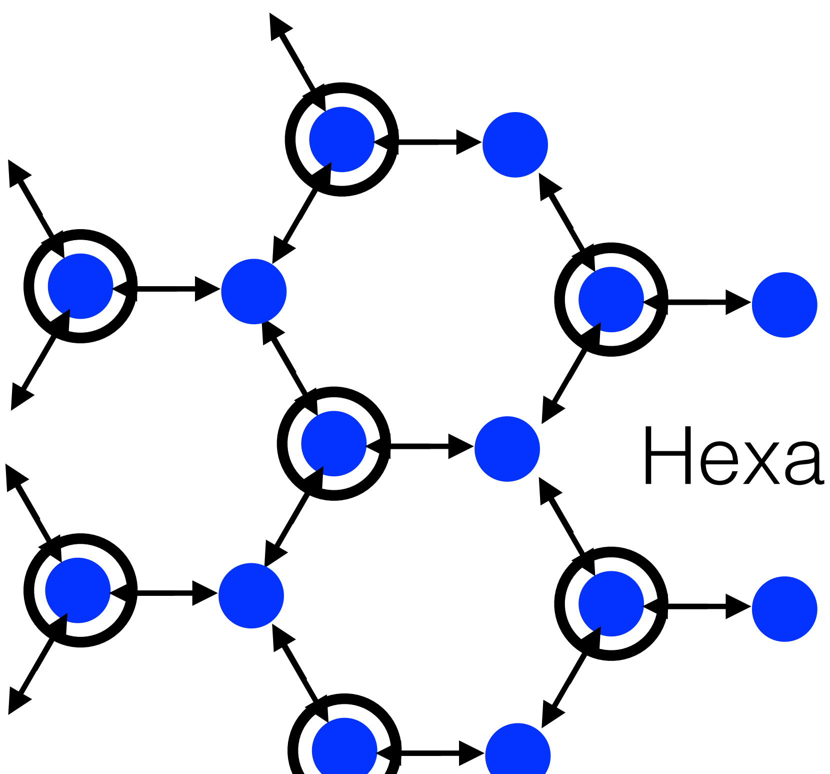
Hubbard model on bipartite lattice

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

Hopping term: no sign problem on any bipartite lattice

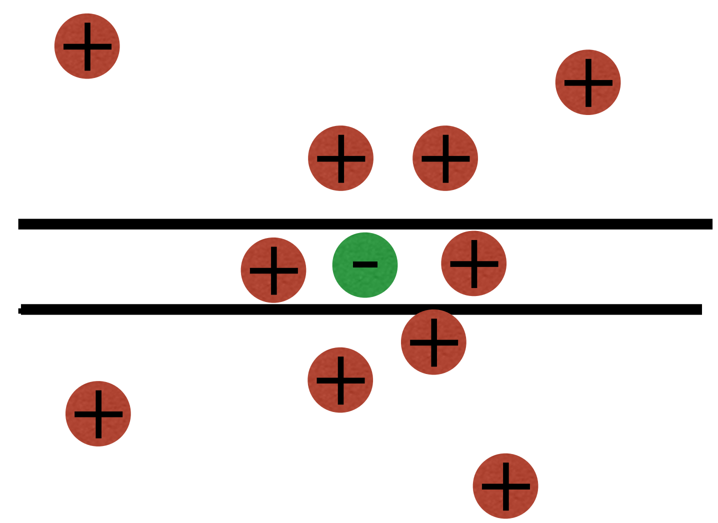


Square

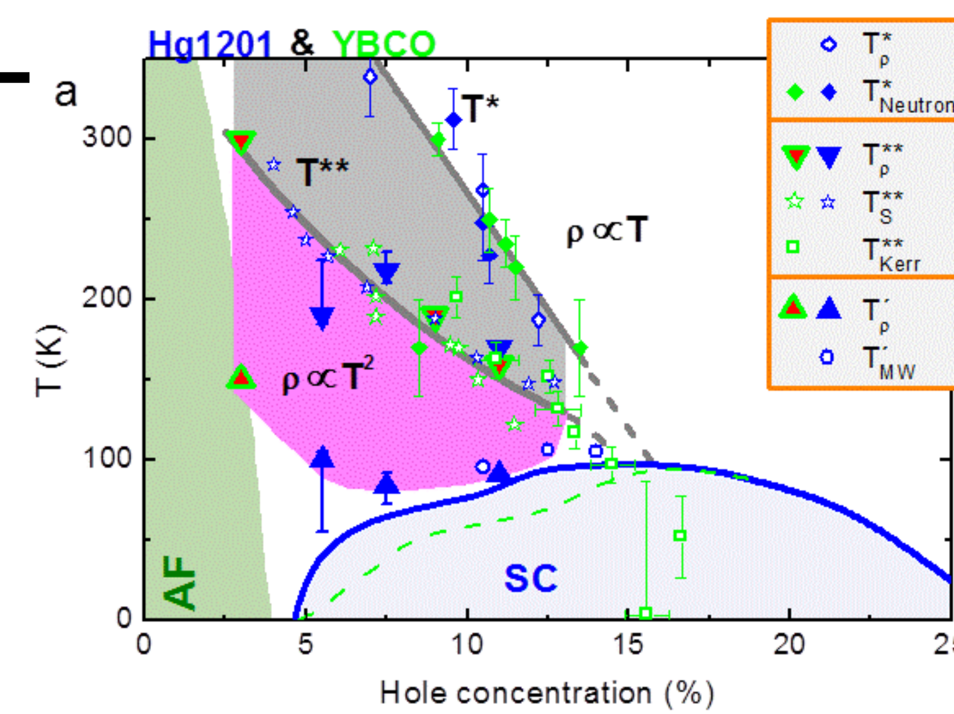


Hexagonal

Only local interaction: long range Coulomb is screened by «plasma» of free electrons at large doping (chemical potential)



Chemical potential: the key ingredient leading to superconductivity

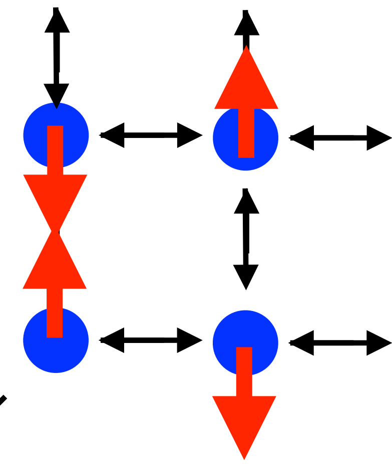


Increasing chemical potential

N. Barišić et al, Proceedings of the National Academy of Sciences 110(30)

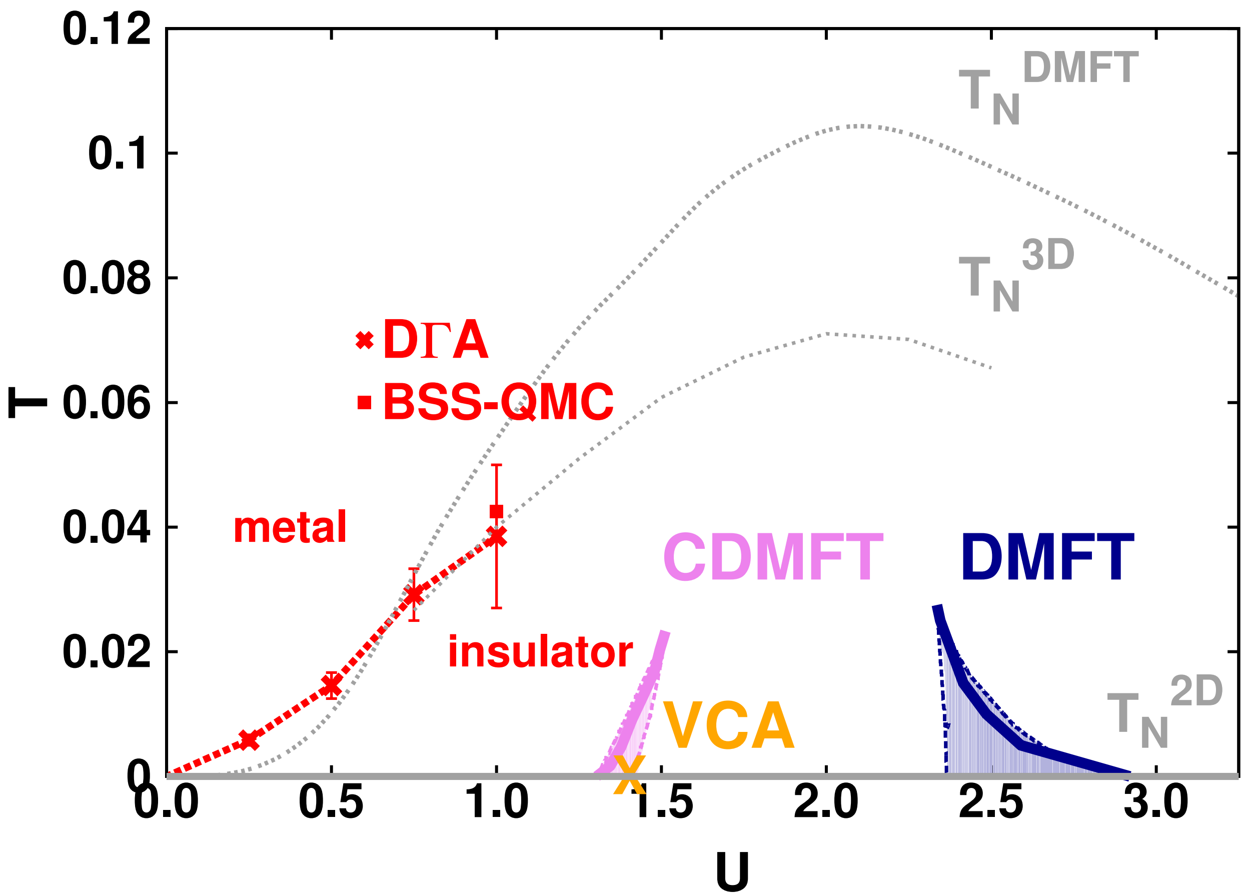
Why do we need approximations ? (1)

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

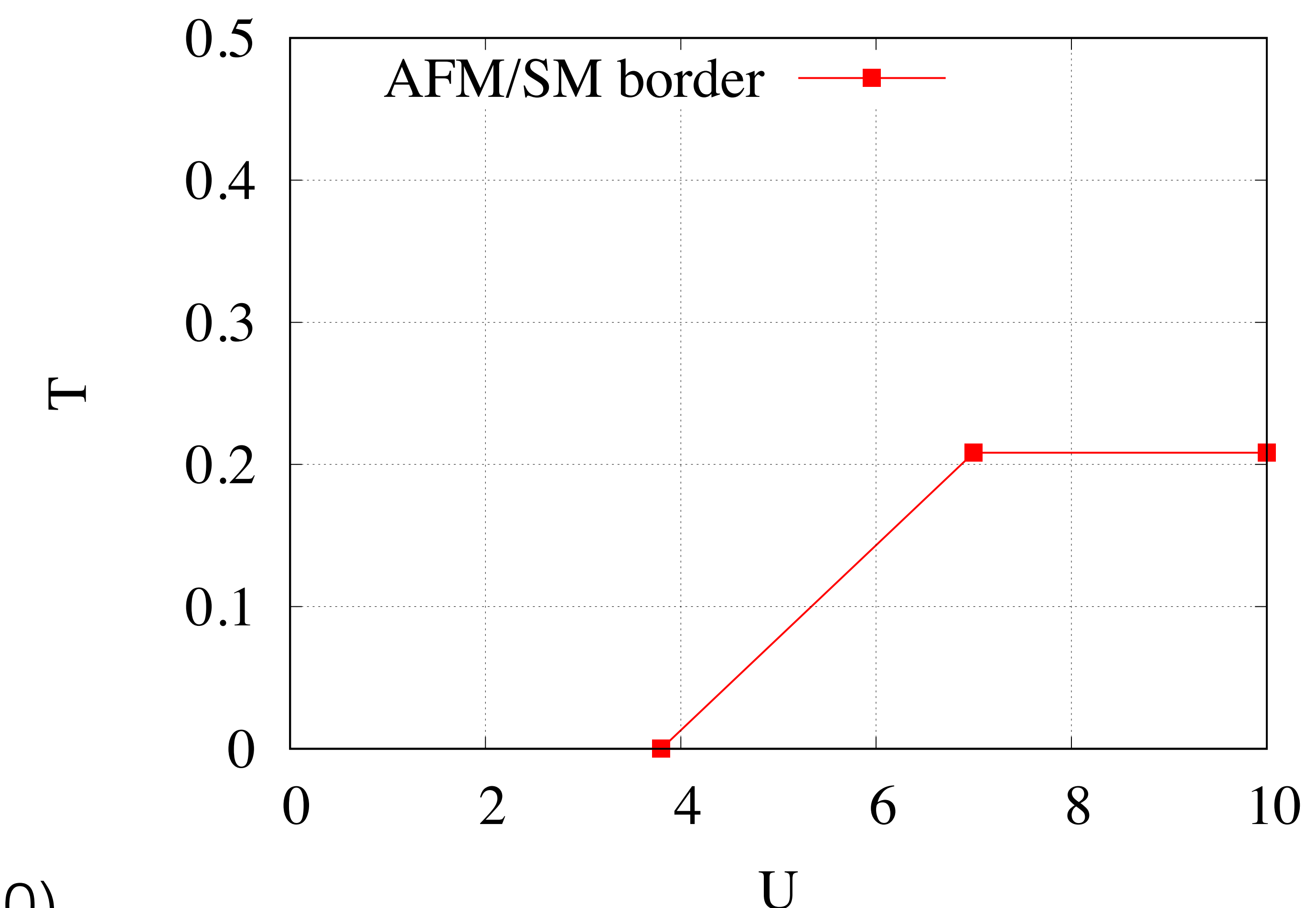


Zero chemical potential («half filling»): Antiferromagnetic (AFM) order, or transition from semimetal to AFM insulator, all identified with exact Quantum Monte Carlo

«Localized spins» assembled in antiferromagnetic order



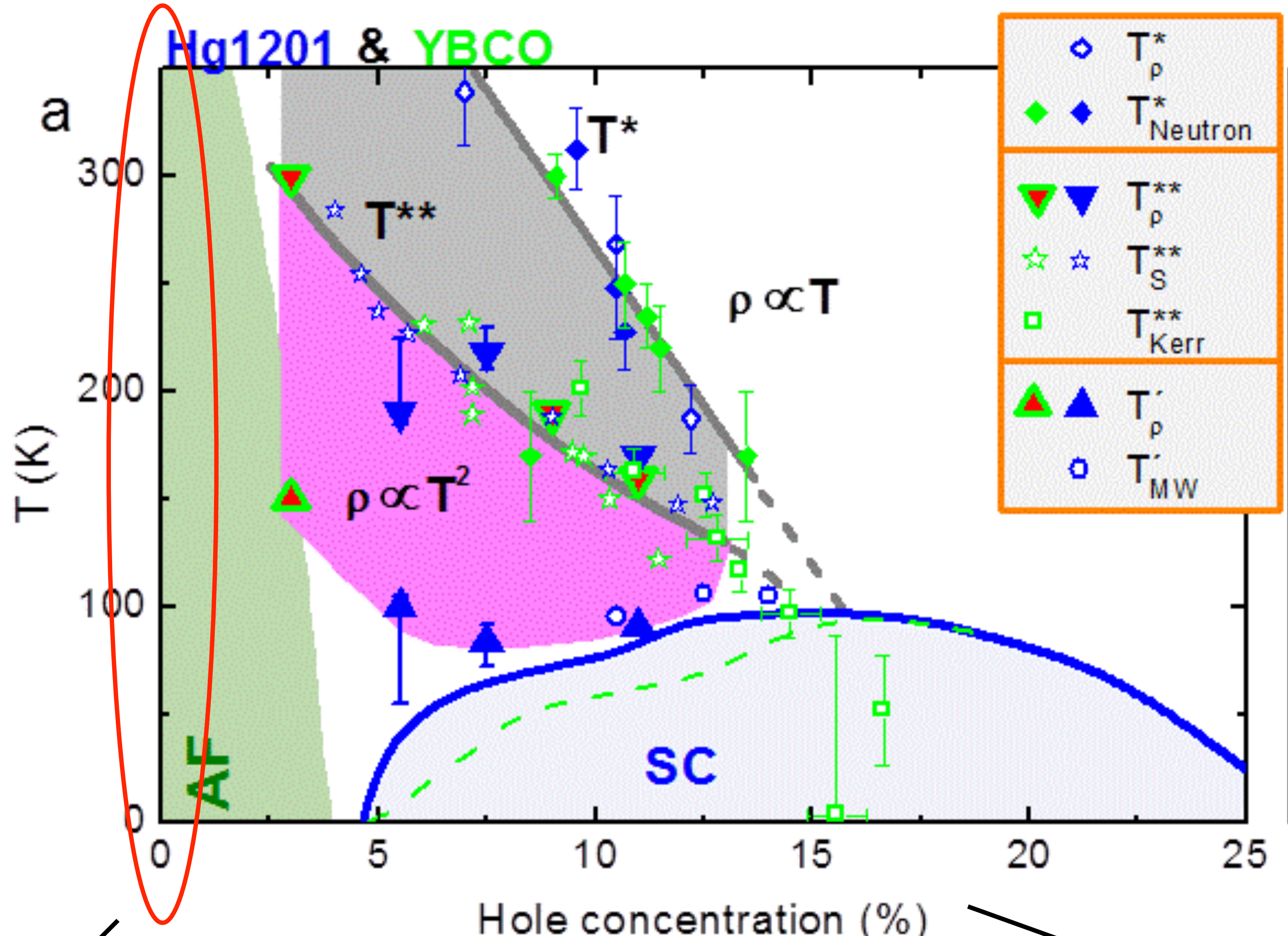
Square lattice (T. Schäfer et al, arXiv:1405.7250)



Hexagonal lattice (zero temperature point from F. Assaad, I. Herbut PRX 3, 031010 (2013))

Why do we need approximations ? (2)

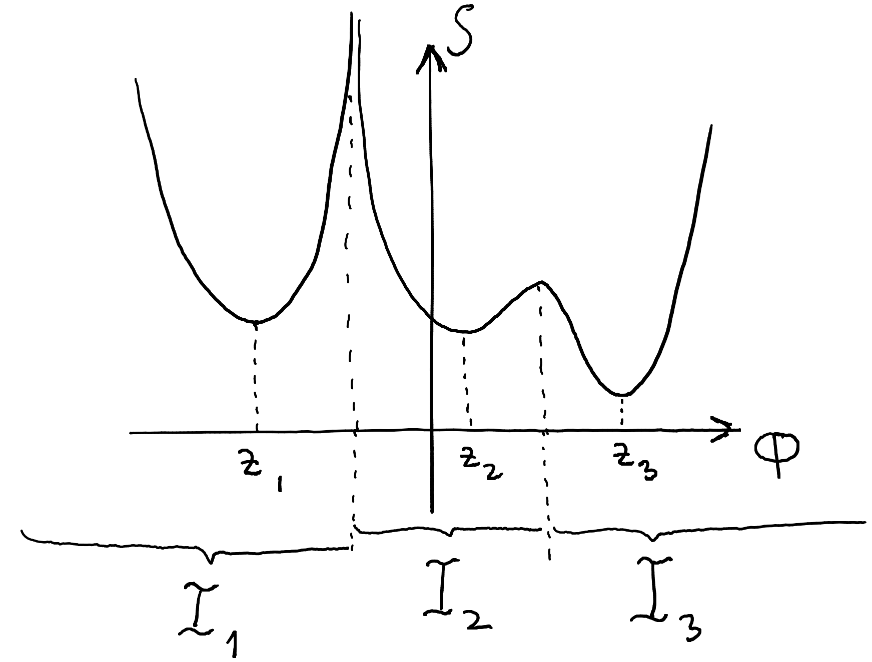
$$\hat{H} = -\kappa \sum_{\langle x,y\rangle,\sigma} (\hat{c}^{\dagger}_{x\sigma}\hat{c}_{y\sigma} + h.c.) + U \sum_{x} \hat{n}_{x\uparrow}\hat{n}_{x\downarrow} - \left(\frac{U}{2} - \mu\right) \sum_{x} (\hat{n}_{x\uparrow} + \hat{n}_{x\downarrow} - 1)$$



Only this tiny region is accessible for the simulations!

Prohibitively expensive simulations due to the sign problem

Another motivation: structure of the thimbles decomposition



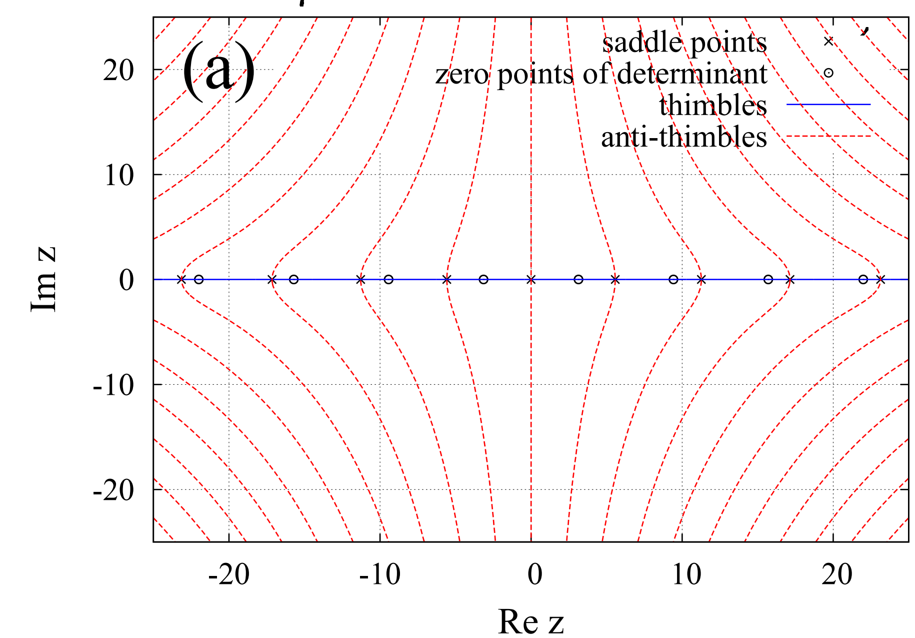
$$\mathcal{Z} = \int_{\mathbb{R}^N} \mathcal{D}\Phi\, e^{-S[\Phi]} = \sum_\sigma k_\sigma \mathcal{Z}_\sigma$$

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

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

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

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



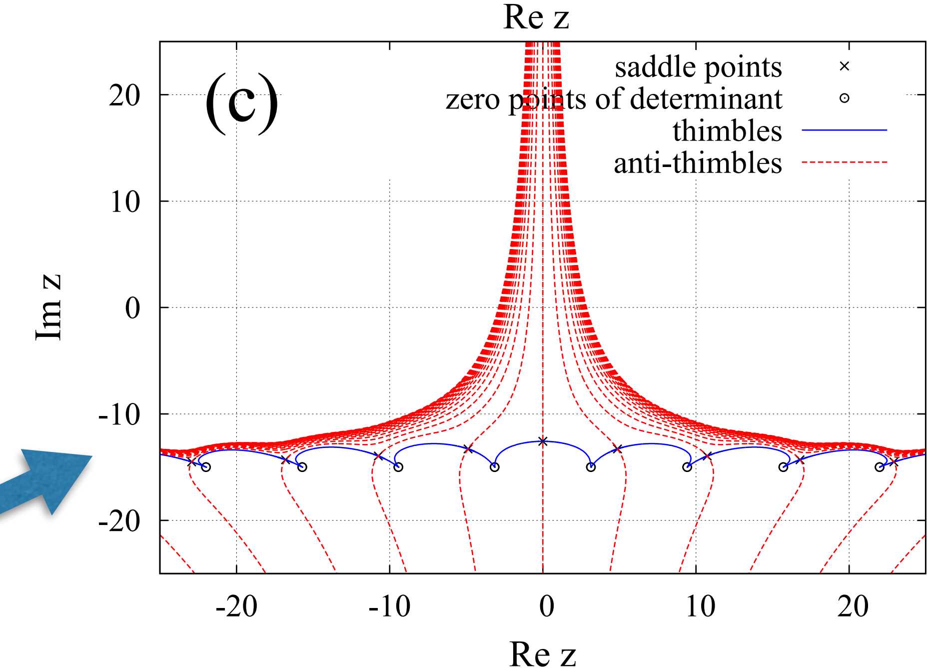
Structure of the thimbles decomposition in the thermodynamic limit for the model with lattice fermions: one- or many-thimble regime?

Spoiler: instanton gas model for the field configurations at saddle points predicts the dominant saddles with reasonable accuracy.

Knowing all relevant saddle points, which physical properties can we describe with this saddle point approximation?

Spoiler: instanton gas model gives good predictions for the localization of electrons, but one needs full integral over just one dominant thimble in order to describe the spontaneous symmetry breaking.

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



Path integrals for the Hubbard model

$$\hat{H} = -\kappa \sum_{\langle \boldsymbol{x},\boldsymbol{y}\rangle} (\hat{a}^\dagger_{\boldsymbol{x}}\hat{a}_{\boldsymbol{y}} + \hat{b}^\dagger_{\boldsymbol{x}}\hat{b}_{\boldsymbol{y}} + \text{h.c}) + \frac{U}{2}\sum_{\boldsymbol{x}} \hat{q}^2_{\boldsymbol{x}} + \mu \sum_{\boldsymbol{x}} \hat{q}_{\boldsymbol{x}} \qquad \hat{q} = \hat{n}_{el.} - \hat{n}_{h.}$$

Trotter decomposition:

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

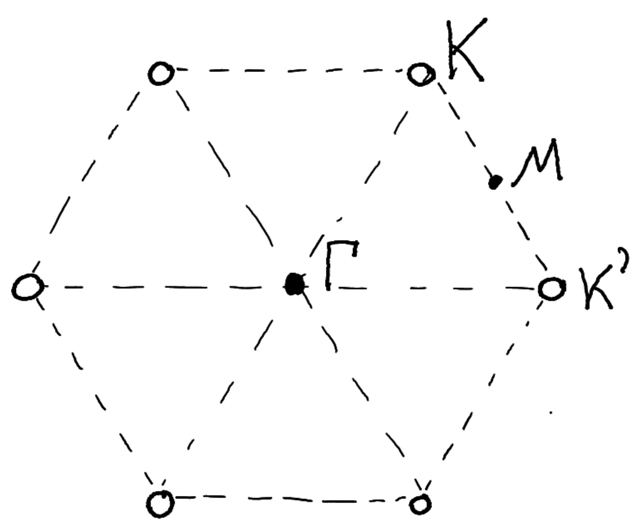
Subsequently, the auxiliary field is introduced via the Hubbard-Stratonovich transformation:

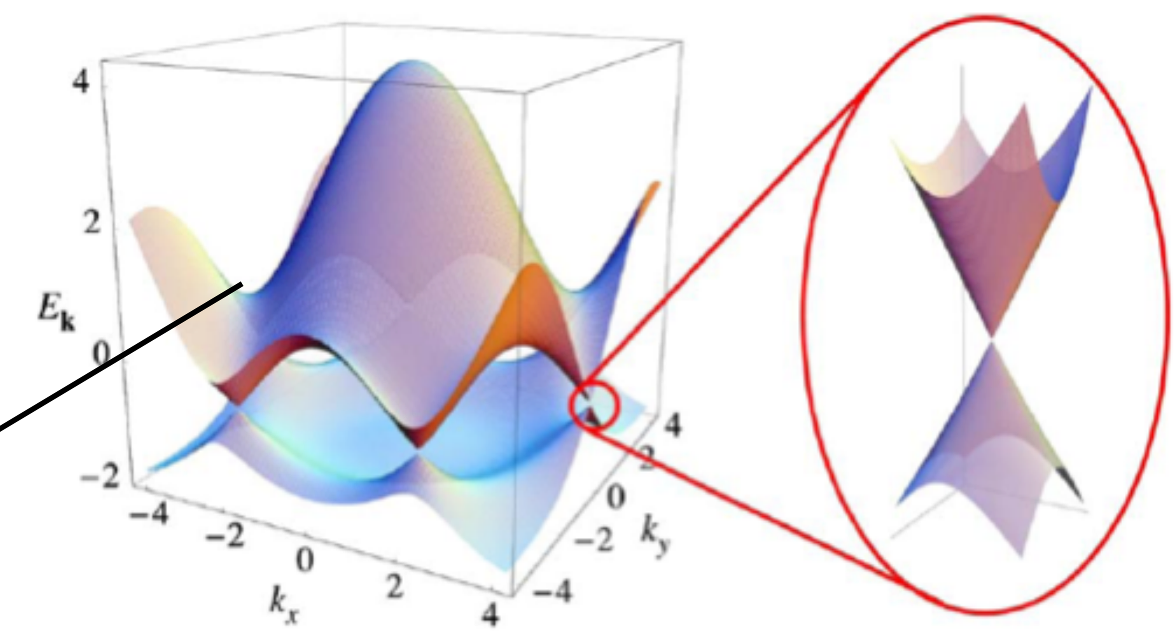
$$e^{-\frac{\Delta\tau}{2} U \hat{q}^2_{\boldsymbol{x}}} \cong \int d\phi_{\boldsymbol{x}} e^{-\frac{\phi^2_{\boldsymbol{x}}}{2U\Delta\tau} + i\phi_{\boldsymbol{x}}\hat{q}_{\boldsymbol{x}}}$$

$$\mathcal{Z} = \int \mathcal{D}\phi e^{-S_B[\phi]} \det M_{el.}[\phi] \det M_{h.}[\phi]$$

Purely Gaussian bosonic action: $S_B[\phi] = \sum_{\boldsymbol{x},\tau} \frac{\phi^2_{\boldsymbol{x},\tau}}{2U\Delta\tau}$ $\qquad S = S_B - \ln(\det M_{el.} \det M_{h.})$

We will work mostly with hexagonal lattice (a bit simpler construction of saddle points):





Lifshitz transition

M. Körner et al., arXiv:1704.03757

Algorithms: exact calculation of fermionic forces

$$S = S_B - \ln(\det M_{el.} \det M_{h.}) \quad \Longrightarrow \quad \frac{d\Phi}{dt} = \overline{\frac{\partial S}{\partial \Phi}}$$

$$S_B[\phi] = \sum_{\boldsymbol{x},\tau} \frac{\phi^2_{\boldsymbol{x},\tau}}{2U\Delta\tau}$$

Purely Gaussian bosonic action does not carry any non-trivial info.
We must take into account fermionic determinant in GF

$$D_{2\tau+1} \equiv e^{-\Delta\tau h} \qquad D_{2\tau} \equiv \mathrm{diag}\left(e^{i\phi_{\boldsymbol{x},\tau}}\right)$$

$$\boldsymbol{M} = \begin{pmatrix} 1 & D_1 & 0 & 0 & 0 & \dots \\ 0 & 1 & D_2 & 0 & 0 & \dots \\ 0 & 0 & 1 & D_3 & 0 & \dots \\ 0 & 0 & 0 & 1 & D_4 & \dots \\ \vdots & & & & \ddots & \\ -D_{2N_\tau} & 0 & 0 & & \dots & 1 \end{pmatrix} \qquad \boldsymbol{M}^{-1} = \begin{pmatrix} g_1 & \dots & \dots & \dots & \dots & \bar{g}_{2N_\tau} \\ \bar{g}_1 & g_2 & \dots & \dots & \dots & \dots \\ \dots & \bar{g}_2 & g_3 & \dots & \dots & \dots \\ \dots & \dots & \bar{g}_3 & g_4 & \dots & \dots \\ \vdots & & & & \ddots & \\ \dots & \dots & \dots & & \dots & g_{2N_\tau} \end{pmatrix}$$

Possible for staggered fermions [Nuclear Physics B 371, 539 (1992)], Wilson fermions, and general tight-binding lattice models in condensed matter physics

Elements of fermionic propagator are computed through the iterations

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

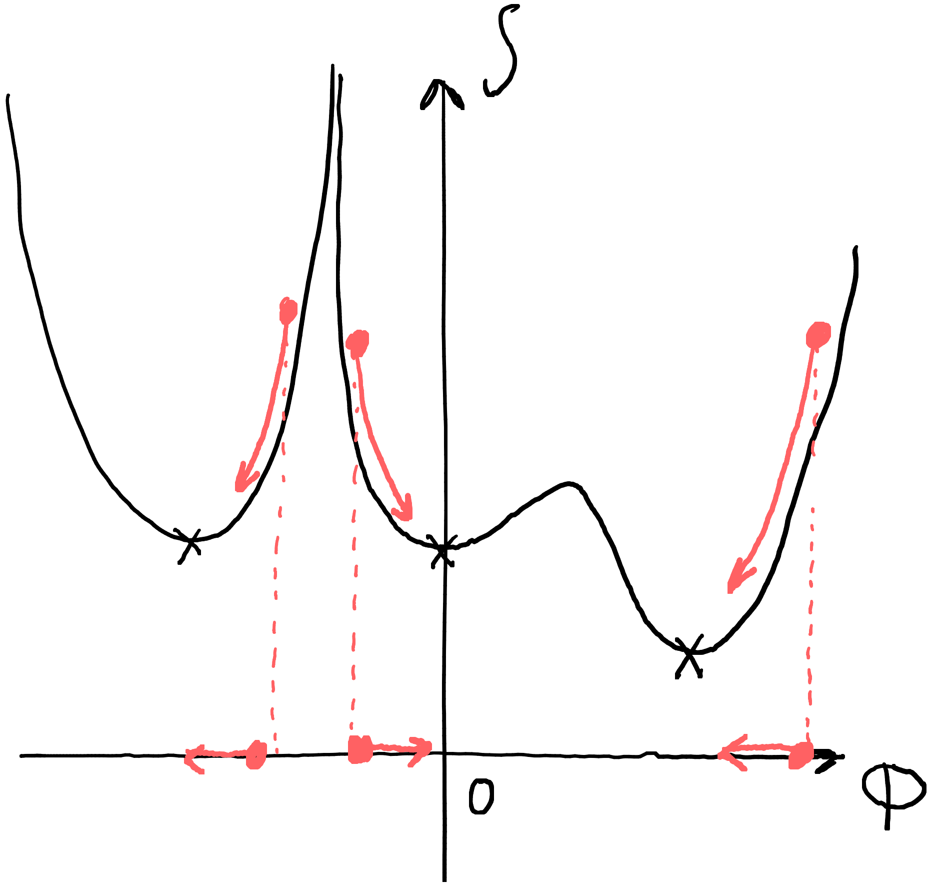
$N_s^3 N_\tau$ - scaling

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

Derivative:

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

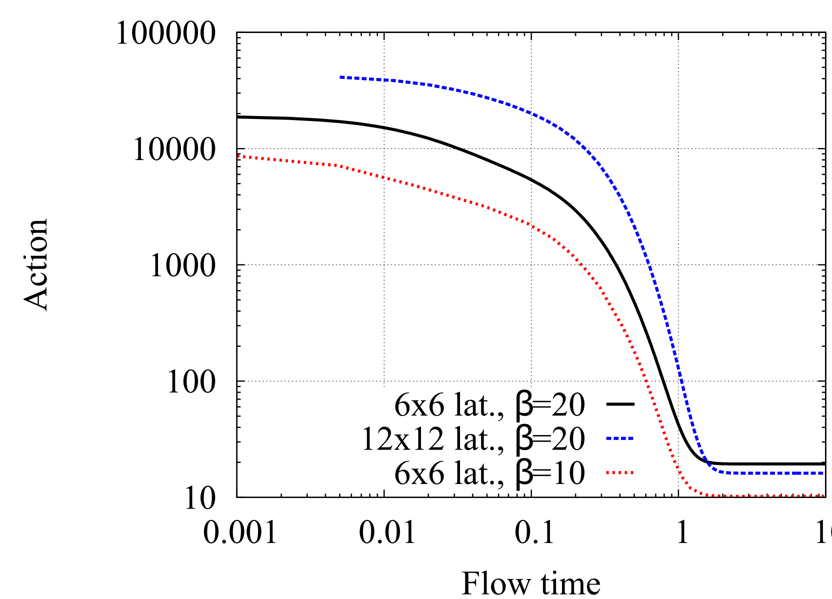
Recovering exact saddle points from Hybrid Monte Carlo data (no sign problem)



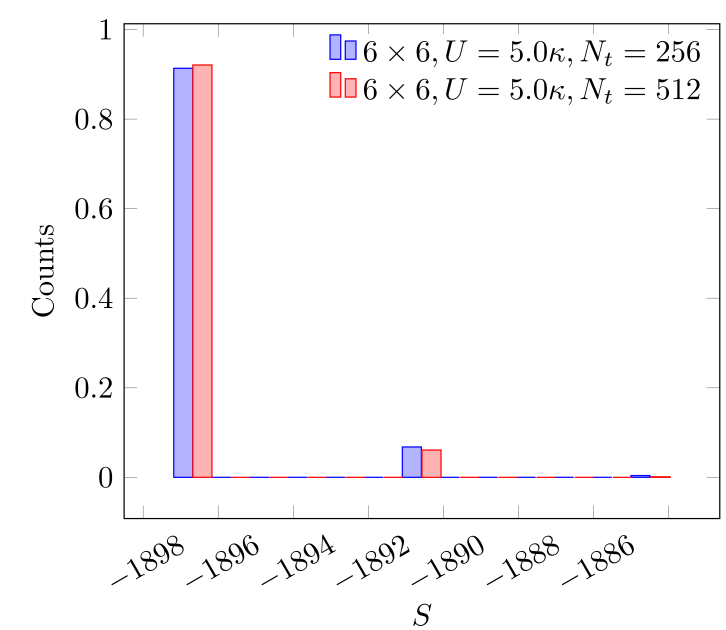
$$\mathcal{Z} = \int_{\mathbb{R}^N} \mathcal{D}\Phi\, e^{-S[\Phi]} = \sum_\sigma k_\sigma \mathcal{Z}_\sigma$$

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

History of the action:



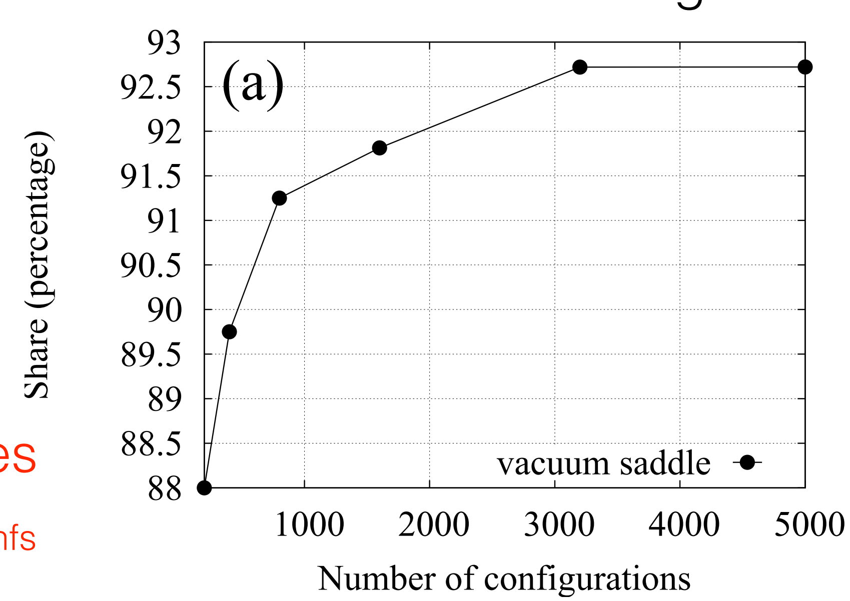
Histogram:

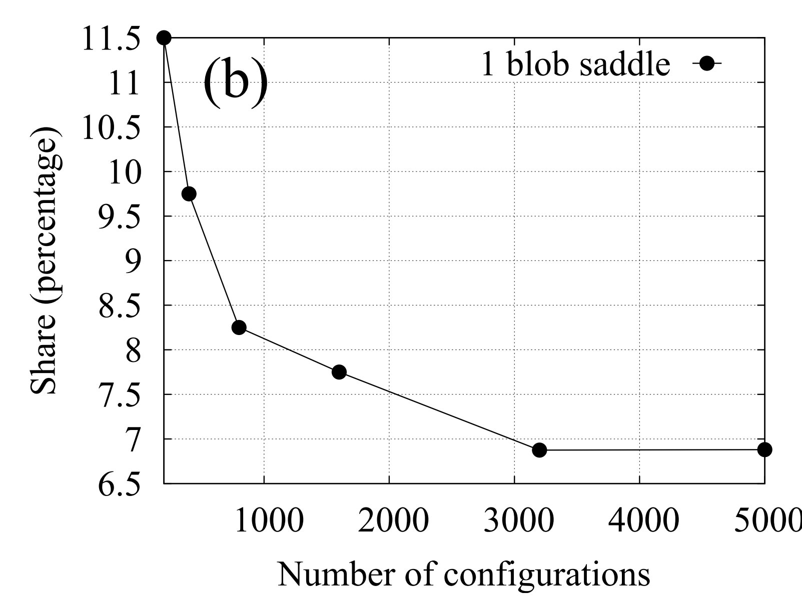


1) generation of lattice field configurations;
2) GF for each configuration;
3) Histogram for the final actions after GF shows

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

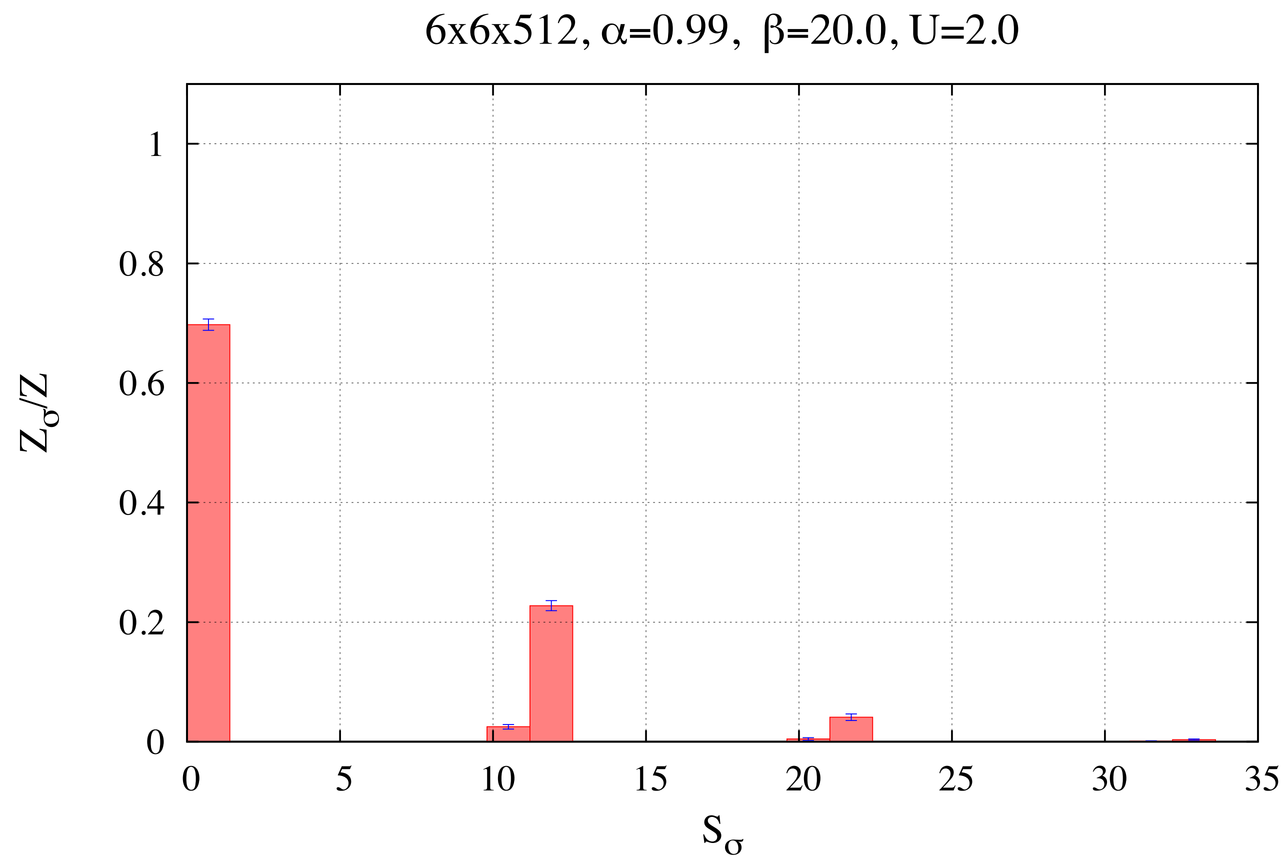
Stabilization of the histogram:

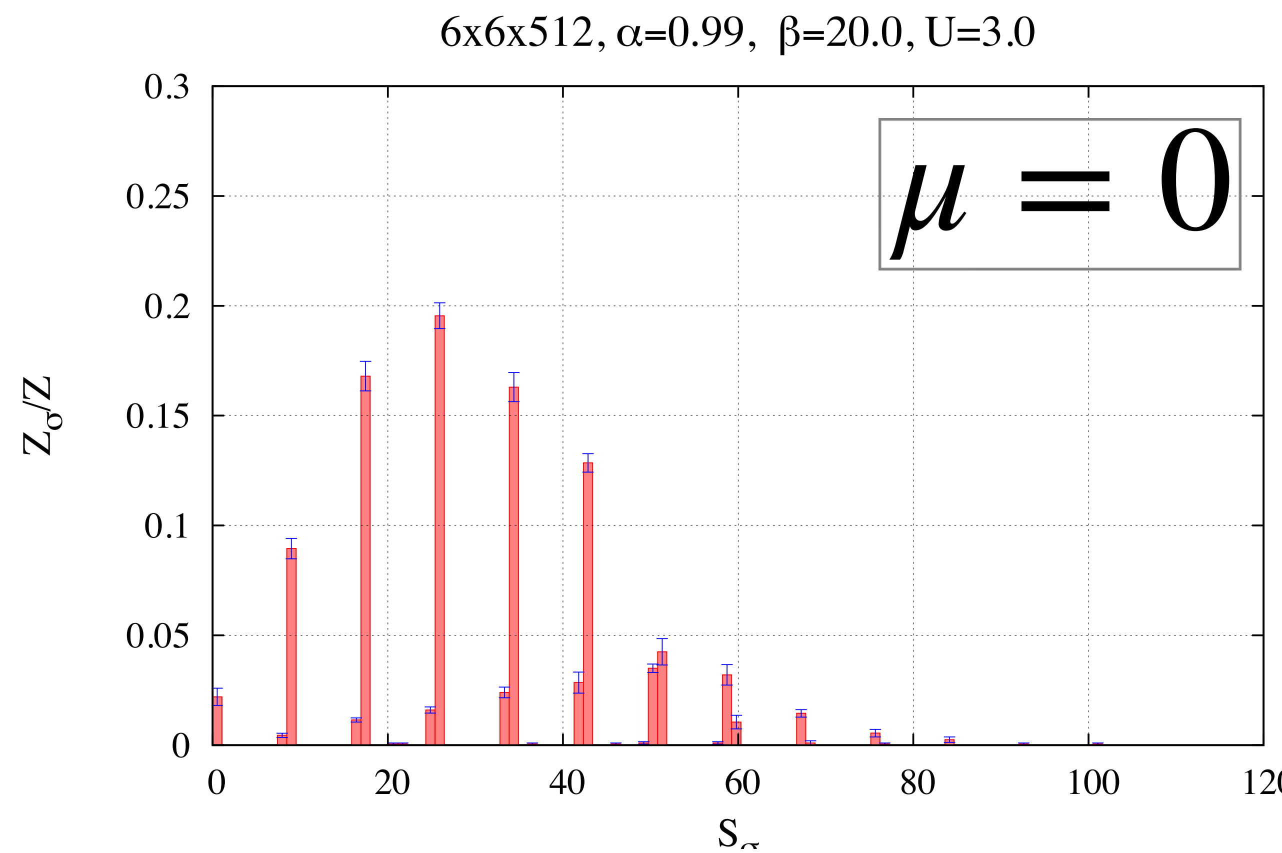


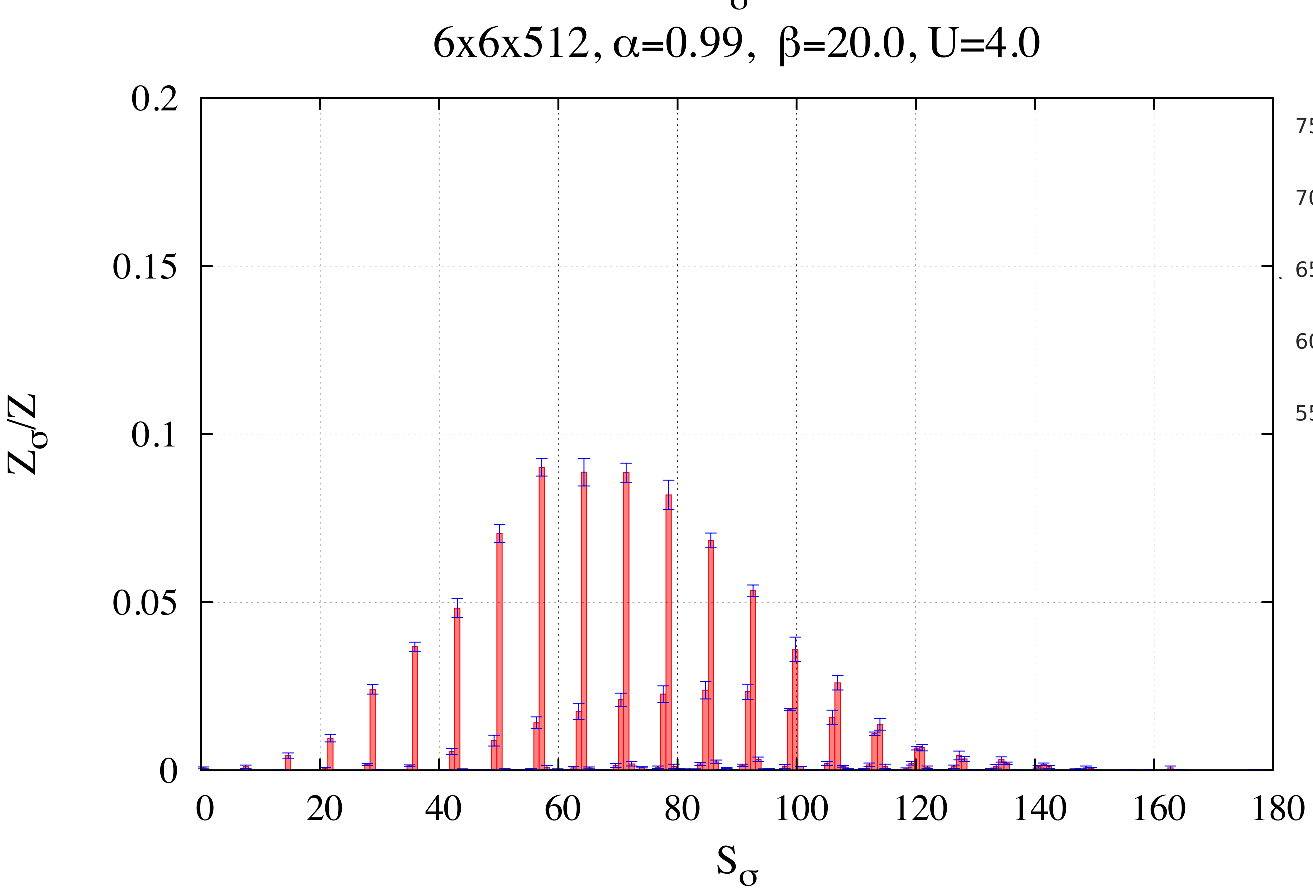


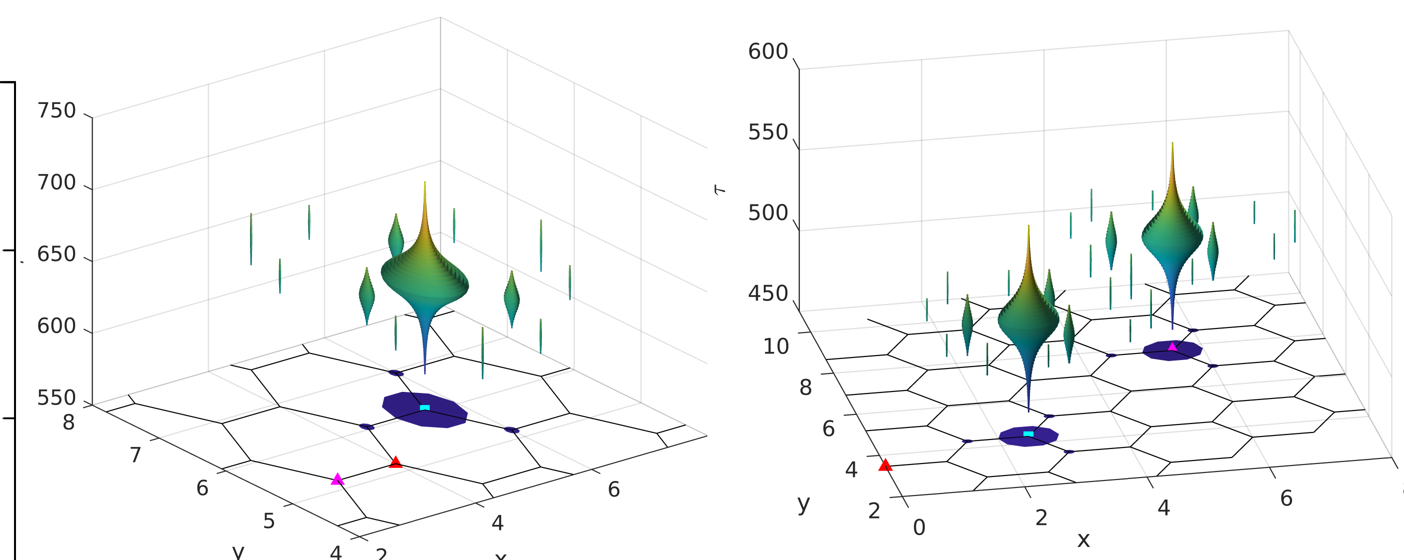
If HMC is ergodic, we can find all saddles with the share in partition function > $1/N_{\text{confs}}$

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

Instantons with back reaction from fermions (1)

$$S = \frac{\sum_{x,\tau} (\phi_x^\tau)^2}{2U\Delta\tau} - \ln\det\left(M_{el.}M_{h.}\right) \qquad \frac{\partial \ln\det M}{\partial \Phi} = \mathrm{Tr}\left(M^{-1}\frac{\partial M}{\partial \Phi}\right)$$

$$M_{el./h.} = \begin{pmatrix} I & e^{-\Delta\tau h} & 0 & 0 & \cdots & \cdots & 0 \\ 0 & I & \{e^{\pm i\phi_x^1}\} & 0 & \cdots & \cdots & 0 \\ \cdots & \cdots & \ddots & \ddots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & I & \{e^{\pm i\phi_x^\tau}\} & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & I & e^{-\Delta\tau h} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots & \ddots \\ \{-e^{\pm i\phi_x^{N_\tau}}\} & \cdots & \cdots & \cdots & \cdots & \cdots & I \end{pmatrix} \qquad M_{el.}^{-1} = \begin{pmatrix} g_1 & \cdots & \cdots & \cdots & \cdots & \cdots & \bar{g}_{2N_\tau} \\ \bar{g}_1 & g_2 & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \bar{g}_2 & g_3 & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \ddots & \ddots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \bar{g}_\tau & g_\tau & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \ddots & \ddots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & g_{N_\tau} \end{pmatrix}$$

Saddle point equations including fermionic forces:

$$\frac{\partial S}{\partial \phi_x^\tau} = \frac{\phi_x^\tau}{\Delta\tau U} - \left(\bar{g}_{xx}^{2\tau} i e^{i\phi_x^\tau} - (\bar{g}_{xx}^{2\tau})^* i e^{-i\phi_x^\tau}\right)$$

Connection between bosonic field and fermionic propagator (in continuum limit $\Delta\tau \to 0$):

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

We need to close the system of equations with the evolution of fermionic propagator:

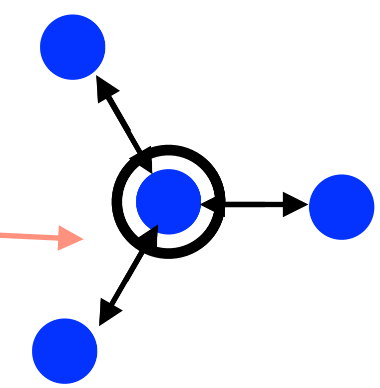
$$\bar{g}^{2(\tau+1)} = \{e^{-i\phi_x^{(\tau+1)}}\}e^{\Delta\tau h}\bar{g}^\tau\{e^{i\phi_x^{(\tau+1)}}\}e^{-\Delta\tau h}$$

Instantons with back reaction from fermions (2)

In the continuous time limit: $\Delta\tau \to 0$

C_3 -symmetry, and rapid decay of propagator: $g_{xy} \to 0, |\vec{x} - \vec{y}| \to \infty$

Only nearest neighbors



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

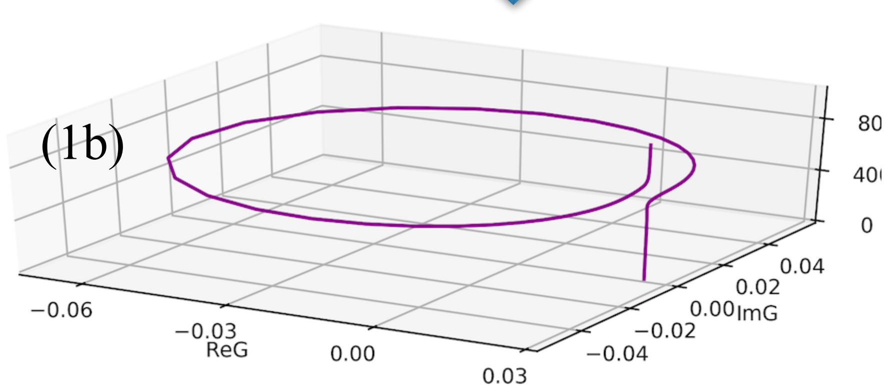
$G = U/\kappa$

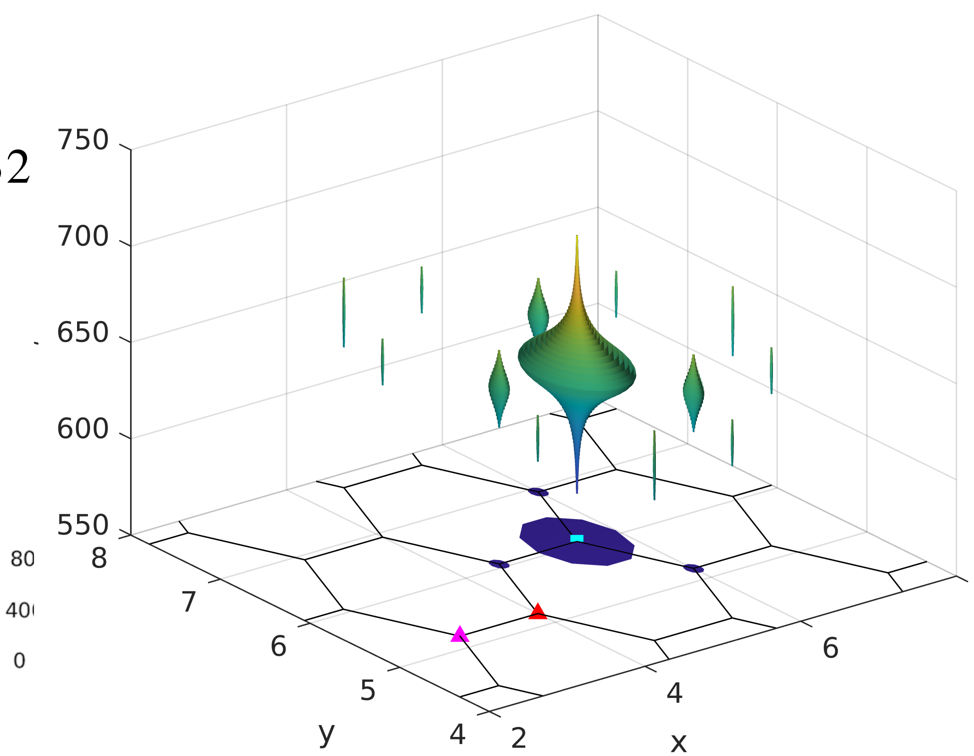
$$\mathrm{Im}\, g_{xx}(\tau) = d(\tau), \quad \mathrm{Re}\, g_{xx}(\tau) = 1/2, \quad g_{xy}(\tau) = a(\tau) + ib(\tau)$$

$$\begin{cases} \dot{d}(\tau) = 6\kappa b(\tau) \\ \dot{a}(\tau) = -Ub(\tau)d(\tau) \\ \dot{b}(\tau) = d(\tau)(\kappa + Ua(\tau)) \end{cases}$$

$$\dot{a}(a + 1/G) = -\dot{b}b$$
$$(a + 1/G)^2 + b^2 = R^2$$

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



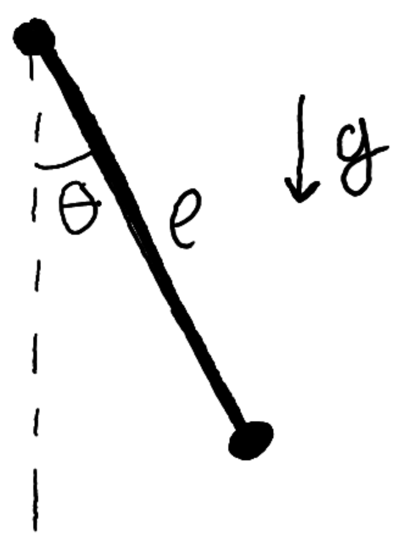


The final equation:

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

Instantons with back reaction from fermions (3)

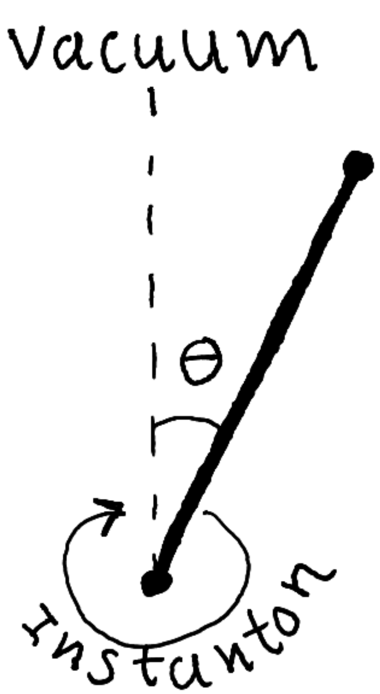
Non-linear pendulum:



$$K = \frac{m(l\dot{\theta})^2}{2}, P = mgl(1 - \cos\theta)$$

$$H = \frac{\dot{\theta}^2}{2} + \frac{g}{l}(1 - \cos\theta)$$

$$\ddot{\theta} = -\frac{g}{l}\sin\theta$$



$$\theta \to \pi + \theta \qquad \ddot{\theta} = \frac{g}{l}\sin\theta$$

Initial condition(vacuum):

$$\operatorname{Im} g_{xy} = 0 \Rightarrow b(\tau = 0) = 0 \Rightarrow \theta(\tau = 0) = 0$$

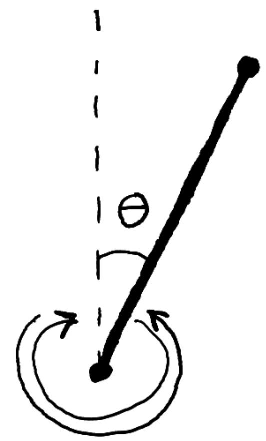
$\dot{\theta}(\tau = 0)$ - defined by the number of instantons and anti-instantons

Instantons with back reaction from fermions (4)

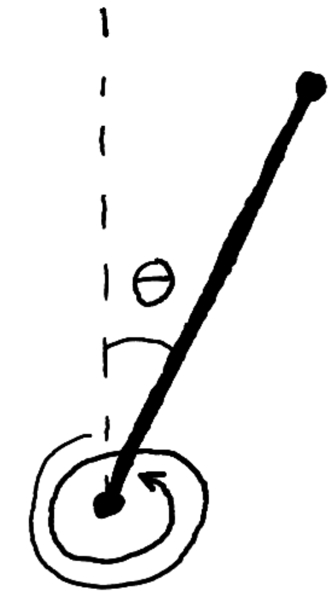
Number of instantons and anti-instantons fixes the initial conditions (time for one full rotation):

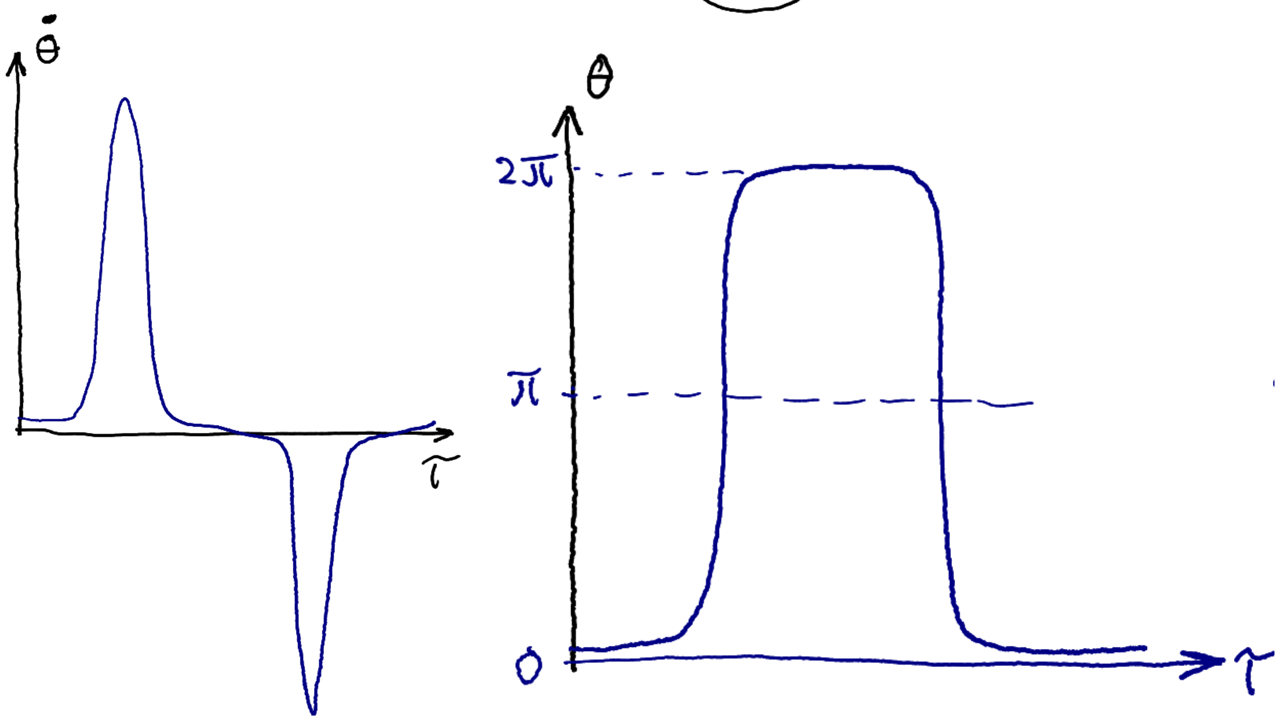
$$\frac{\dot{\theta}^2}{2} + \cos\theta = E_0 \qquad \beta/N_{inst.} = 2\int_0^{\pi} \frac{d\theta}{\sqrt{2(E_0 - \cos\theta)}}$$

Instanton and anti-instanton:

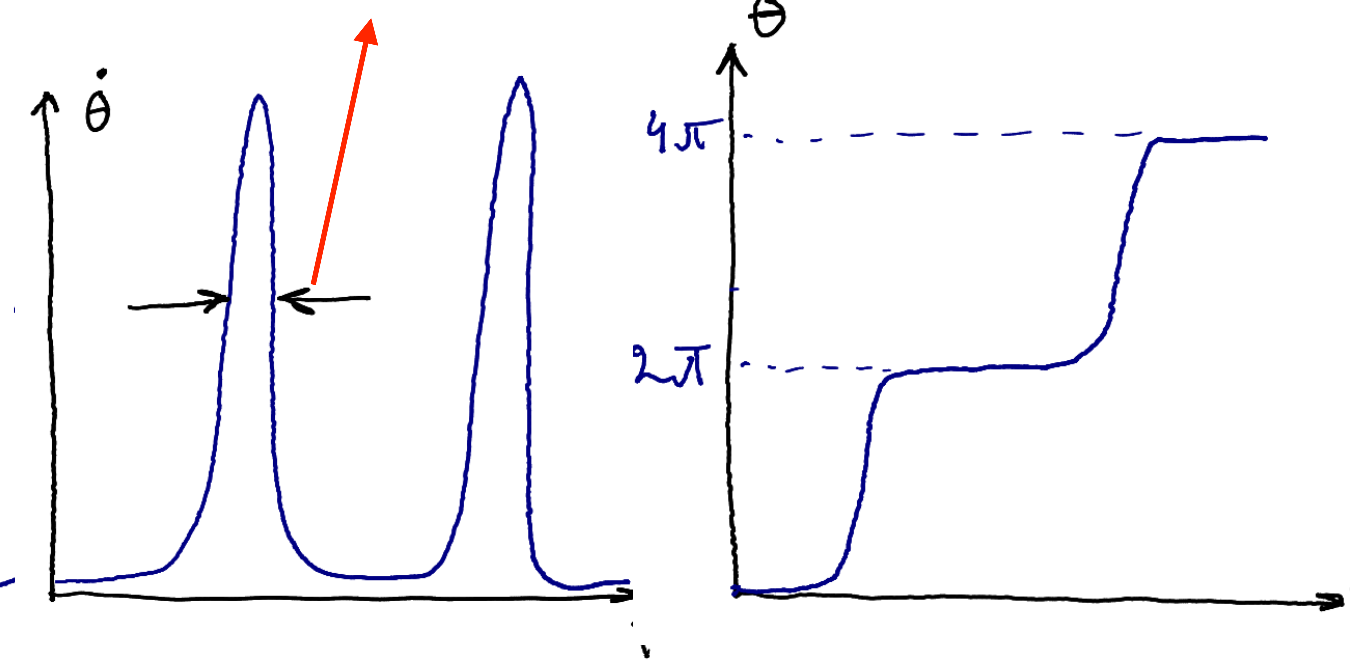


Two instantons:





Width of the instanton

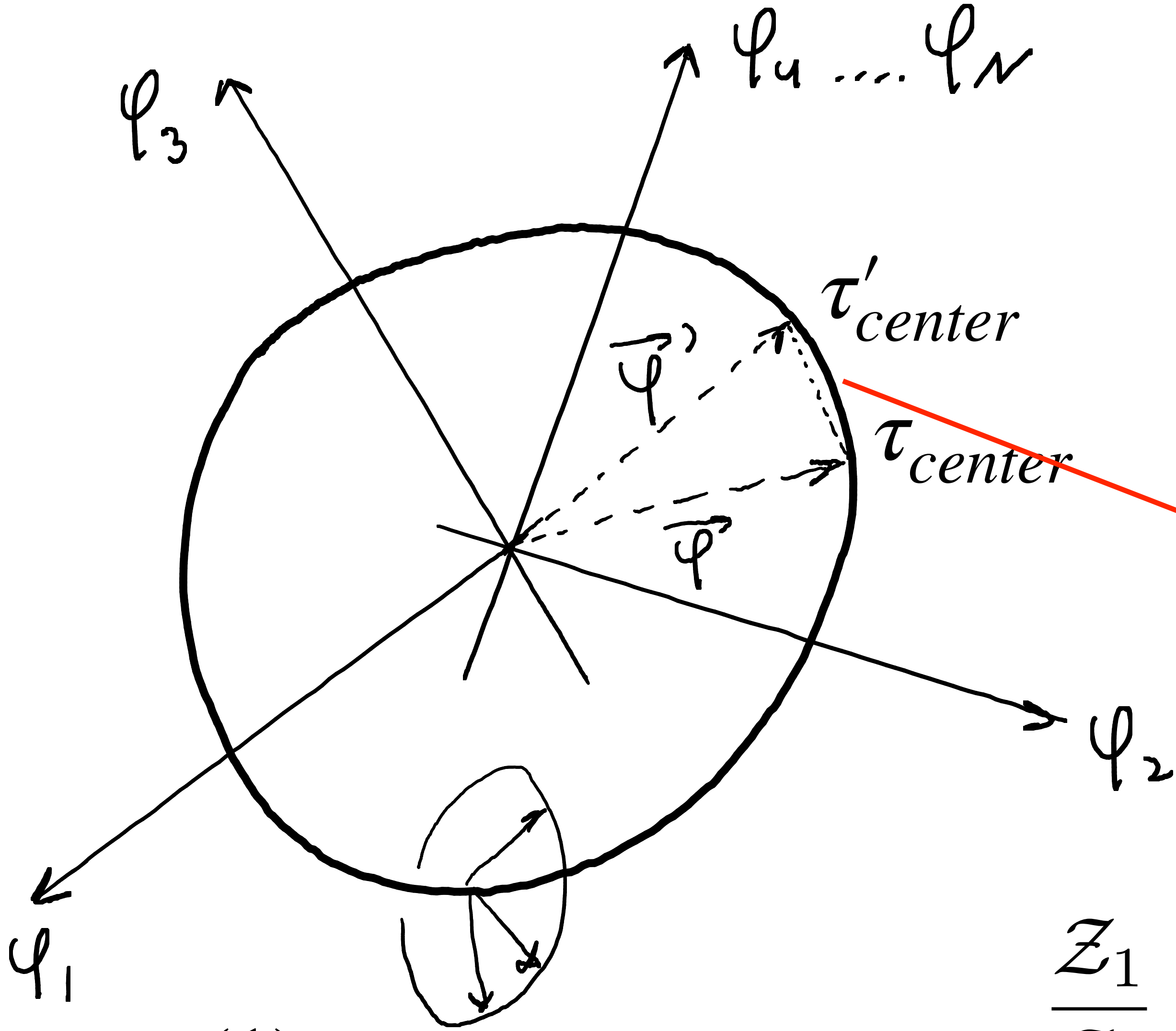


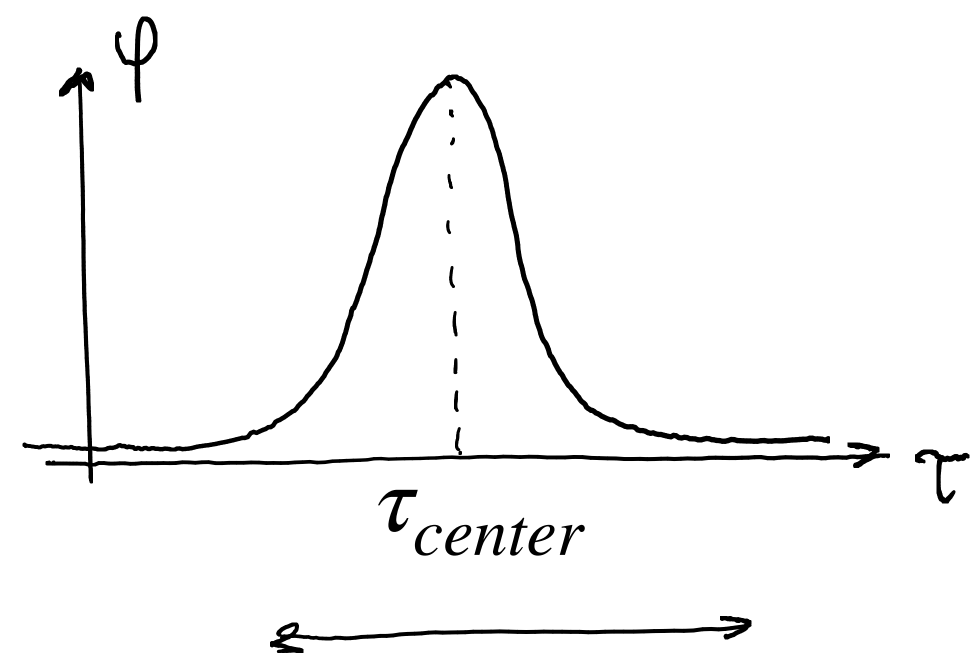
Winding number: $W = \frac{1}{2\pi}\int_0^{\beta} d\tau \theta(\tau)$

Gaussian fluctuations around instanton (1)

$$S \approx S(\phi^{(X,T)}) + \frac{1}{2}\left(\phi_{\boldsymbol{x},\tau_1} - \phi^{(X,T)}_{\boldsymbol{x},\tau_1}\right)\mathcal{H}^{(1)}_{(\boldsymbol{x},\tau_1),(\boldsymbol{y},\tau_2)}\left(\phi_{\boldsymbol{y},\tau_2} - \phi^{(X,T)}_{\boldsymbol{y},\tau_2}\right)$$

Instanton saddle is in fact degenerate:





Continuous symmetry: zero mode in Hessian $\mathscr{H}$

$$L^{(1)} = N_\tau \,|\, \overrightarrow{\phi}(\tau_c) - \overrightarrow{\phi}(\tau'_c) \,|$$

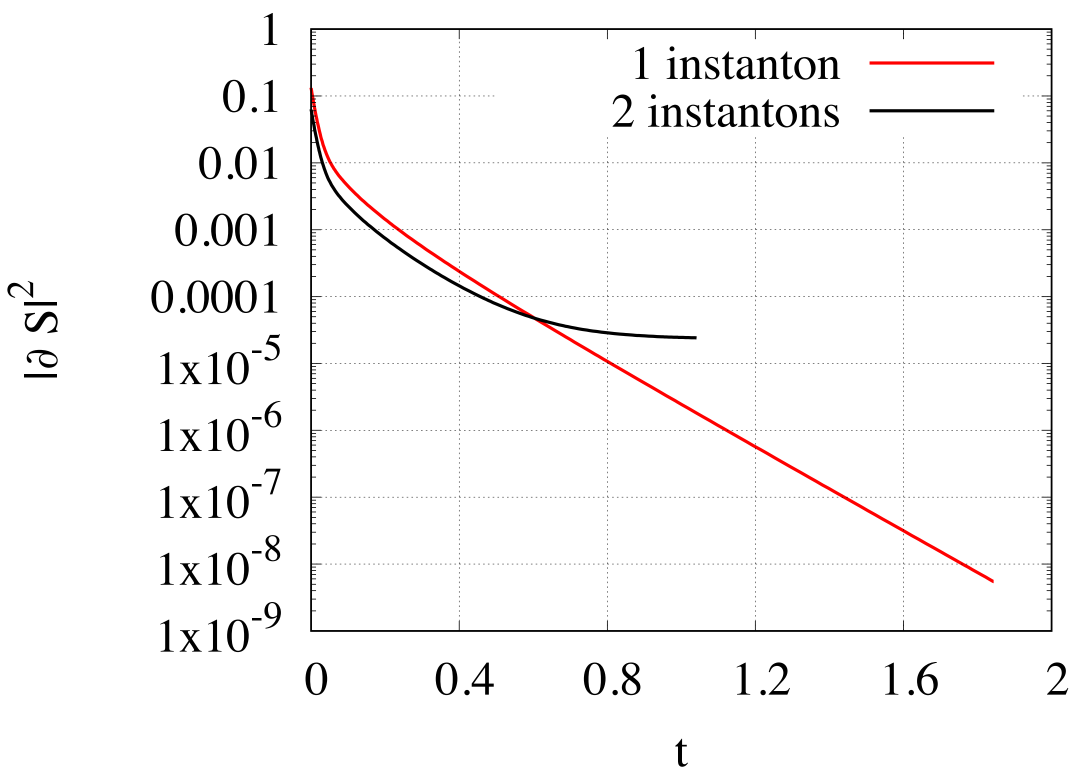
$\mathscr{H}^{(1)}_{\perp}$ - includes all directions except zero mode

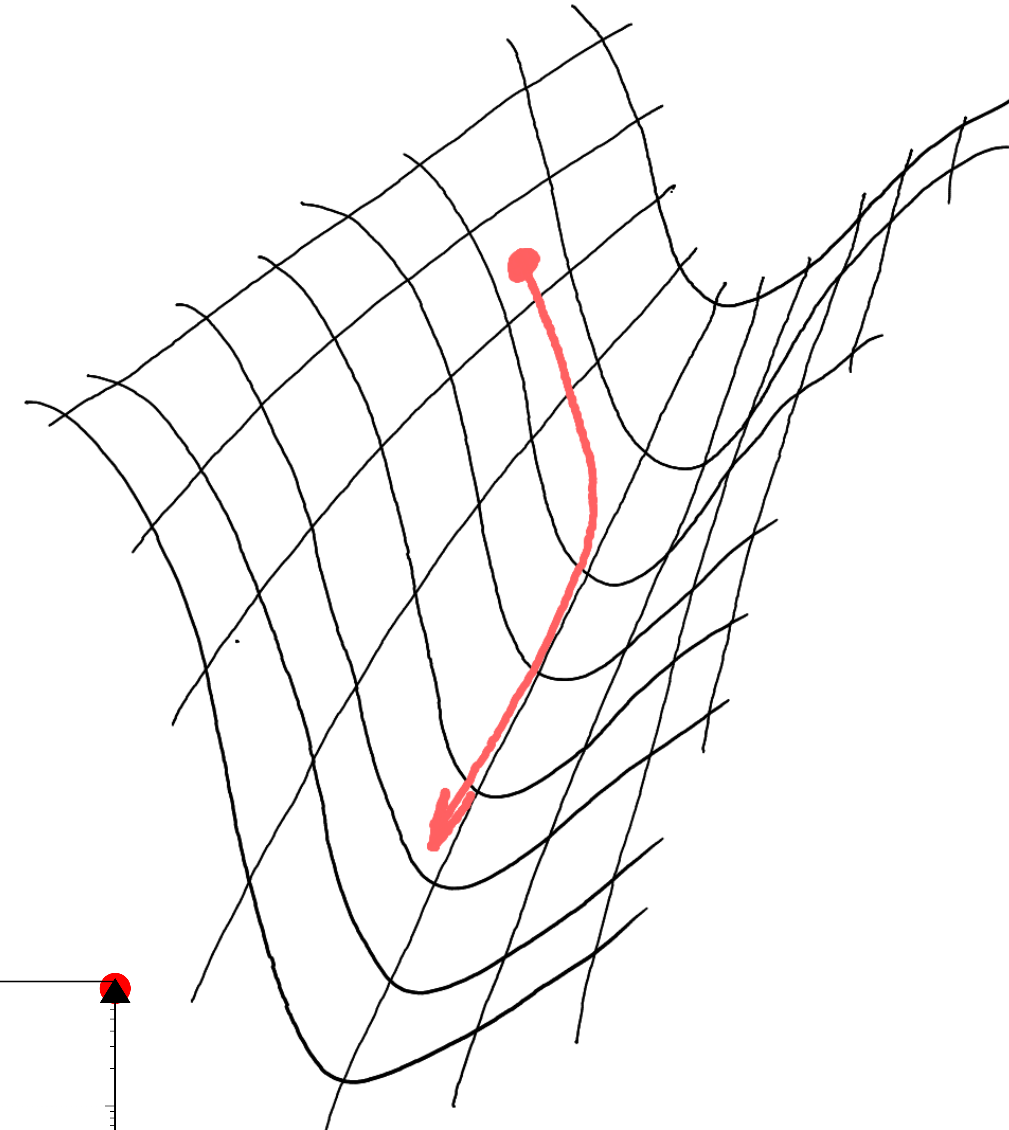
$$\frac{\mathcal{Z}_1}{\mathcal{Z}_0} = 2N_S L^{(1)} e^{-\tilde{S}^{(1)}} \left(2\pi \frac{\det \mathcal{H}^{(1)}_{\perp}}{\det \mathcal{H}^{(0)}}\right)^{-1/2}$$

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

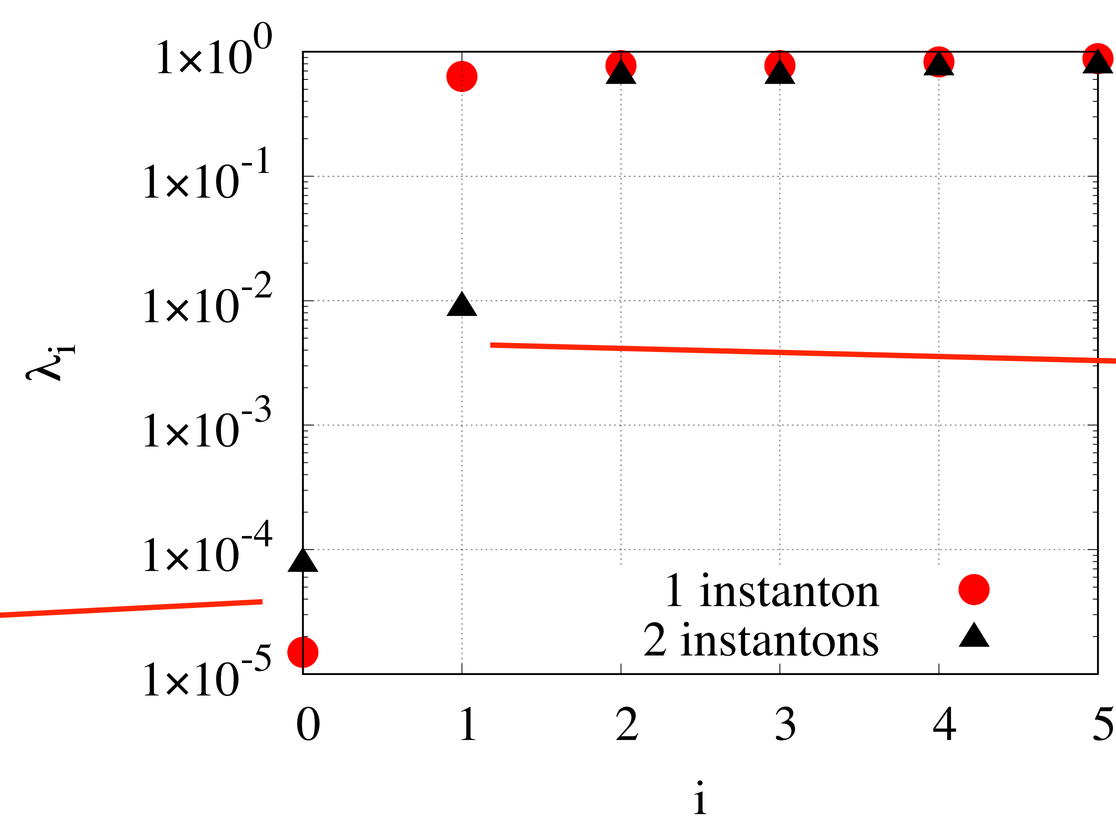
Gaussian fluctuations around instanton (2)

History of the flow:





Eigenvalues of the Hessian:



Quasi-zero mode, corresponding to the relative shift of the instantons

True zero modes

Hessians for multi-instanton saddles

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

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

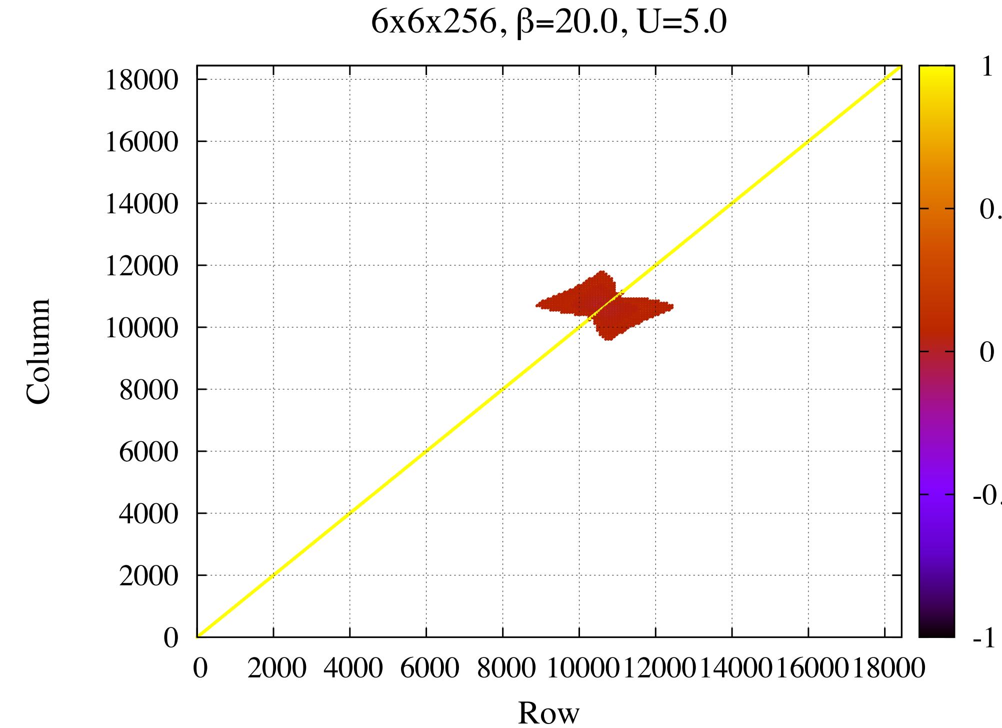
$$\frac{\det \mathscr{H}_{\perp}^{(1)}}{\det \mathscr{H}^{(0)}} = \det\left(\left(\mathscr{H}^{(1)} + \mathscr{P}^{(1)}\right)\left(\mathscr{H}^{(0)}\right)^{-1}\right)$$

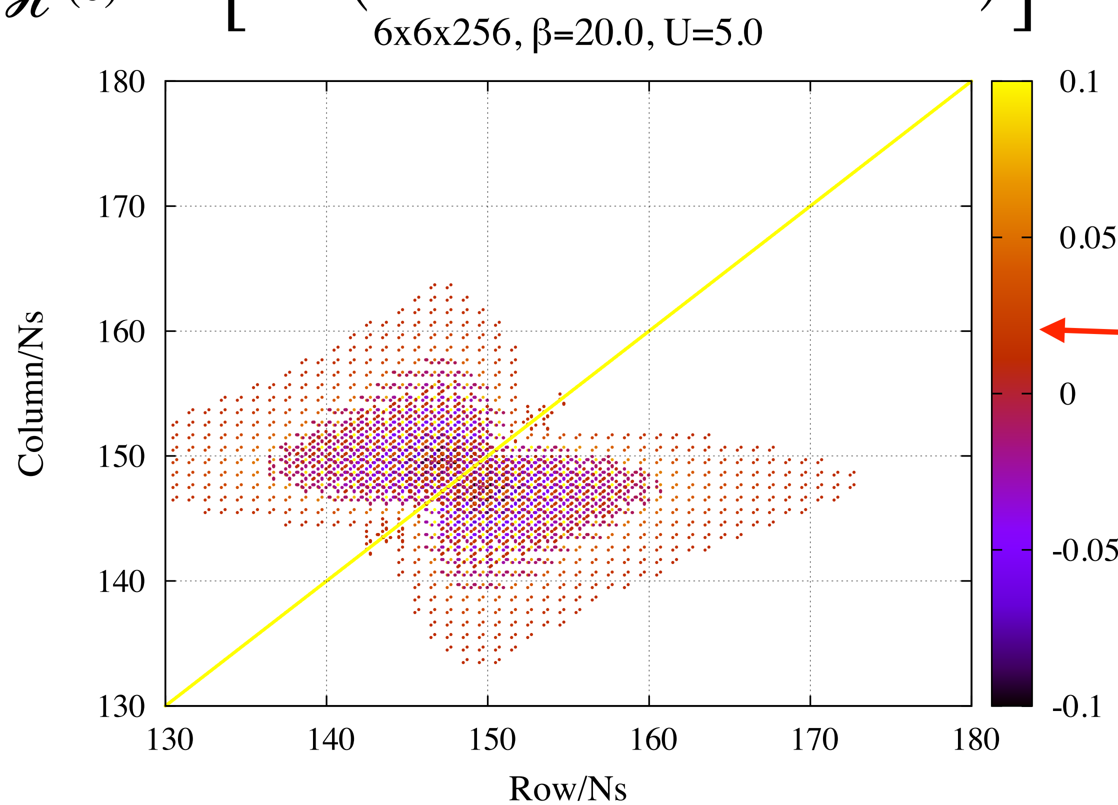
$$\det \mathscr{H}_{\perp}^{(N)} \approx \det\left(\mathscr{H}^{(N)} + \sum_{q=1}^{N} \mathscr{P}_q^{(N)}\right)$$

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

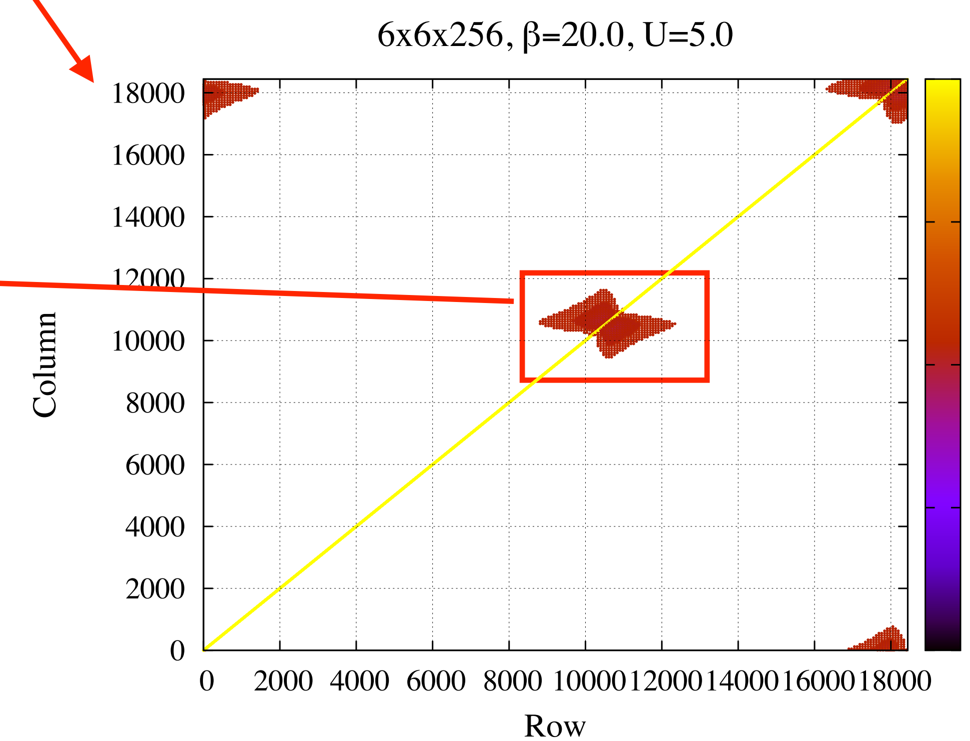
$$\frac{\det \mathscr{H}_{\perp}^{(N)}}{\det \mathscr{H}^{(0)}} \approx \left[\det\left(\left(\mathscr{H}^{(1)} + \mathscr{P}^{(1)}\right)\left(\mathscr{H}^{(0)}\right)^{-1}\right)\right]^N$$

1 instanton (elements>0.01):





2 instantons:

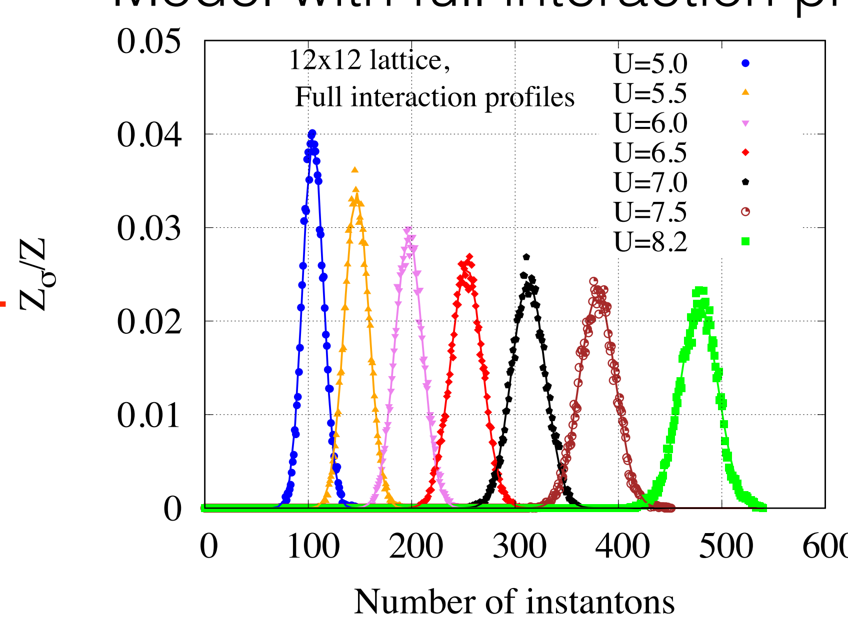


Ways to formulate the classical instanton gas model

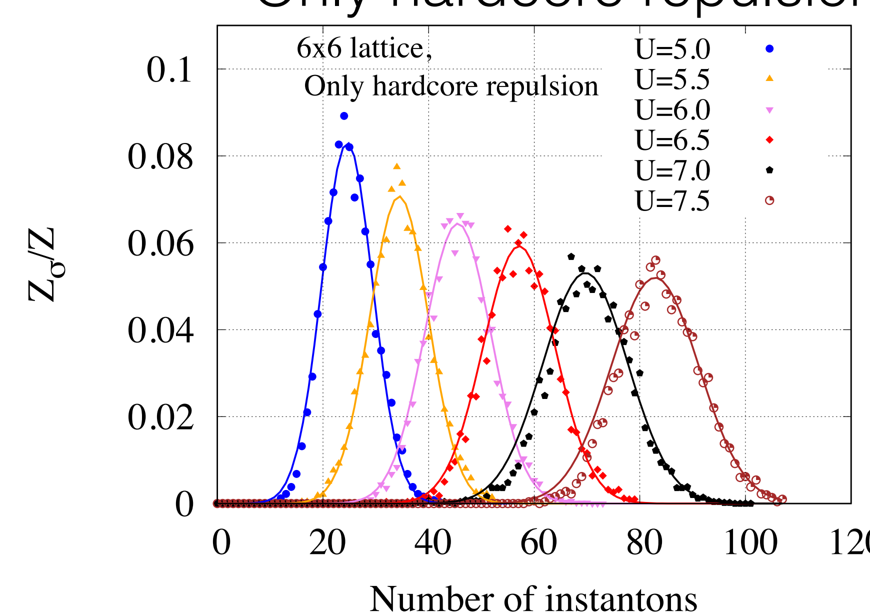
Analytical expression for the free energy of instanton gas with hardcore repulsion (no lattice structure, U-dependence only from input parameters: action of the instanton, etc.)

Classical grand canonical Monte Carlo (updates of instanton positions and number of instantons)

Model with full interaction profiles

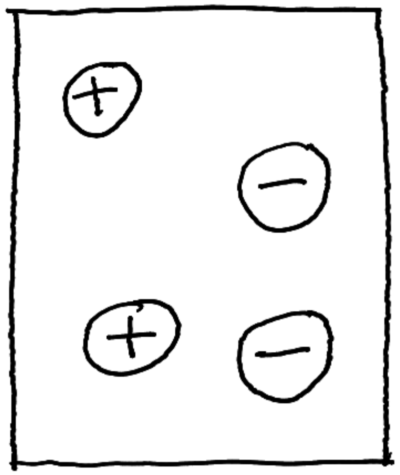


Only hardcore repulsion

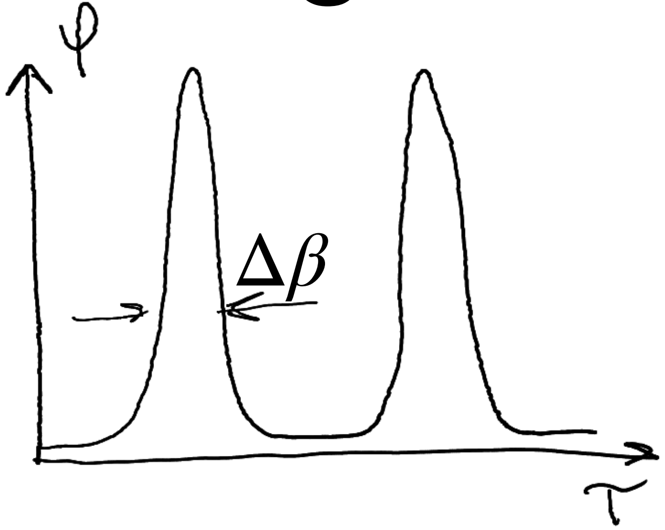


Both: only pairwise interaction of instantons

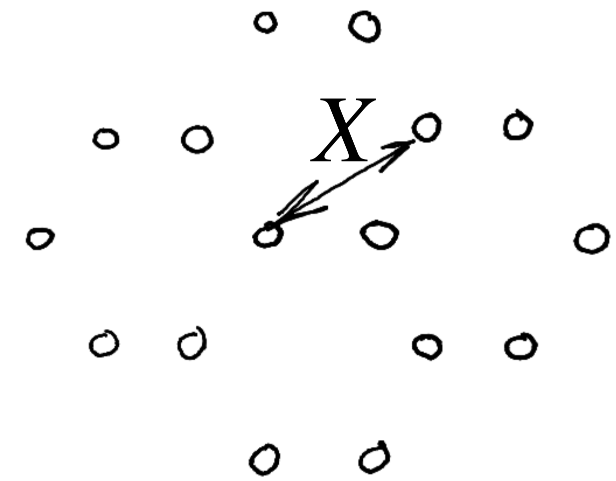
Analytical expression for the partition function for non-interacting instantons



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



Minimal distance in Euclidean time ~ instanton width



Minimal distance in space ~ lattice step

$$\frac{Z}{Z_0} =$$

«vacuum» partition function: integral over vacuum thimble

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

instanton number

Equivalence of instantons

Combinatorial factors including sublattice and instanton - anti-instanton indexes

instanton action

Hessians and valley length, using:

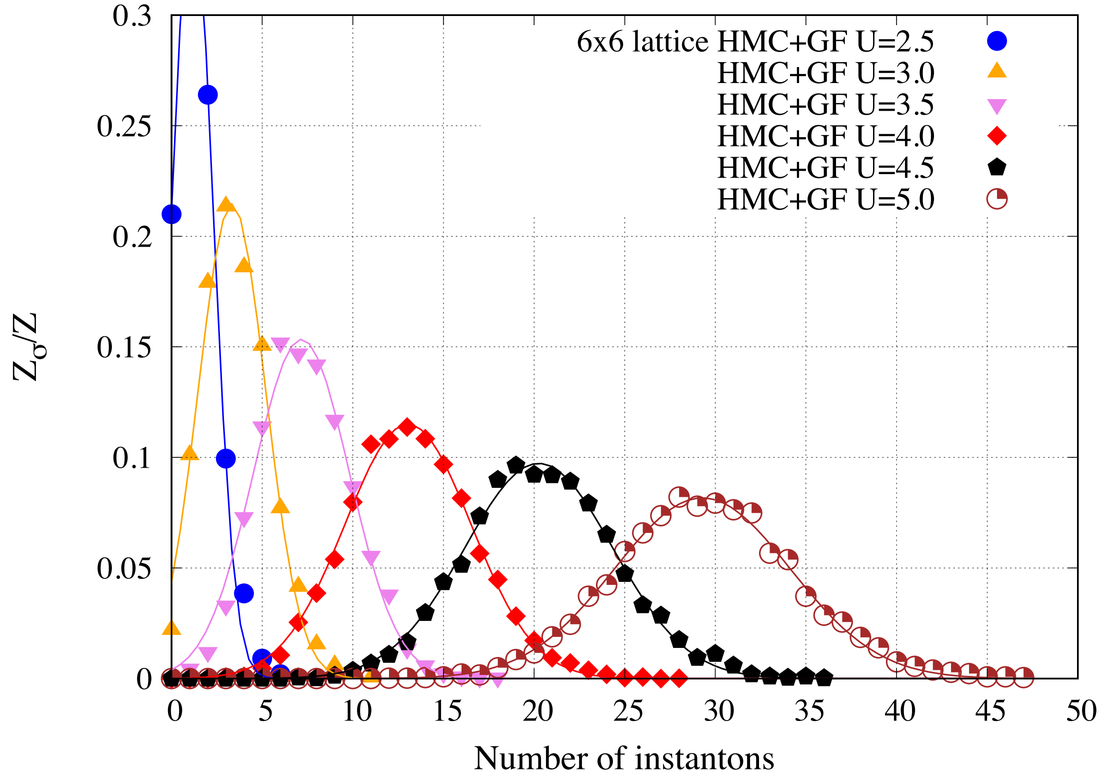
$$\frac{\det \mathscr{H}^{(N)}_{\perp}}{\det \mathscr{H}^{(0)}} \approx \left[\det\left(\left(\mathscr{H}^{(1)} + \mathscr{P}^{(1)}\right)\left(\mathscr{H}^{(0)}\right)^{-1}\right)\right]^{N}$$

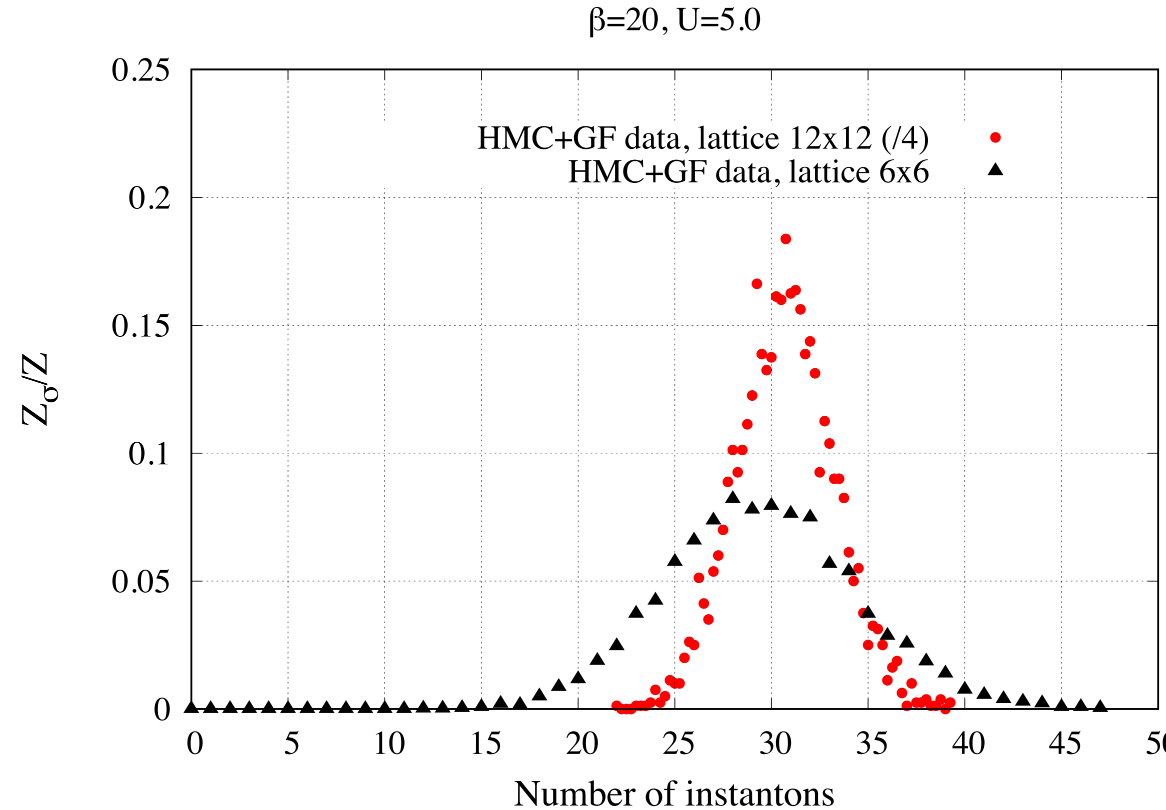
If we sum up to completely filled lattice (all slots are taken):

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

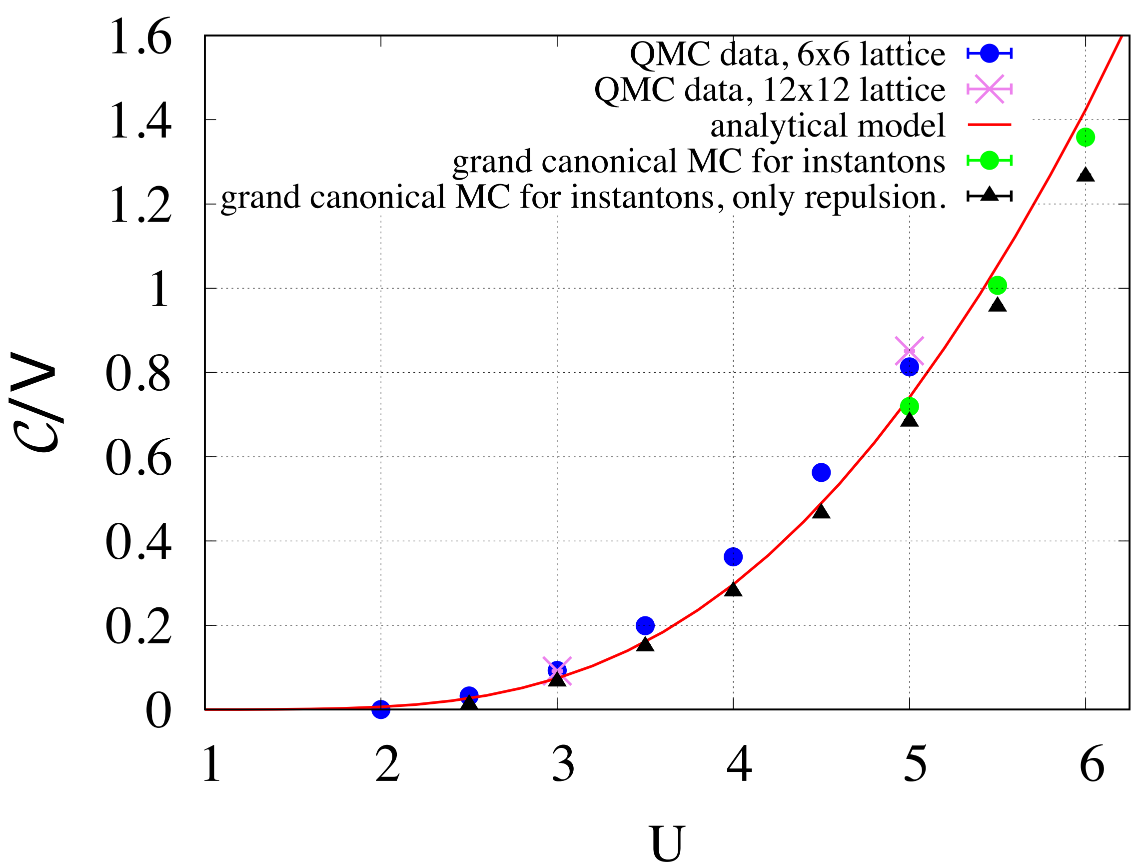
Free energy density: $f = f_0 - \dfrac{1}{\Delta\beta X}\ln\left(1 + \dfrac{2e^{-S_1}\Delta\beta X L}{\beta\sqrt{2\pi\det\left(\mathscr{H}^{(1)}_{\perp}(\mathscr{H}^{(0)})^{-1}\right)}}\right)$

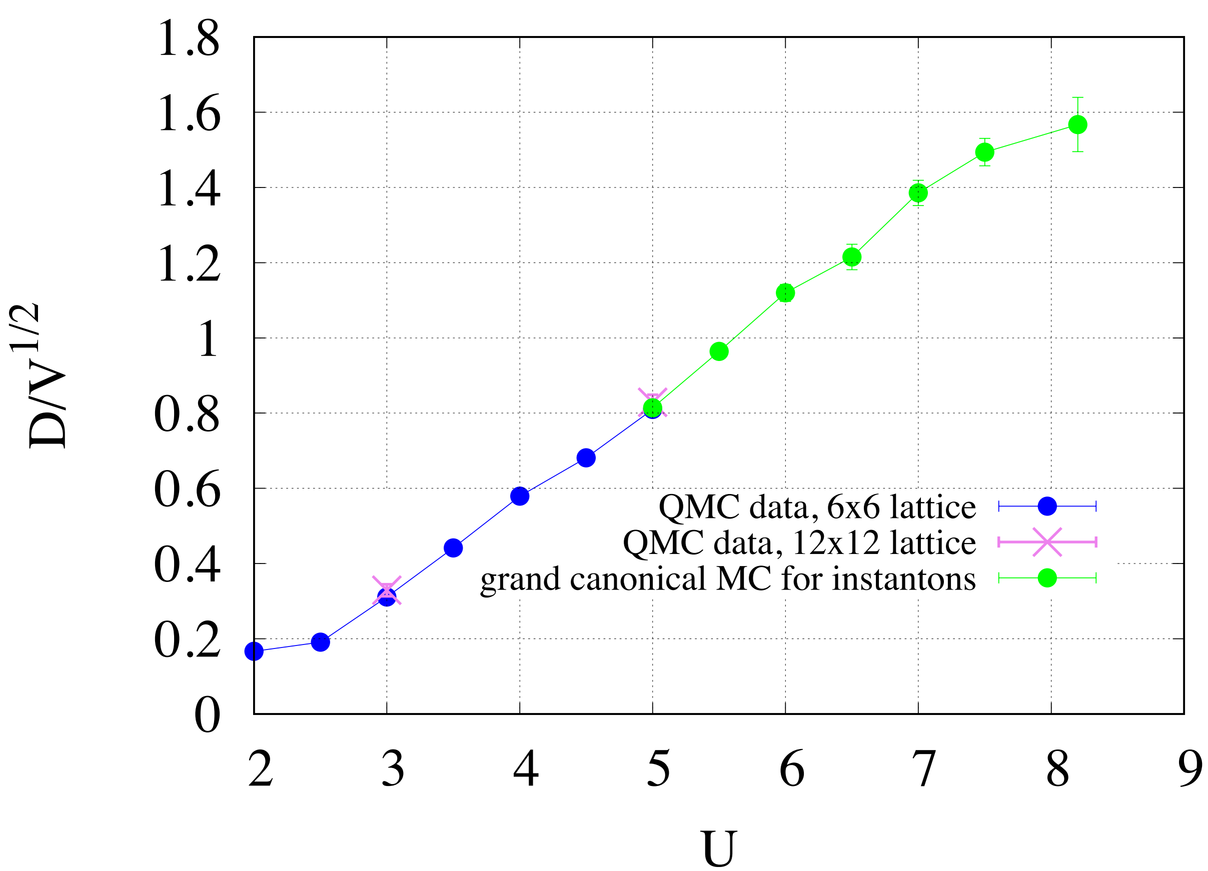
Benchmark: distribution of instantons



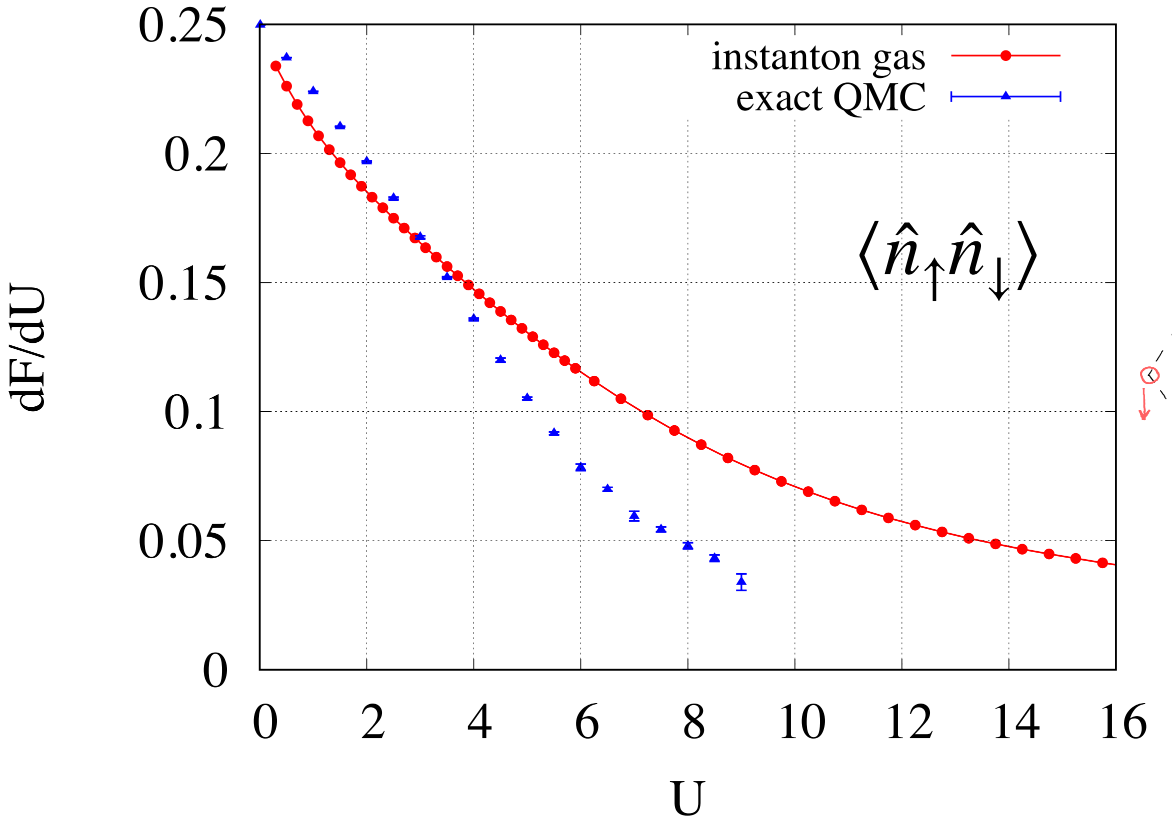


Distribution for the number of instantons and its comparison vs analytical and classical MC predictions:

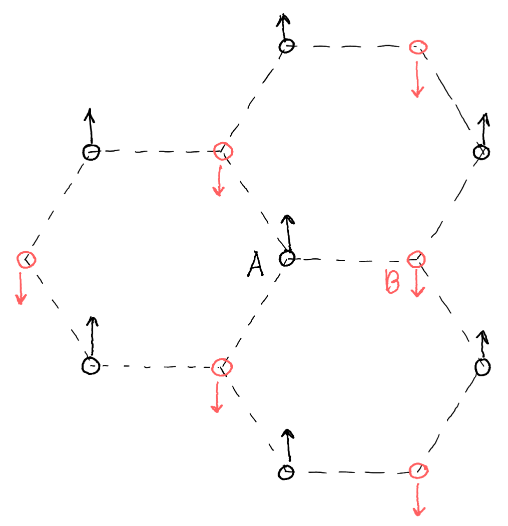


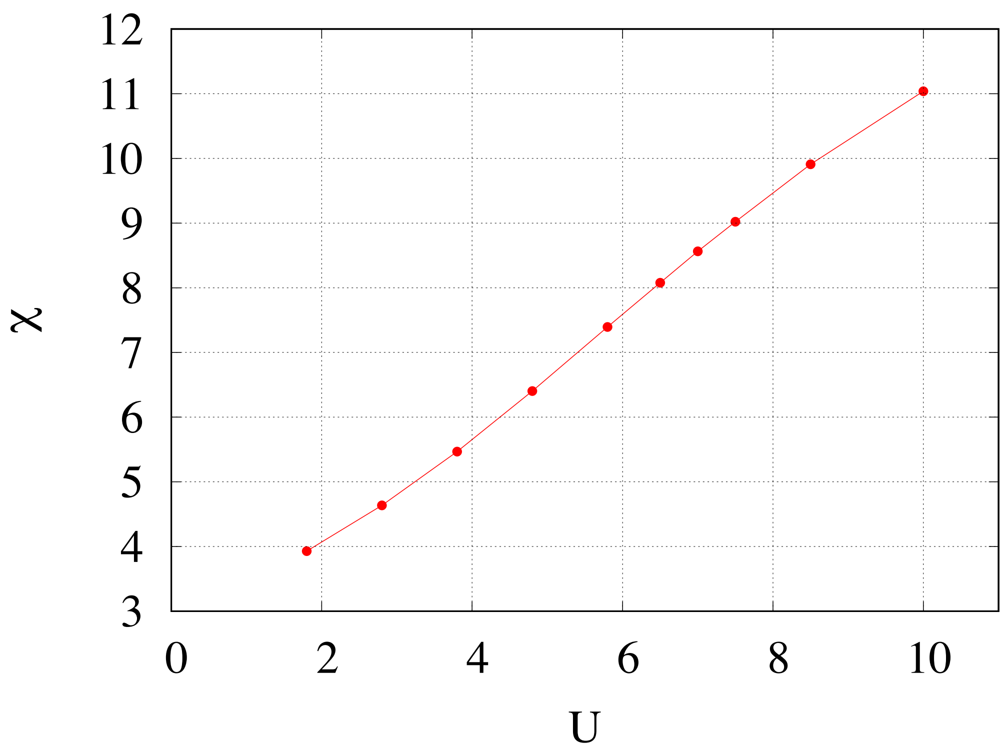


Physics from weakly interacting instanton gas model: spin localization and susceptibility

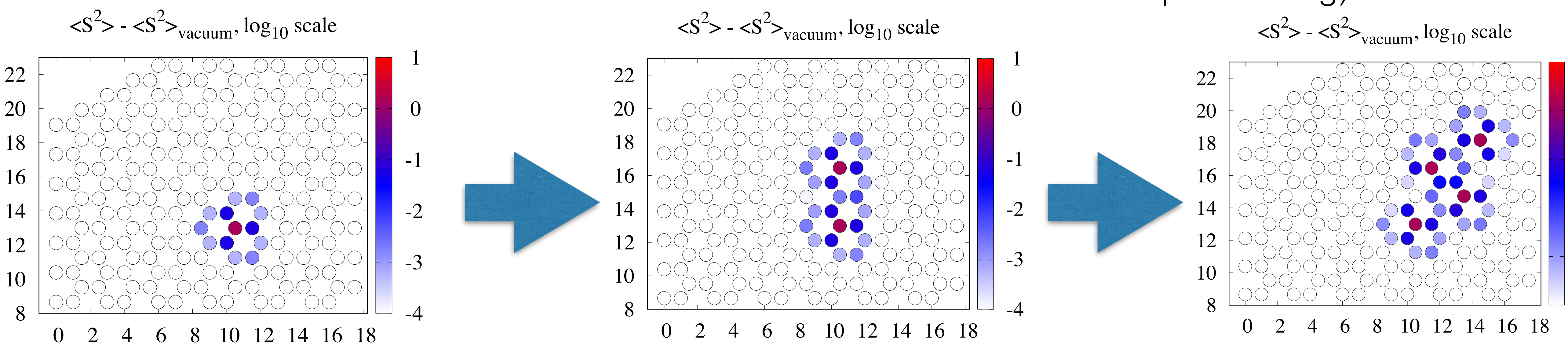


Double occupancy



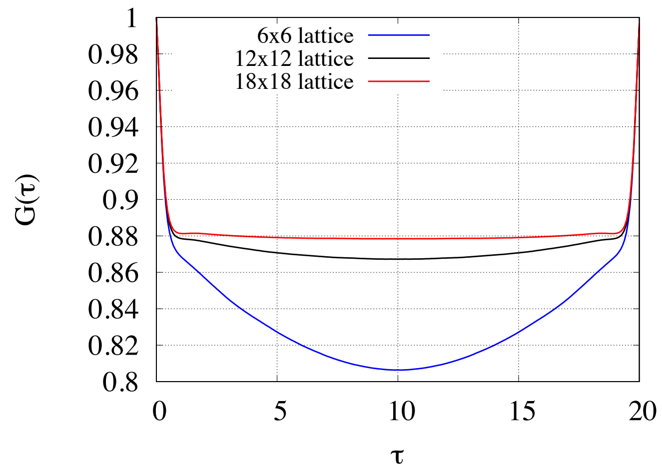


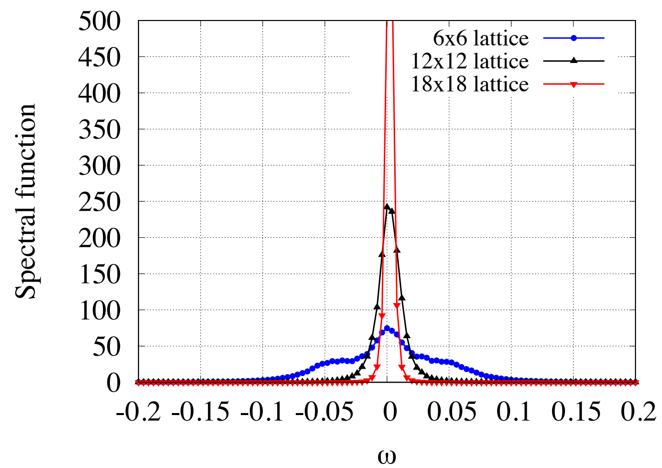
Magnetic susceptibility doesn't diverge at any point: no description of the phase transition (AFM spin ordering)



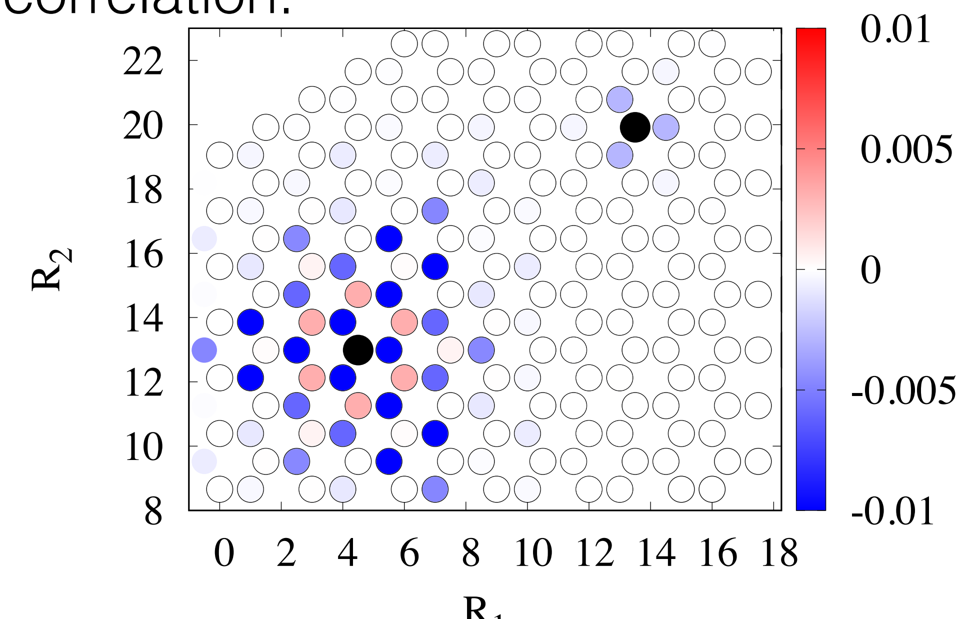
We described the increased spin localization, but local spins are still in paramagnetic phase

Spectral functions: comparison with QMC



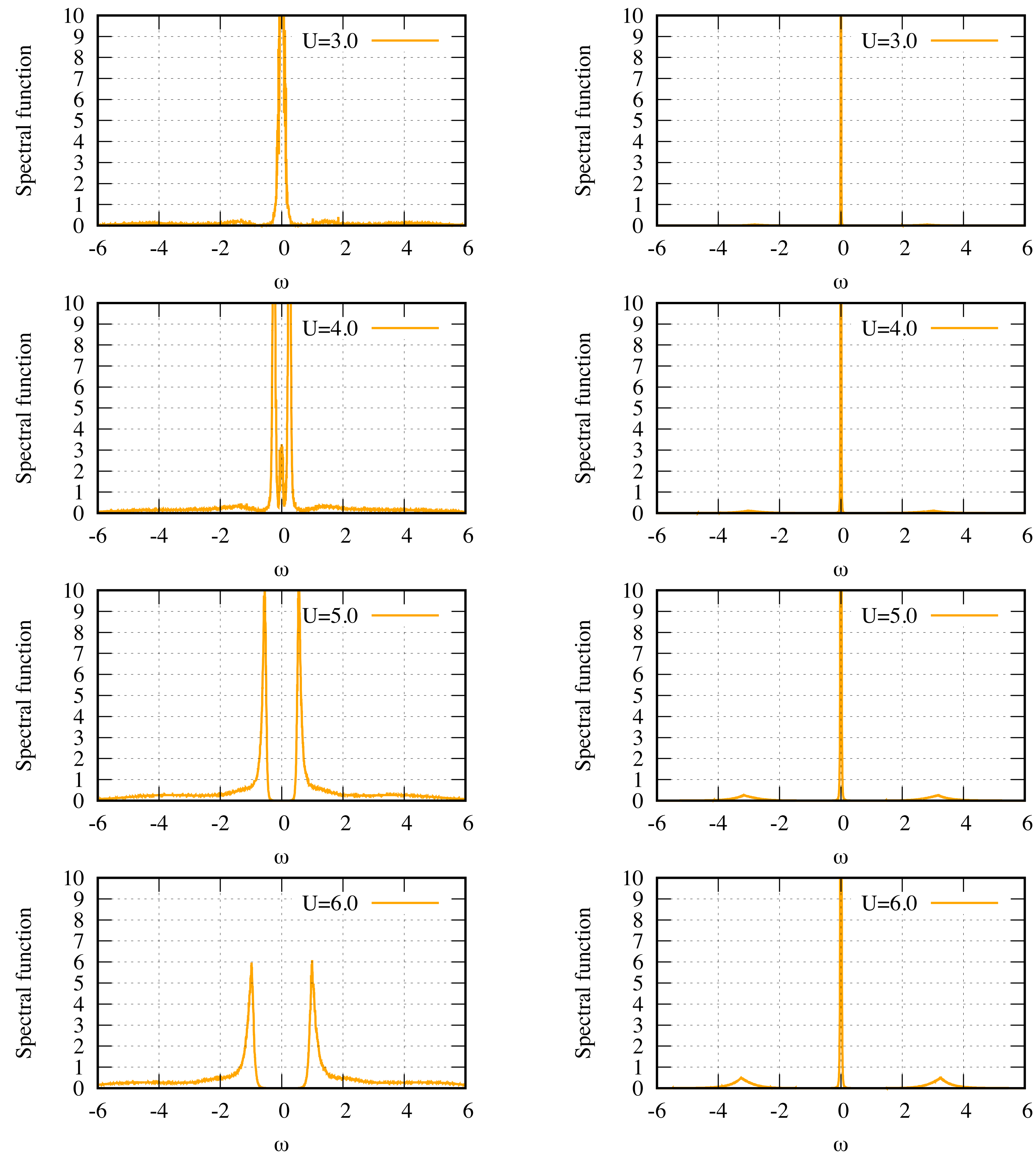


Broadening of the spectral function on smaller lattices: local AFM correlation.

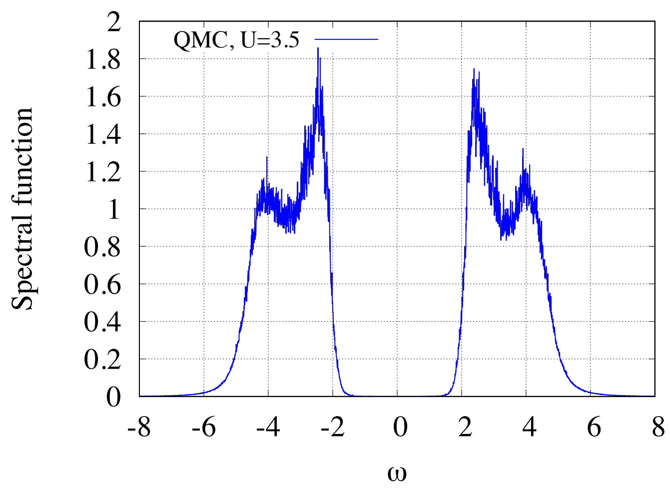


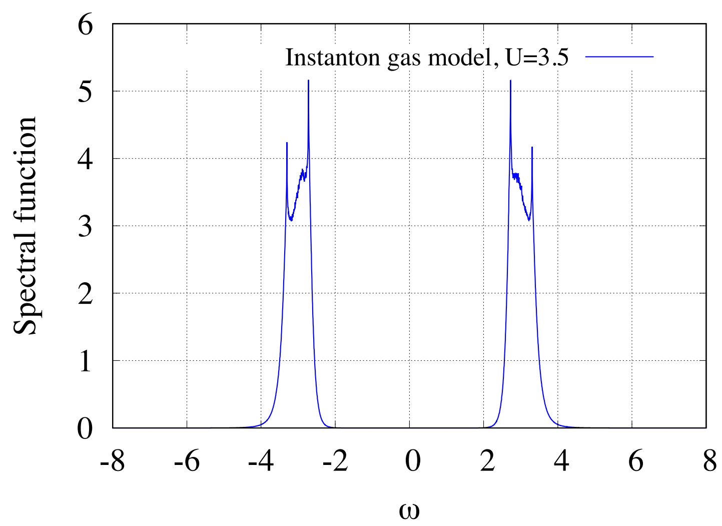
$\frac{1}{3}\langle \hat{\boldsymbol{S}}_{\boldsymbol{x}_0}(T) \cdot \hat{\boldsymbol{S}}_{\boldsymbol{x}_0+\boldsymbol{x}}(T)\rangle$

Spectral functions at K point (12x12 lattice):

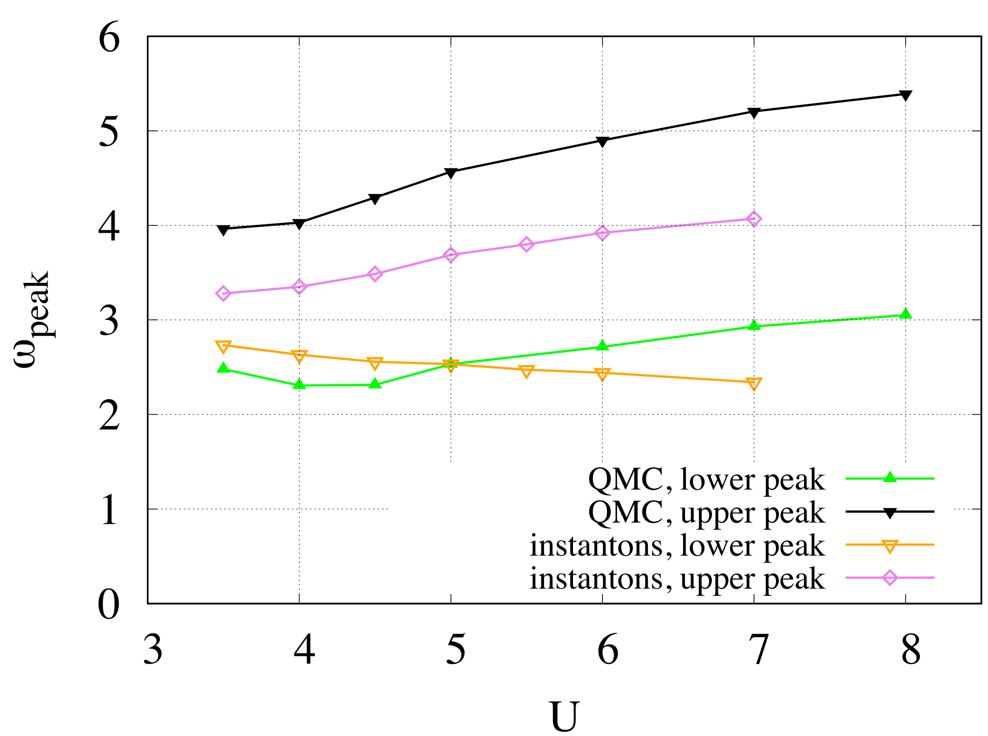


Spectral functions away of Dirac point (1)



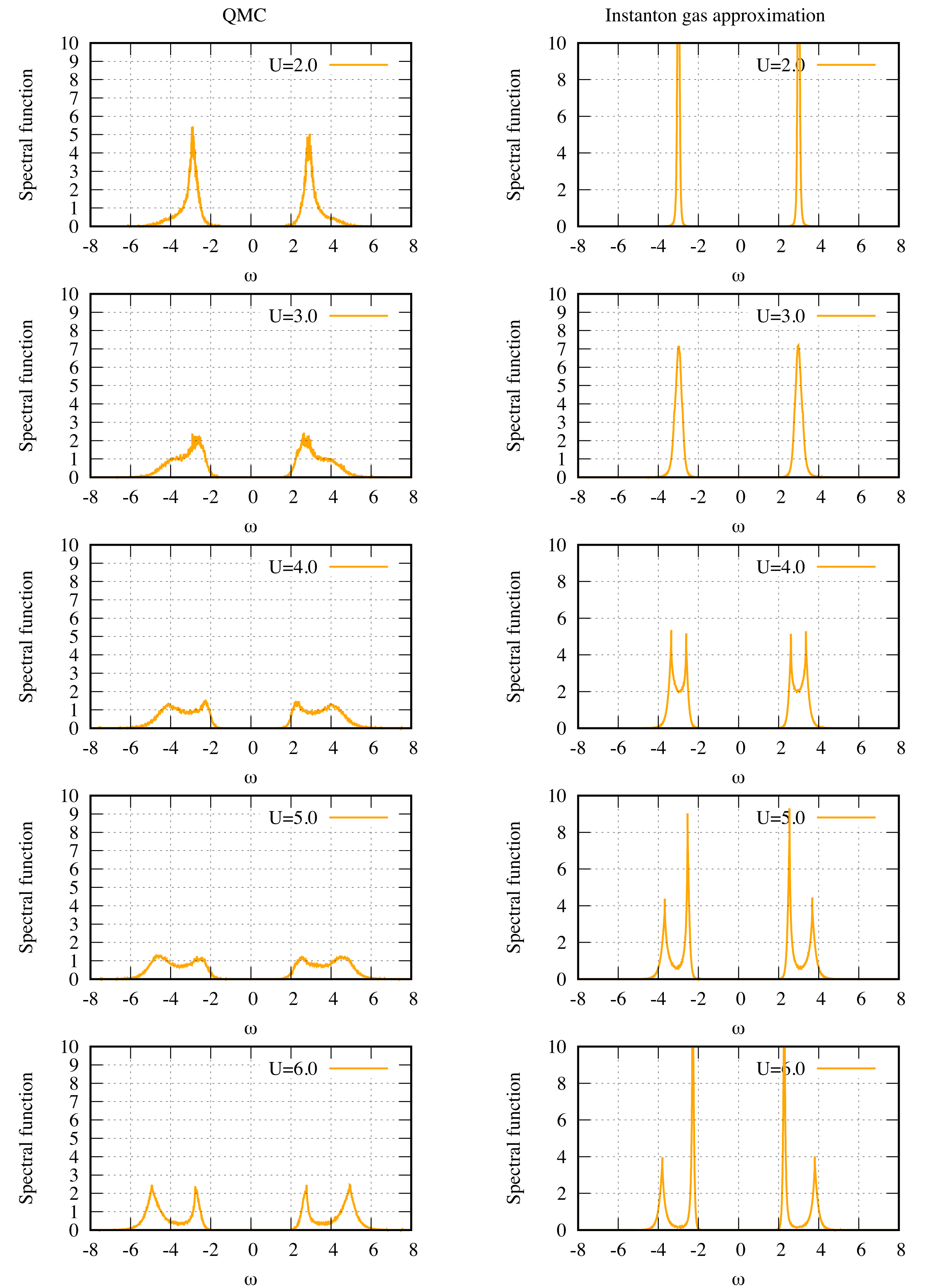


Appearance of the precursor for the upper Hubbard band at around U=3.5

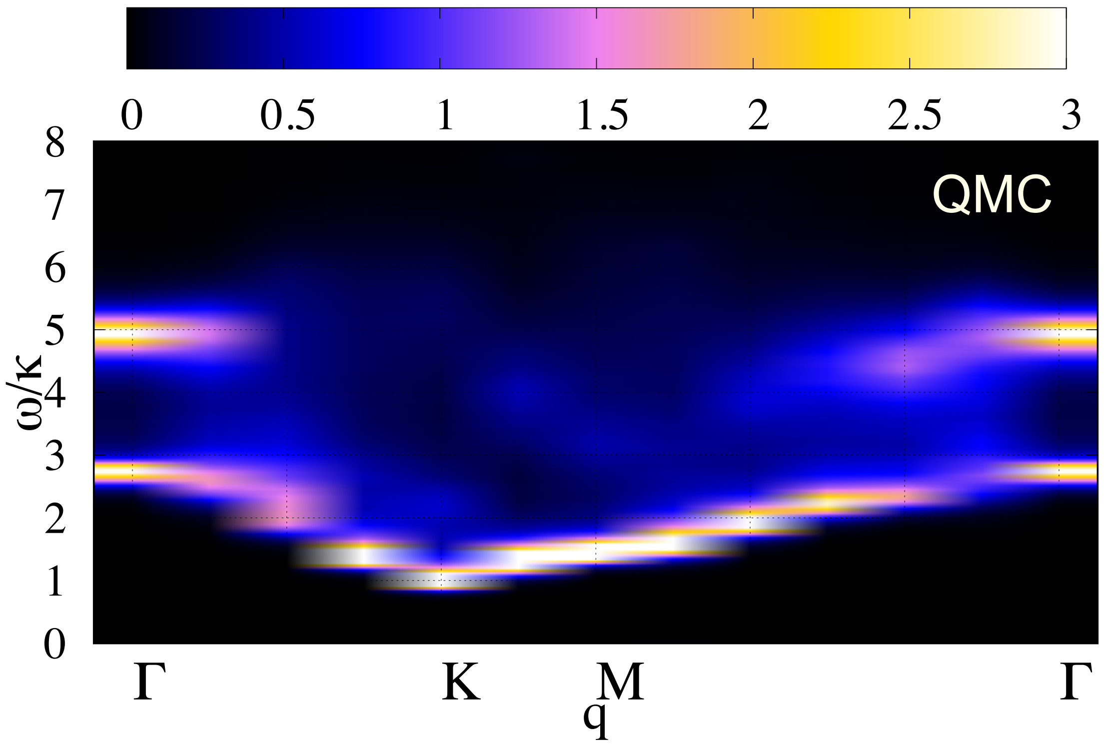


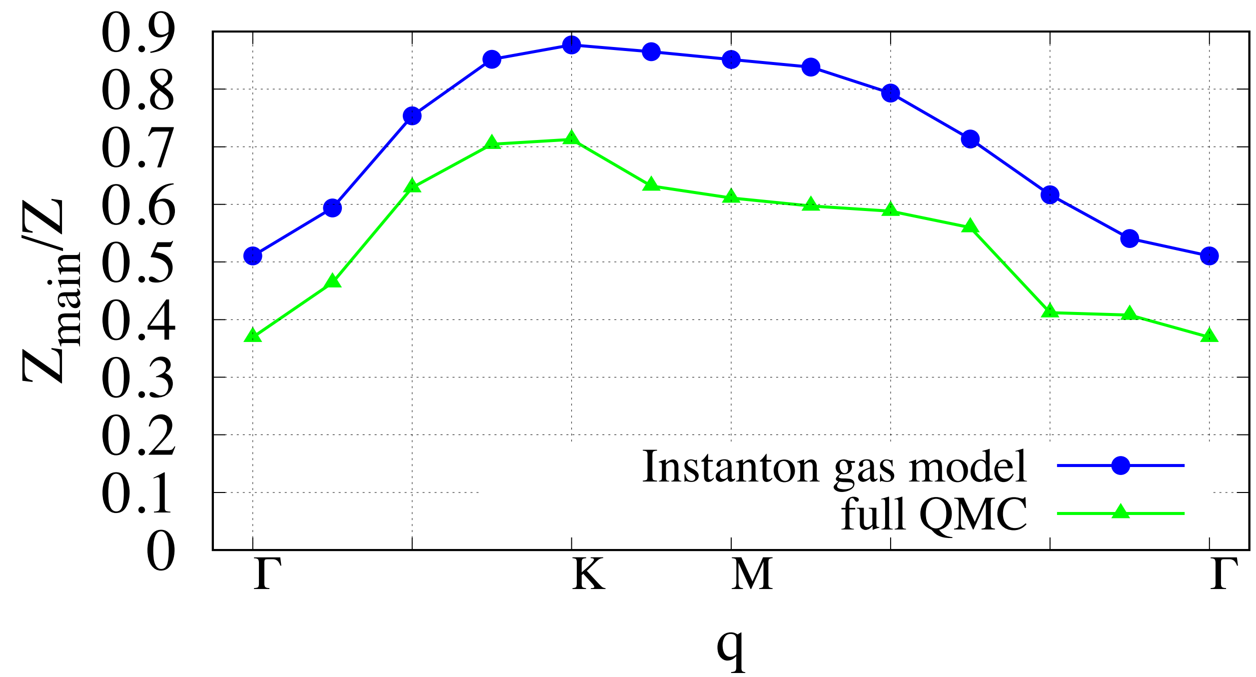
Energies and spectral weights of the peaks at Γ- point

Spectral functions at Γ-point (12x12 lattice):

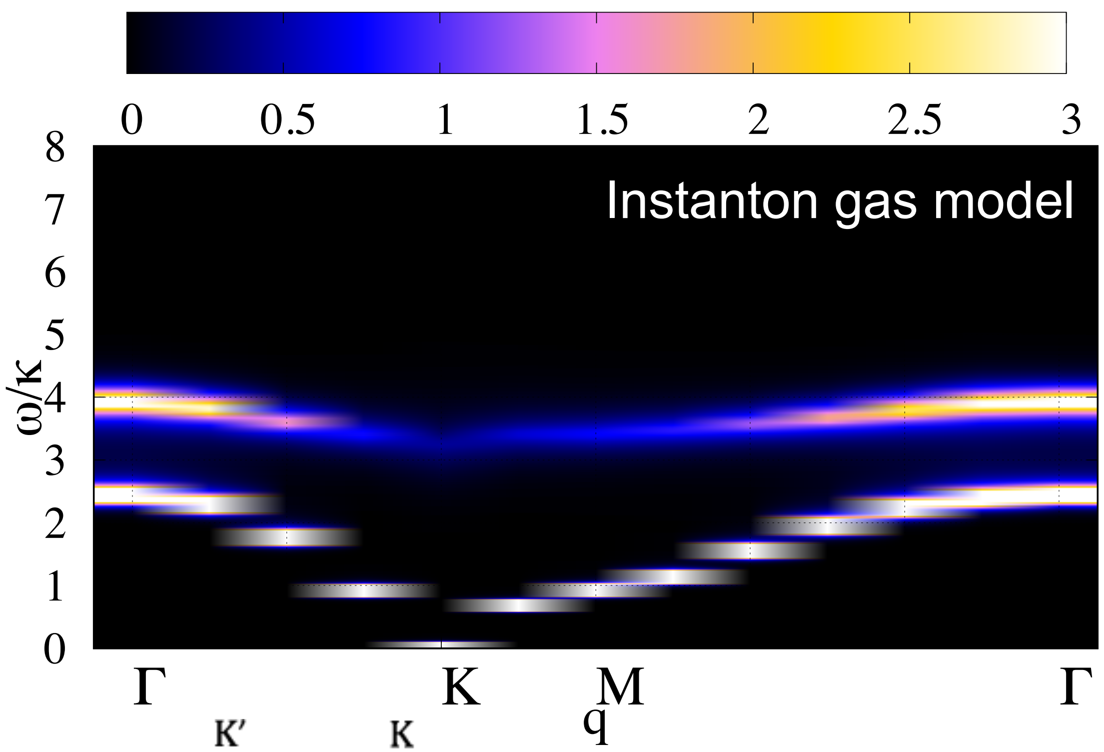


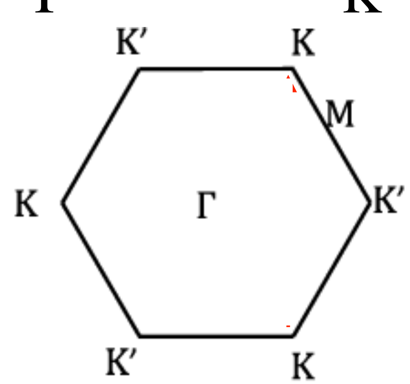
Spectral functions away of Dirac point (2)





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





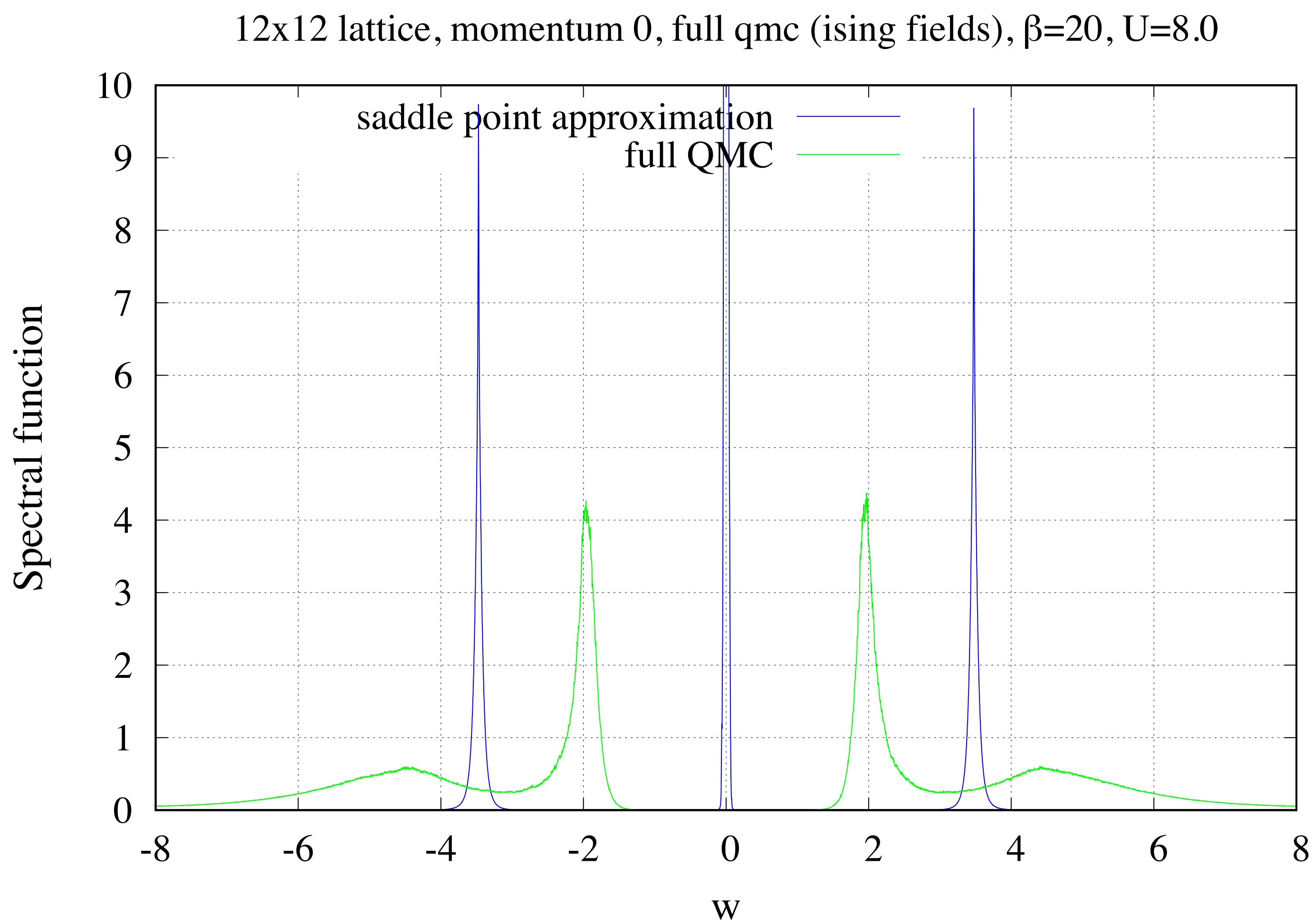
Instanton gas approximation works just fine away of Dirac points.

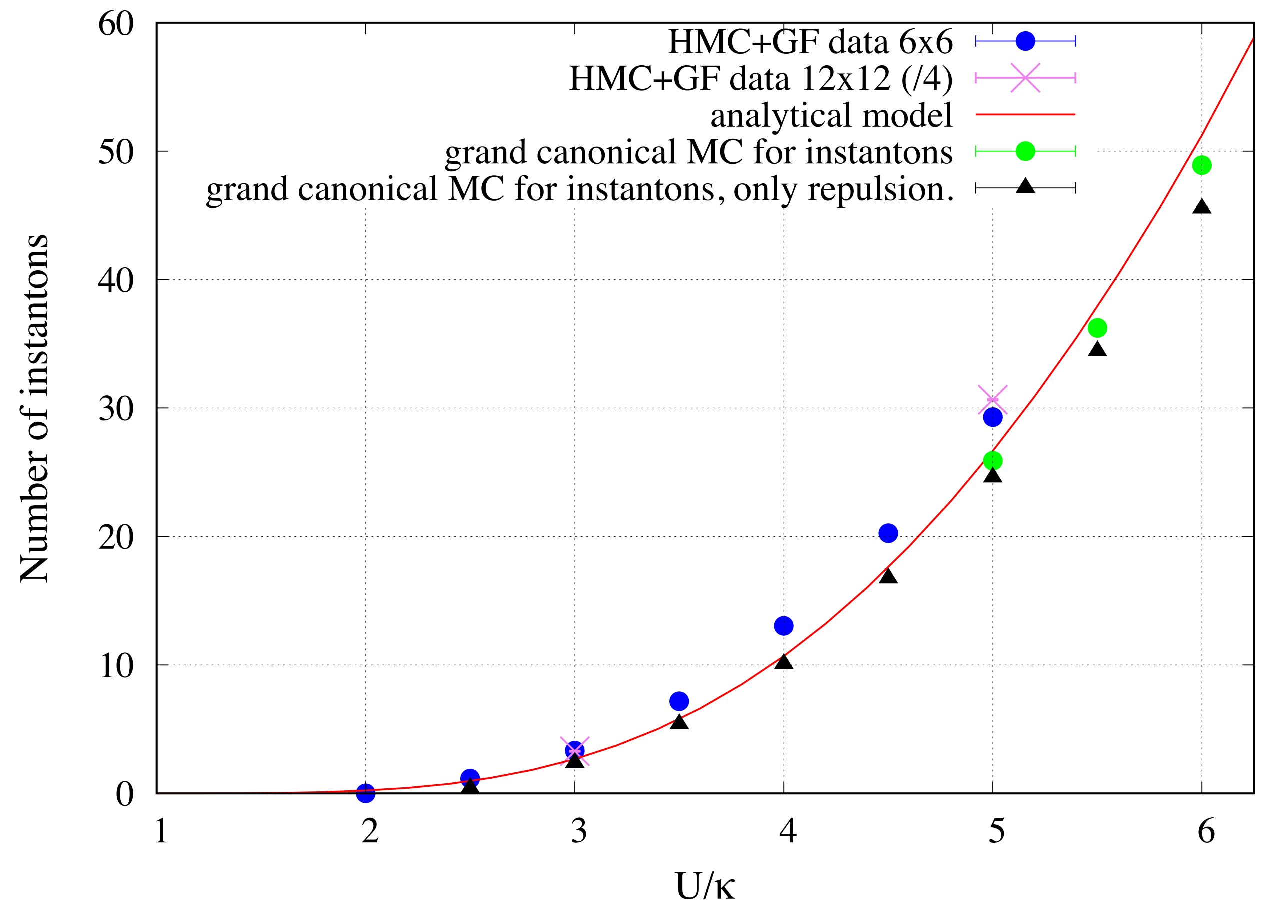
It can be used for more precise inquires into the nature of the excited states via (projection) QMC+MEM in saddle point approximation

$$\frac{\mathrm{Tr}\left(e^{-\hat{H}_{full}\beta}\hat{A}e^{-\hat{H}_{full}\tau}\hat{A}^{\dagger}\right)}{\mathrm{Tr}\left(e^{-\hat{H}_{full}(\beta+\tau)}\right)} = \sum_m |C_m|^2 e^{-\tau(E_m-E_0)}$$

$$\hat{A}|O_{int.}\rangle = \sum_m C_m |m\rangle \qquad \hat{A} = \hat{a}^{\dagger}_{k,\uparrow}; \quad \hat{a}^{\dagger}_{-k_1,\uparrow}\hat{a}_{k_1,\downarrow}\hat{a}^{\dagger}_{k,\uparrow}\ldots$$

Spontaneous symmetry breaking and the generation of mass

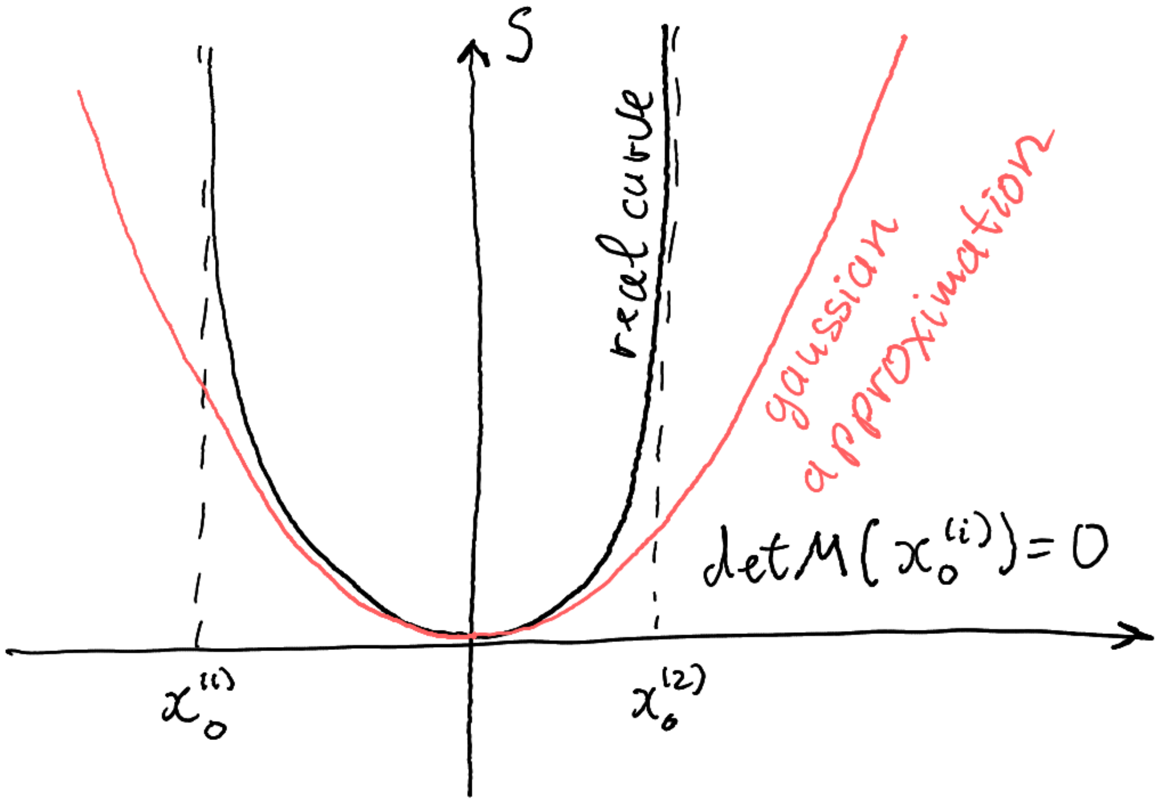




?

Beyond Gaussian approximation: full integral over one dominant thimble

We do not take into account fluctuations of the field in observables, and in fact we can not do so in fermionic observables (easily)

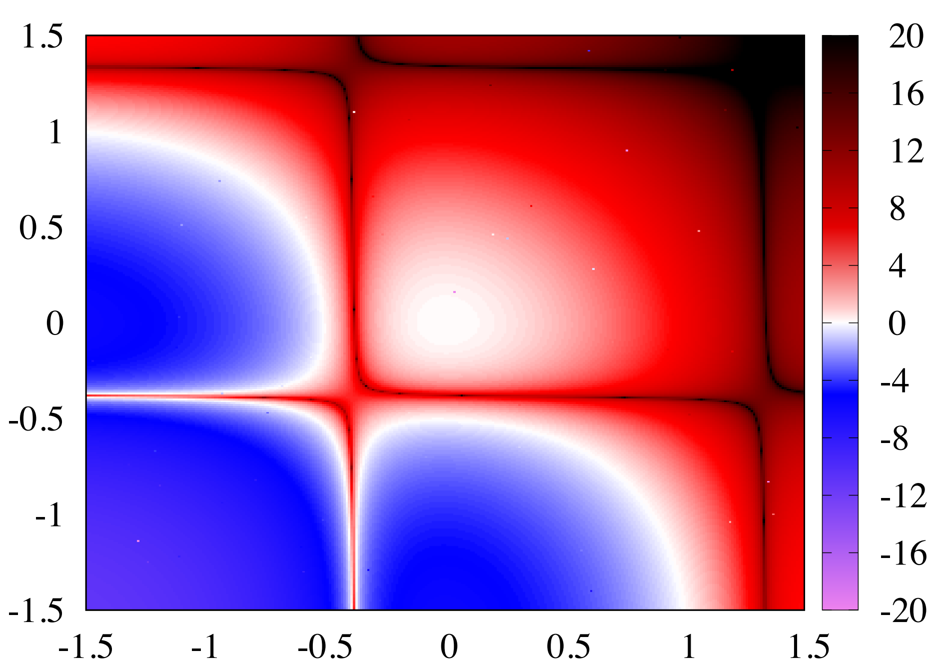


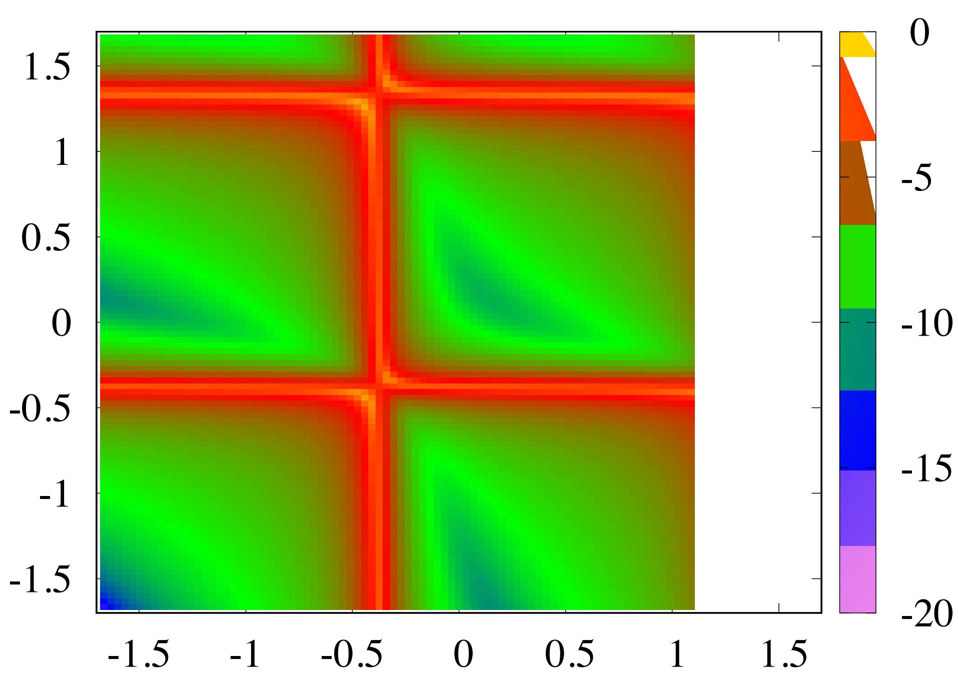
$$\int O(x)P(x)dx$$

$O(x) \to \infty$ as $1/x$

$$P(x) \to const\,.$$

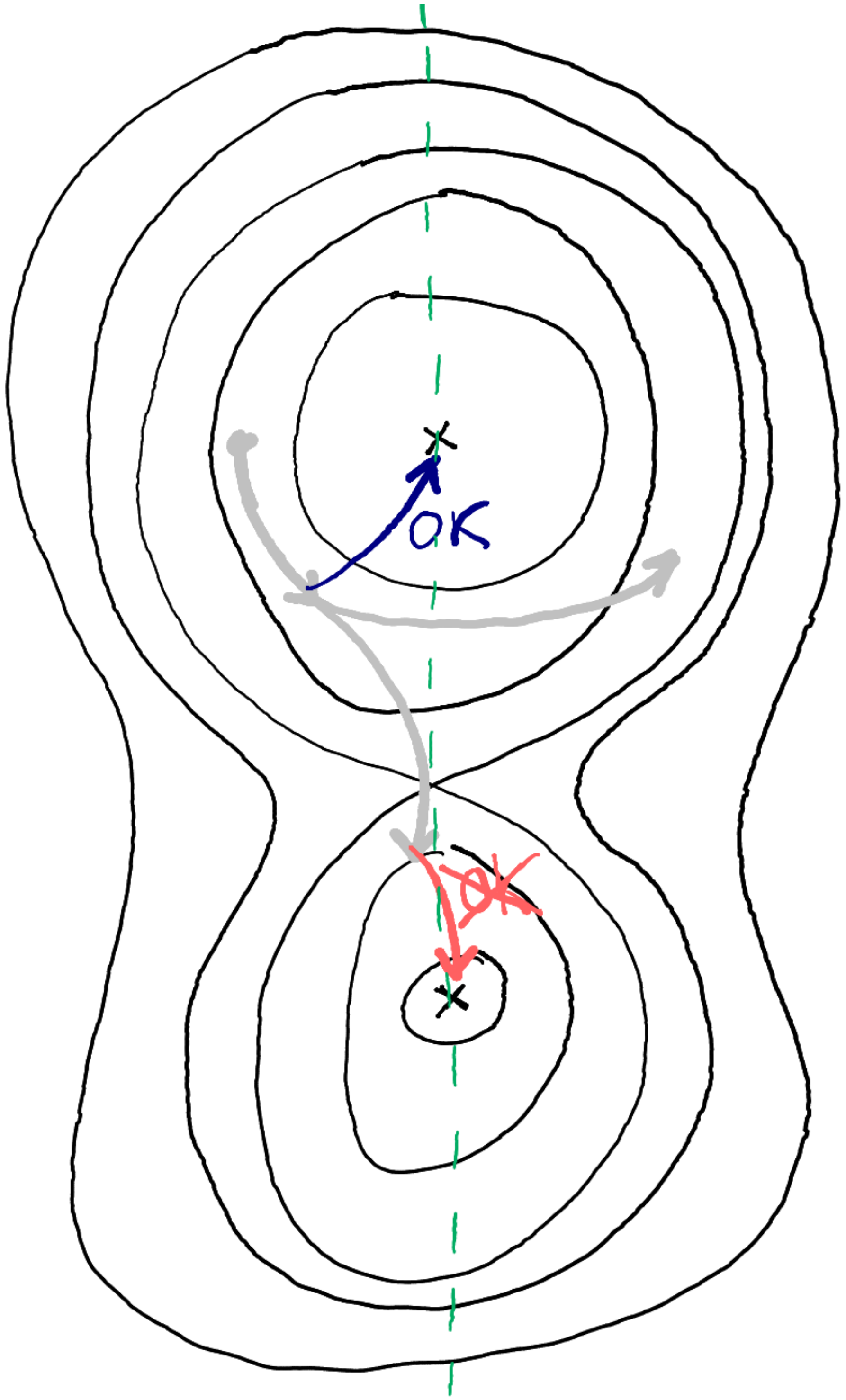
$$x \to x_0$$

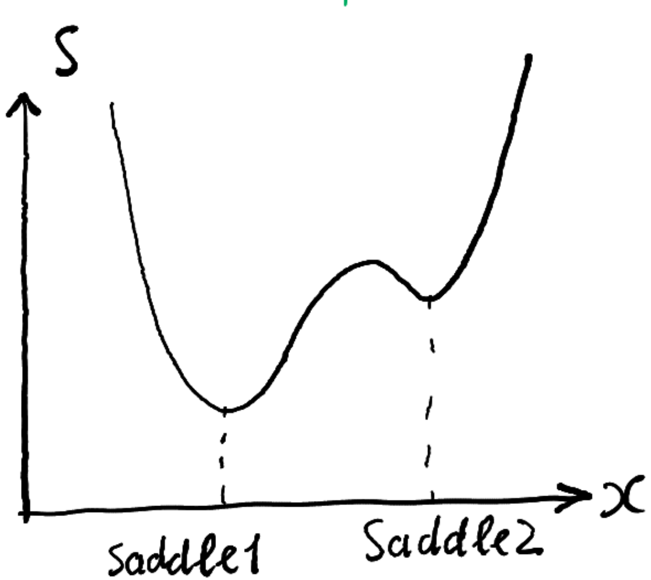




Propagator diverges at the zeros of fermionic operator, thus fermionic observables also diverge

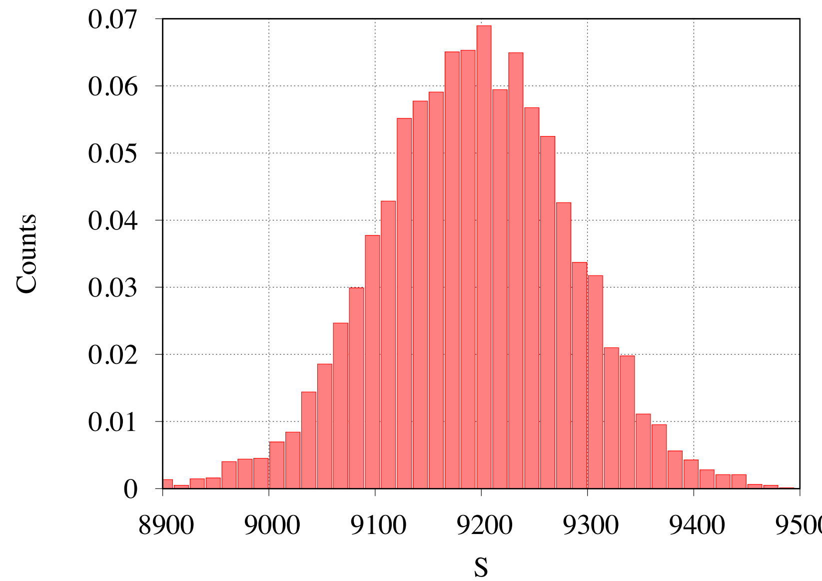
Full integral over one dominant thimble: algorithms



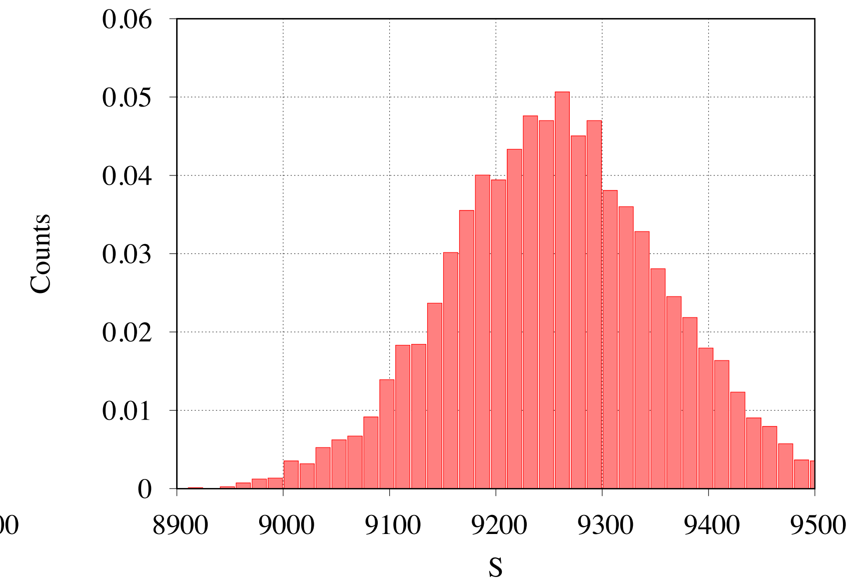


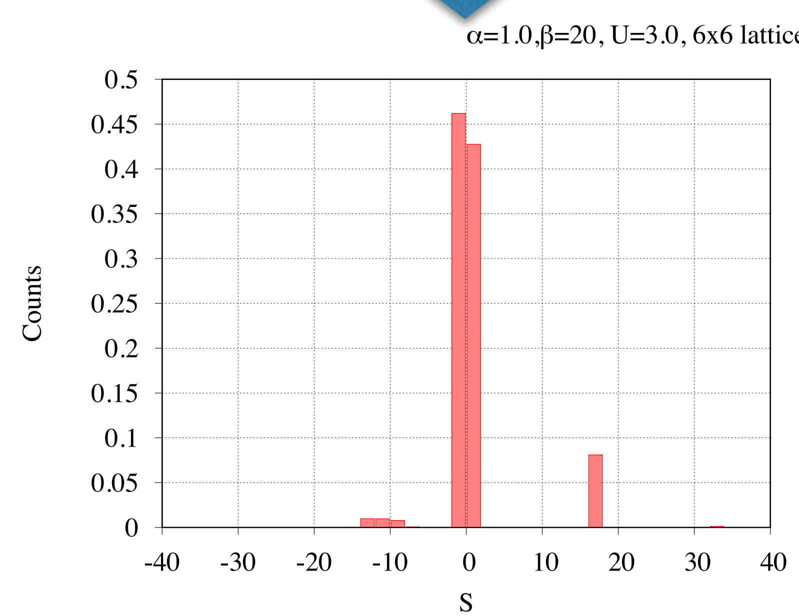
Check that we are still within the same thimble via GF after HMC update:

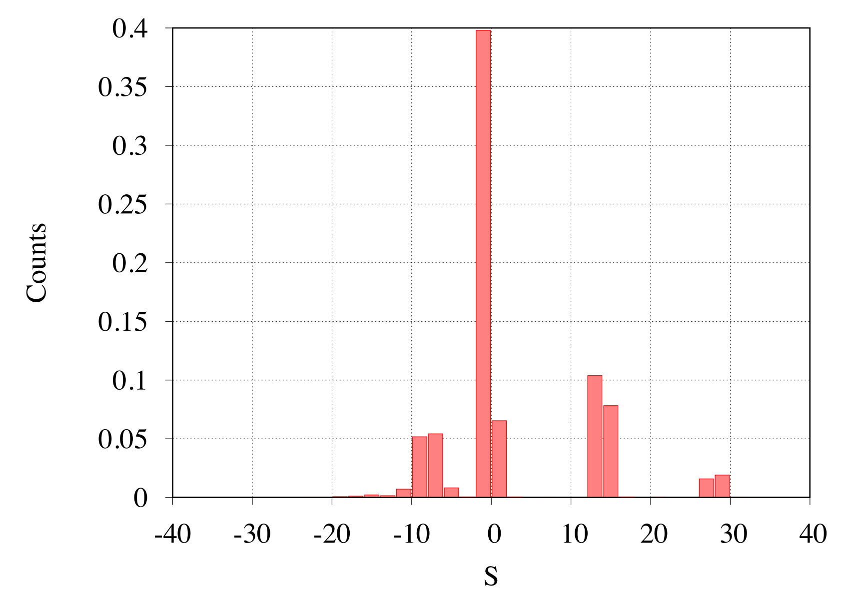
U=3.0



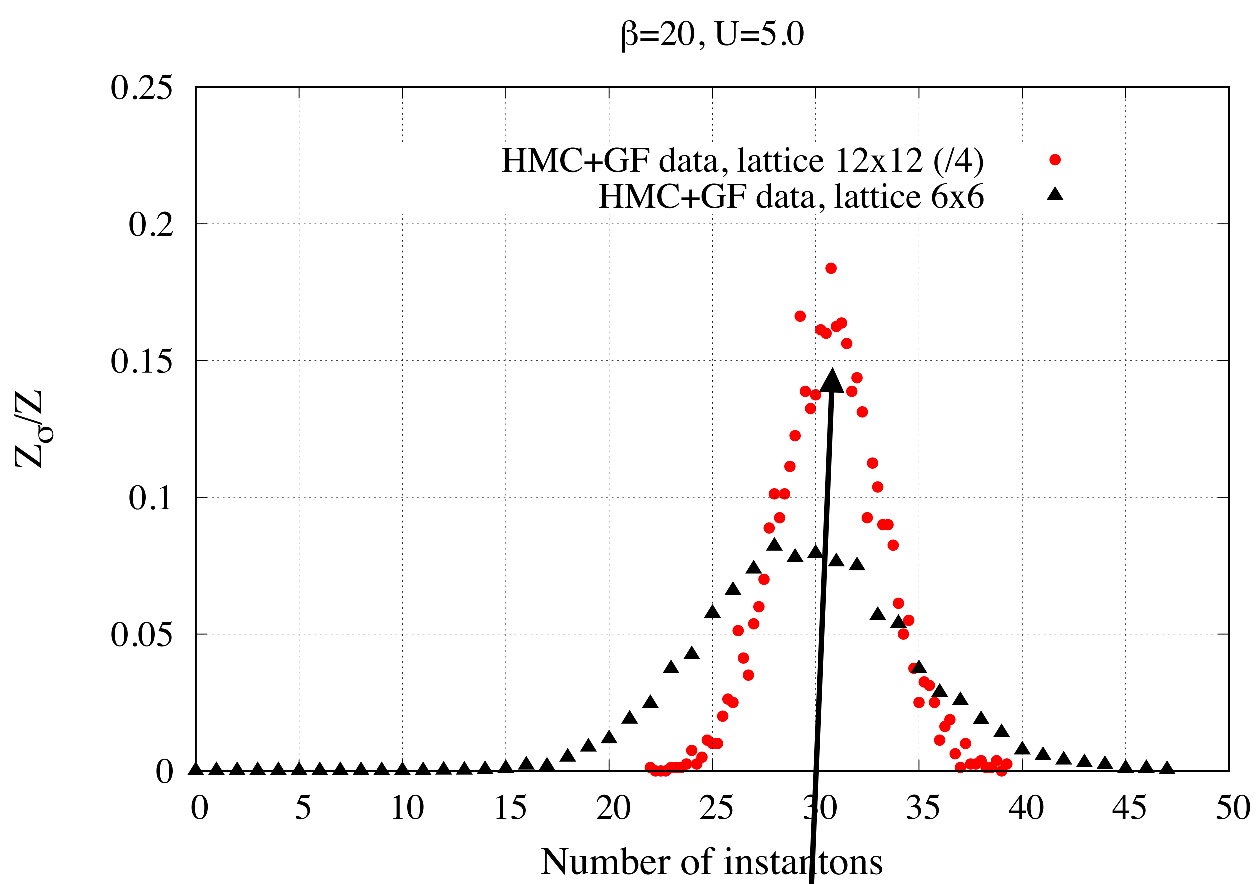
U=4.0



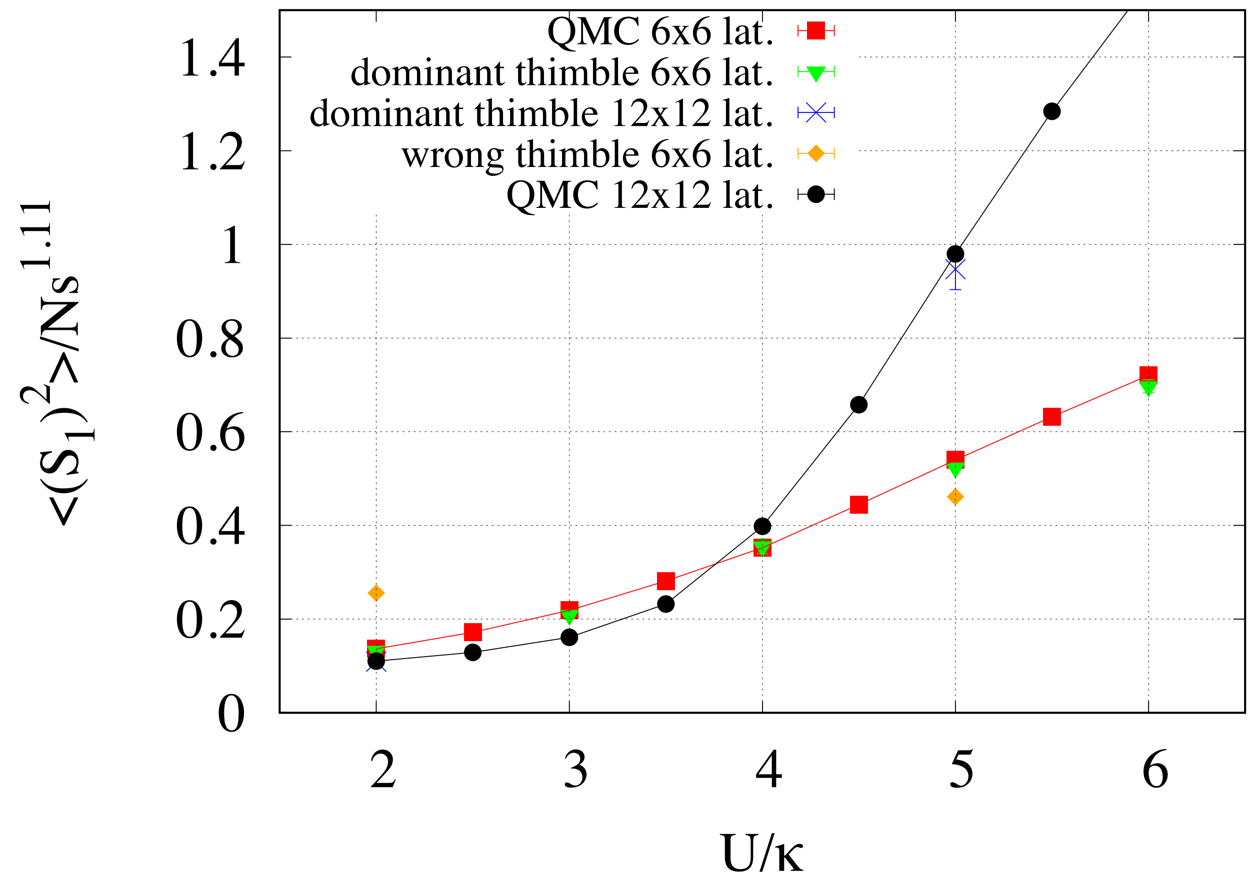


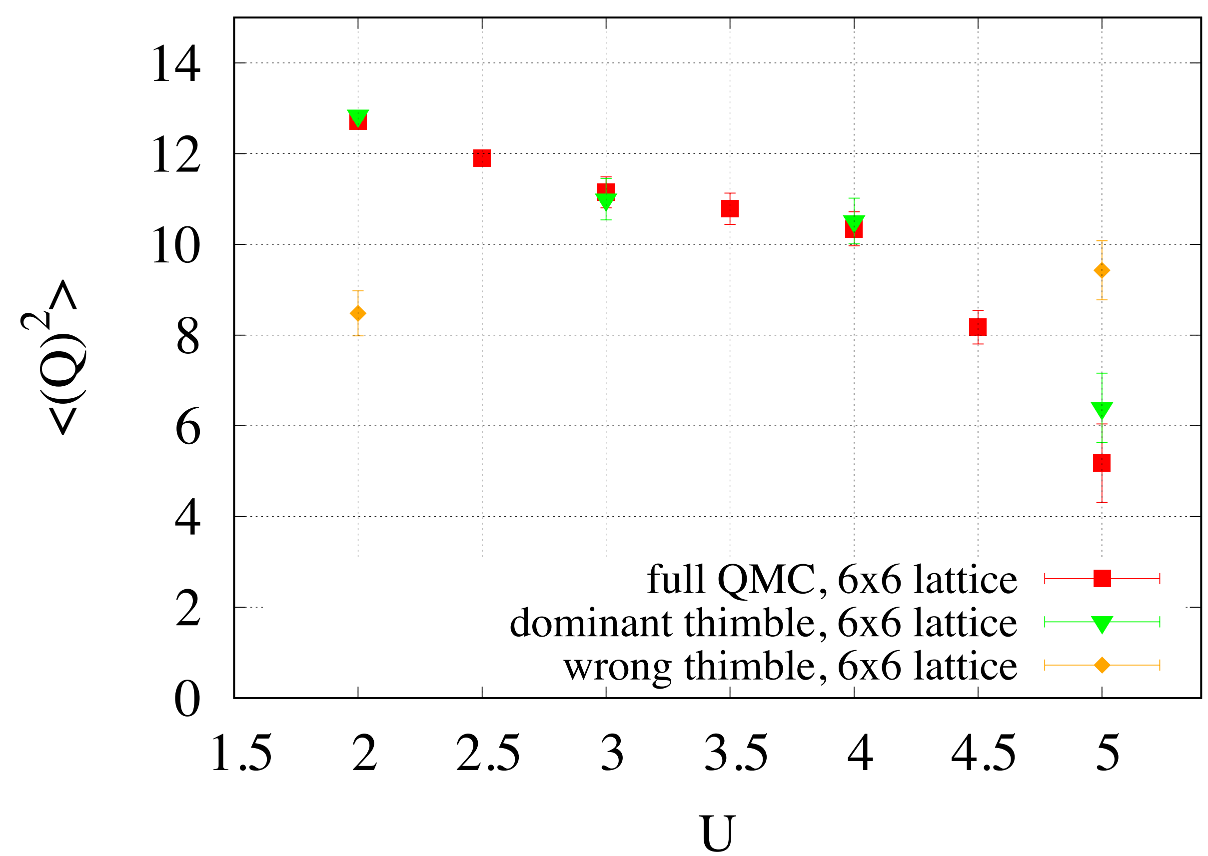


Full integral over one dominant thimble: results (1)



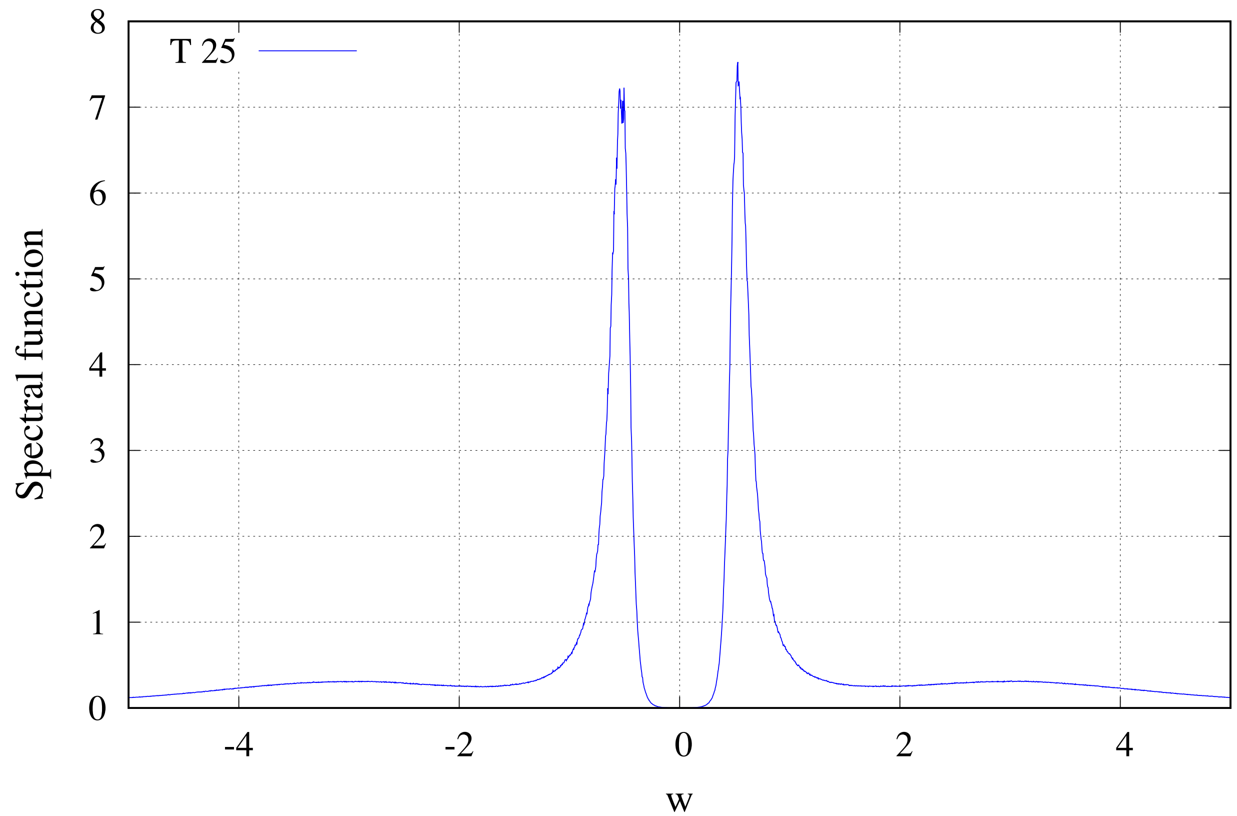
The form of dominant saddle is taken from classical MC for instanton gas





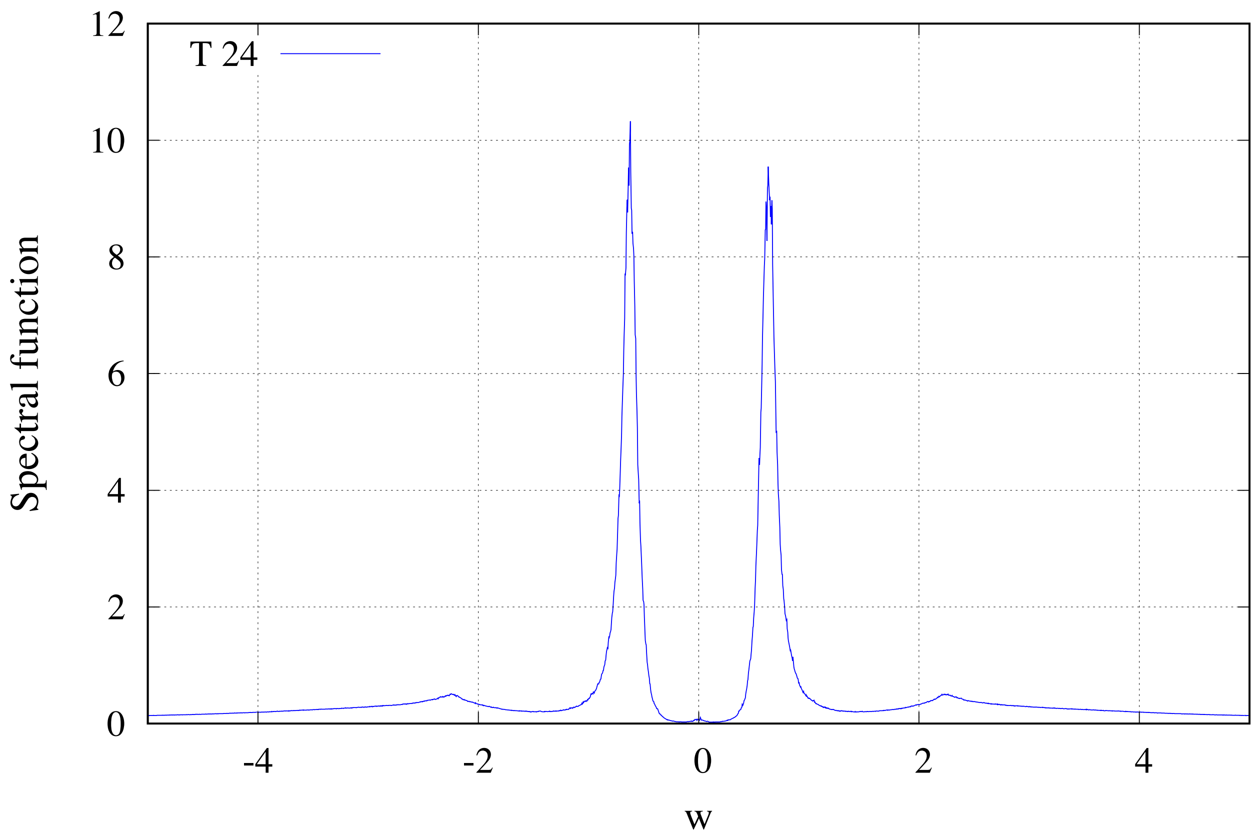
Full integral over one dominant thimble: results (2)

12x12 lattice, momentum 0, 1 thimble HMC, β=20, U=5.0

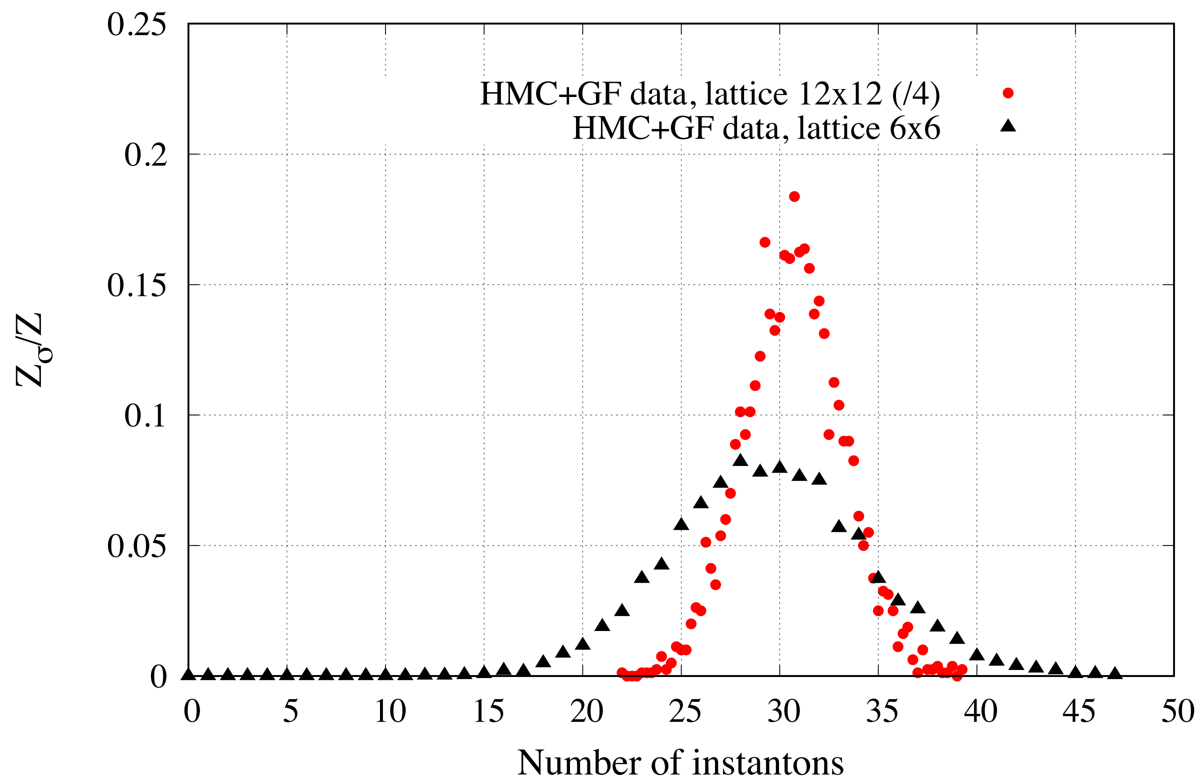


Integral over just one thimble attached to the «dominant» saddle randomly picked up from the peak of instanton number distribution, provides us with almost entirely correct information on mass gap.
Saddle is generated from simple classical MC (grand canonical MC for instanton gas), which doesn't have the sign problem. The reason for the success is the increasing sharpness of the distribution of instantons once we approach the thermodynamic limit.

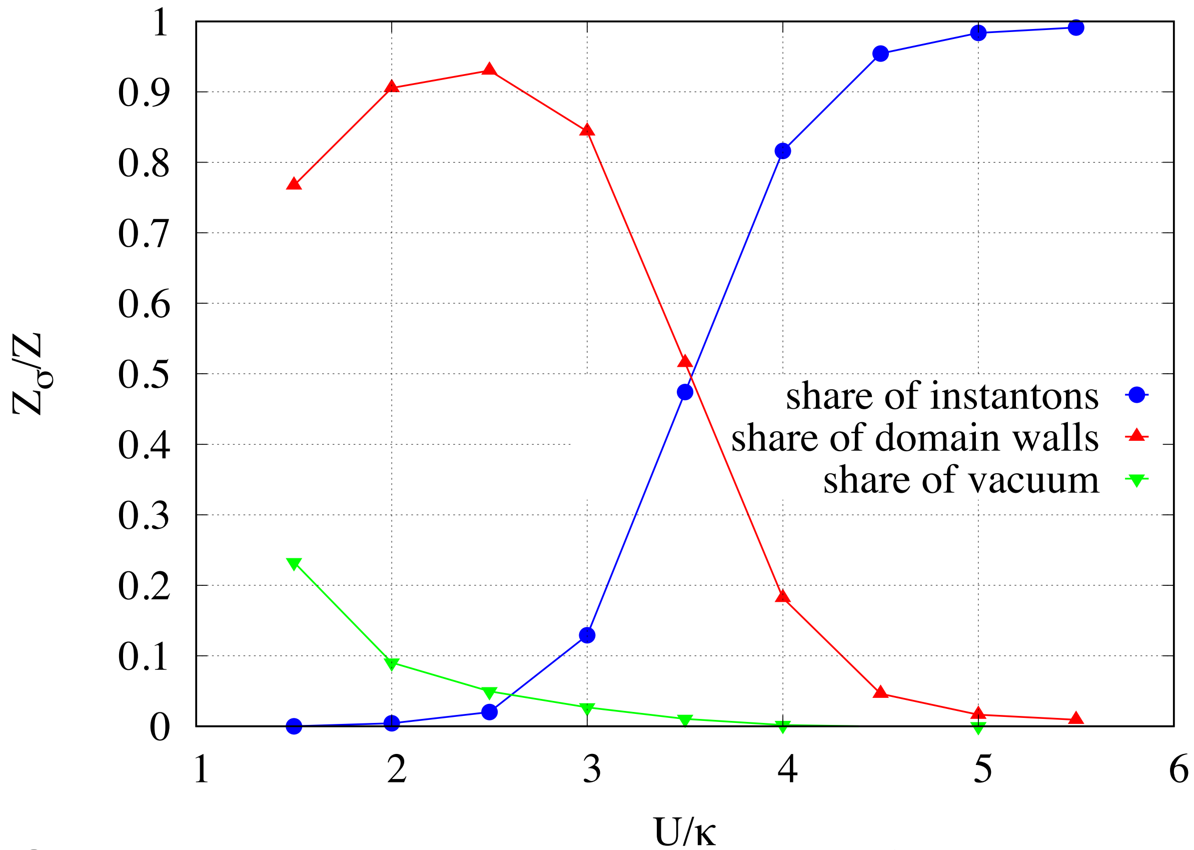
12x12 lattice, momentum 0, full QMC (ising fields), β=20, U=5.0

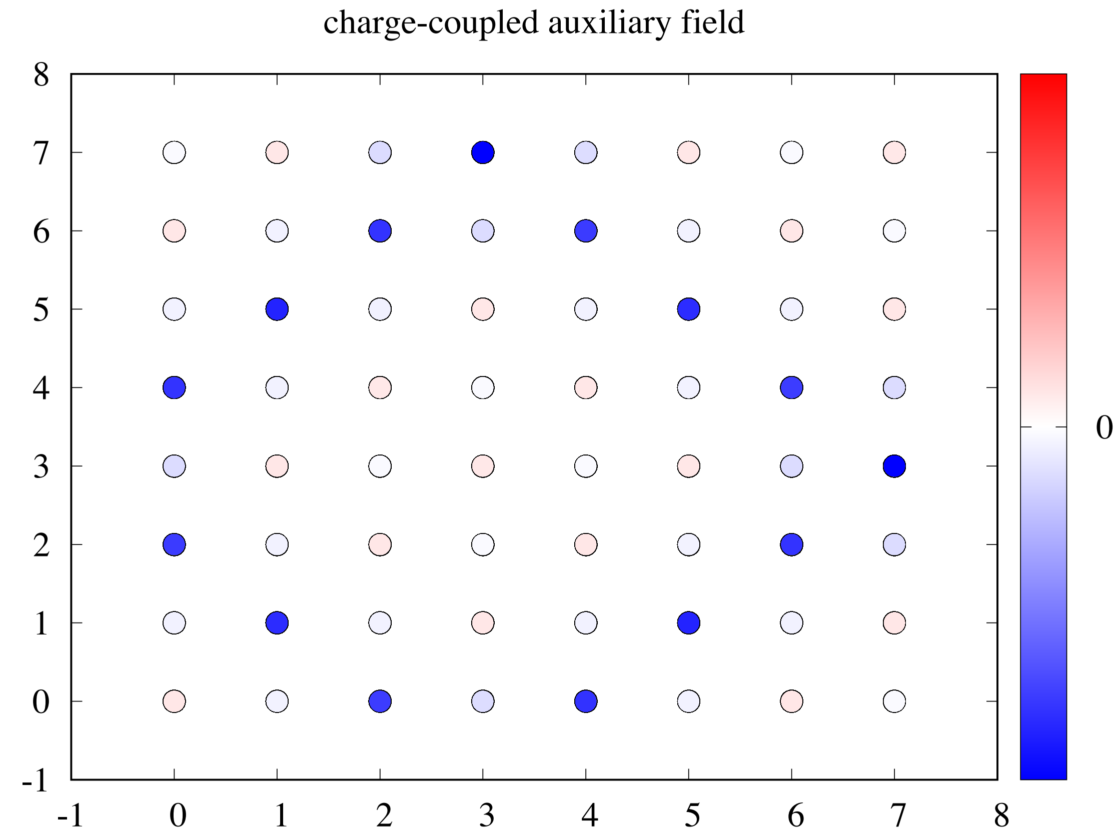


β=20, U=5.0



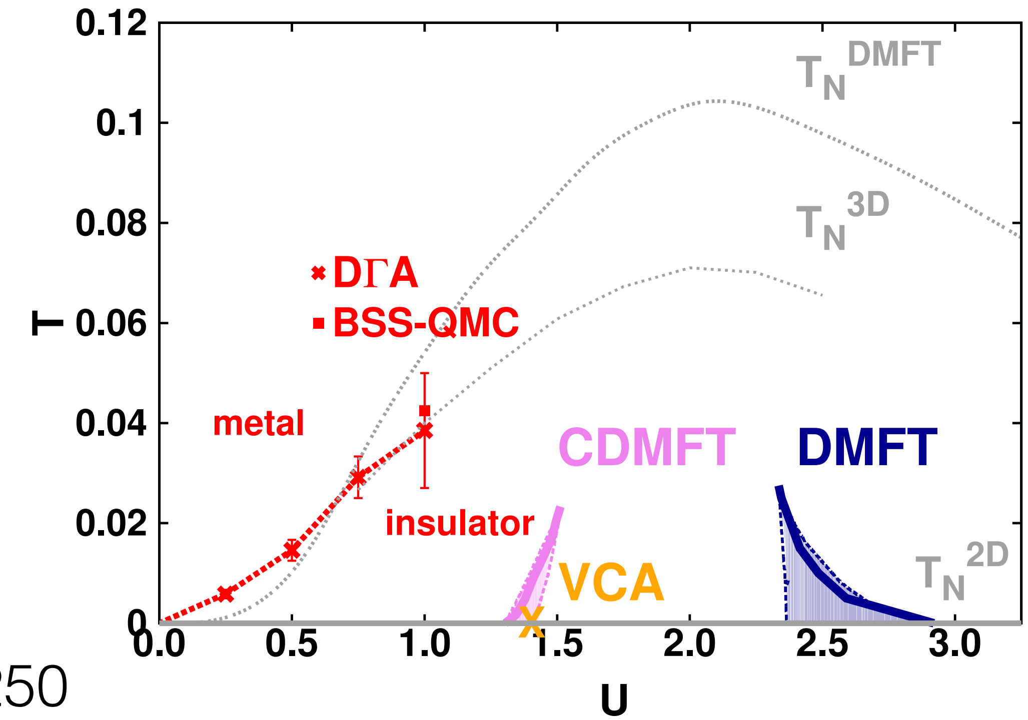
Applications for other systems: square lattice Hubbard model





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

Insulator survives until zero U at zero temperature:



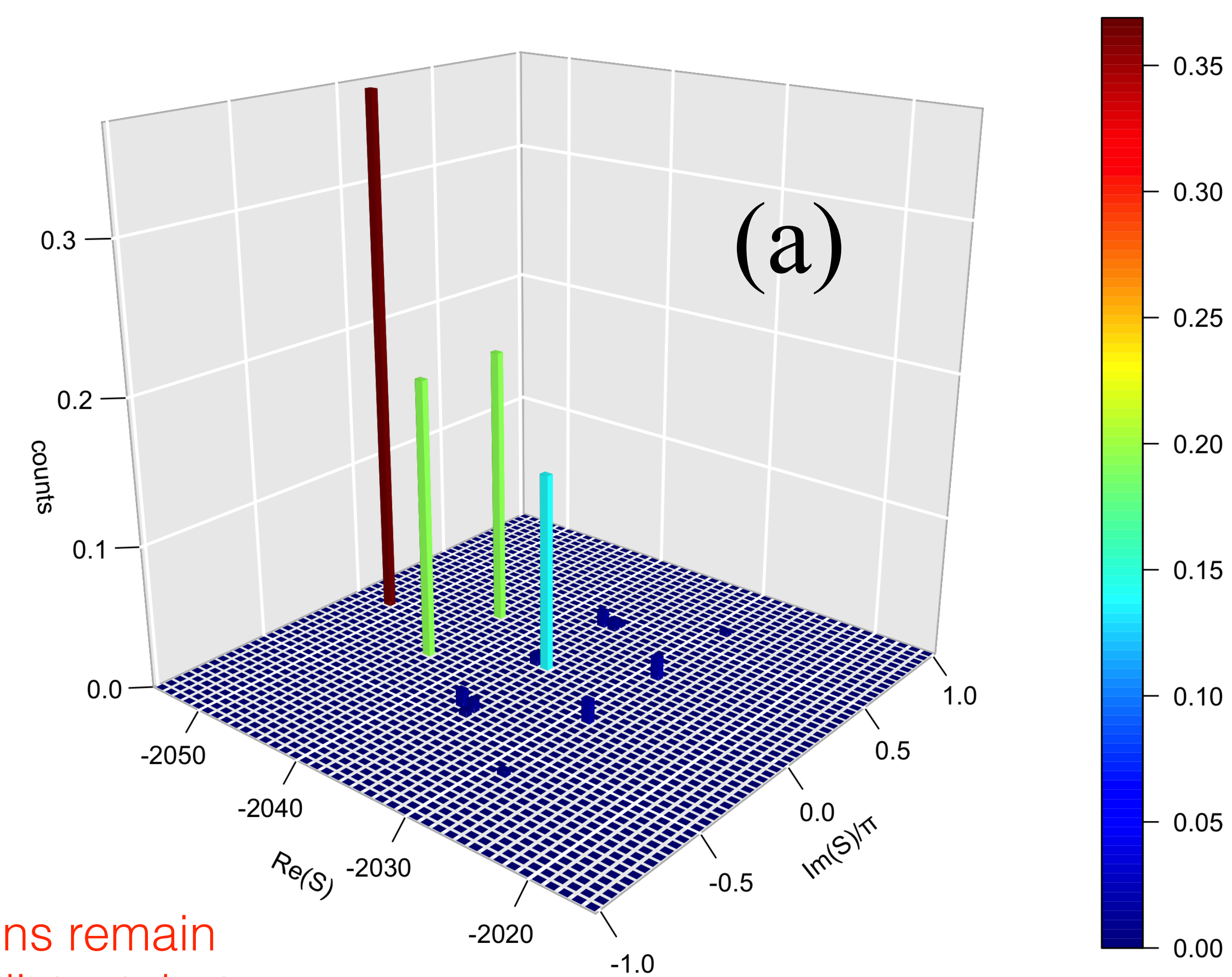
arXiv:1405.7250

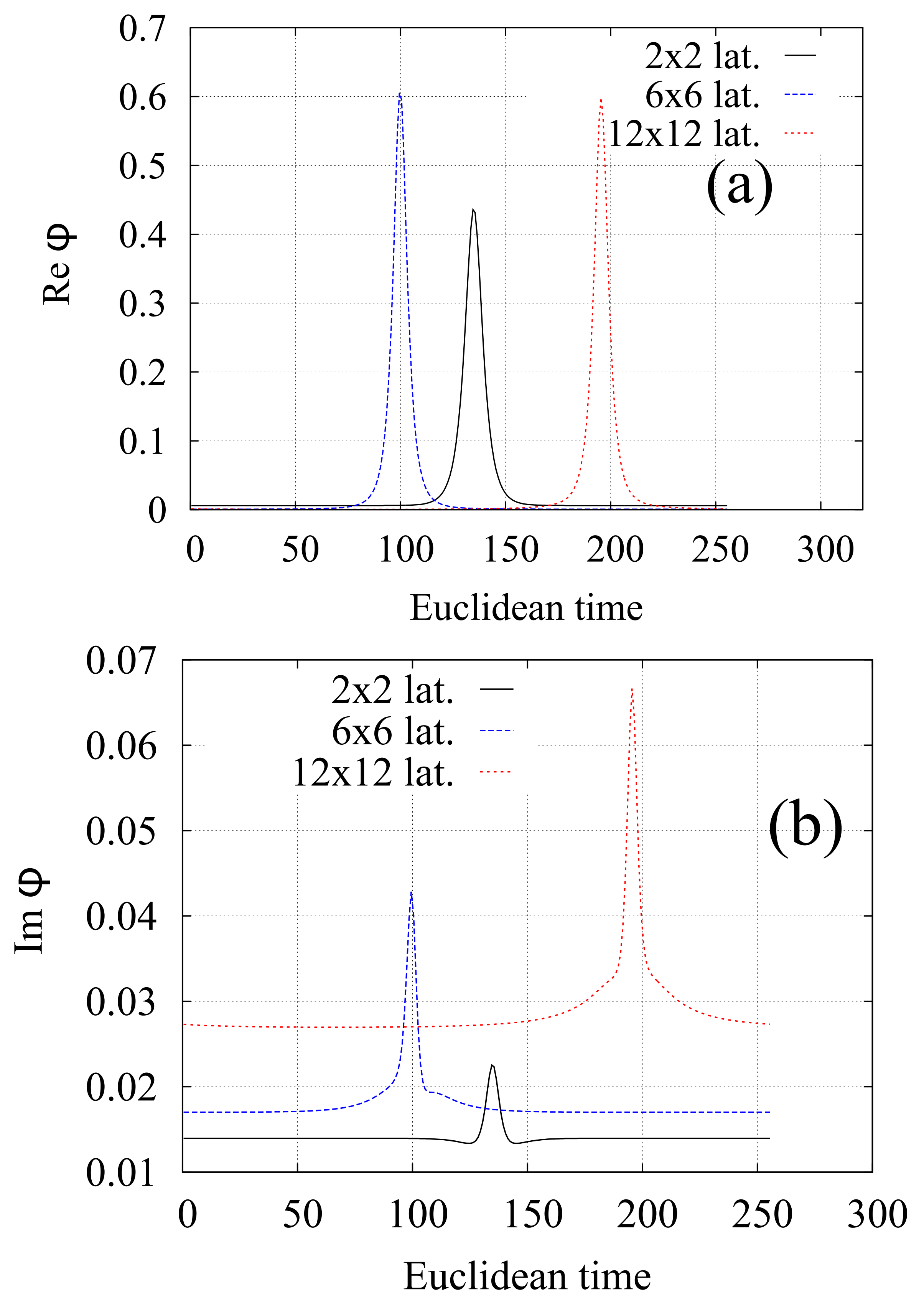
Further perspectives: complex instantons at finite chemical potential

$$\boxed{U = 3.8\kappa}$$

$$\boxed{\mu = \kappa}$$

Distribution of actions:

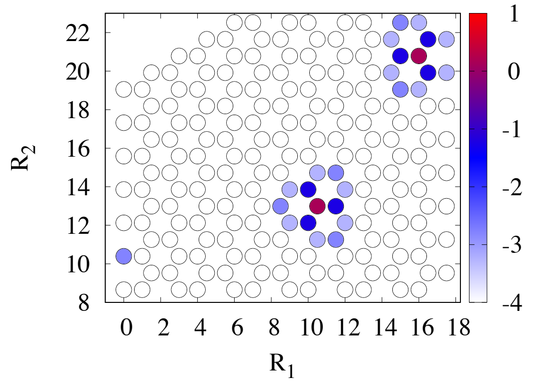




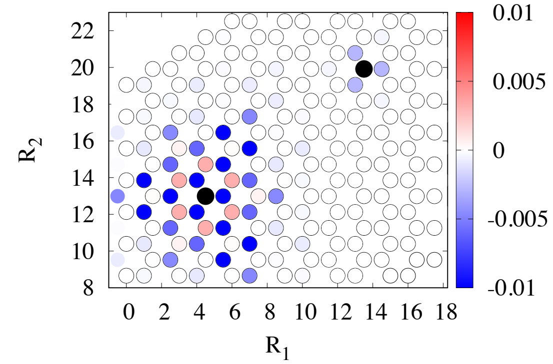
Actions remain equidistant, but now in complex plane

Summary

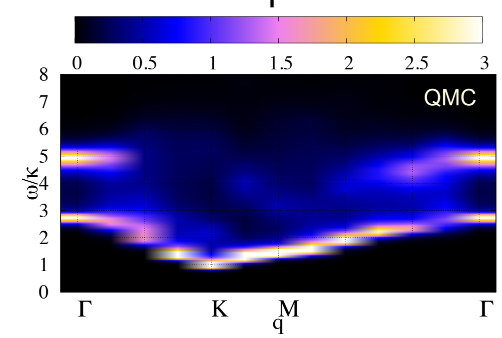
1) Physically, instanton gas model corresponds to increasingly localized spins, distributed through the lattice, with weak interaction between them.

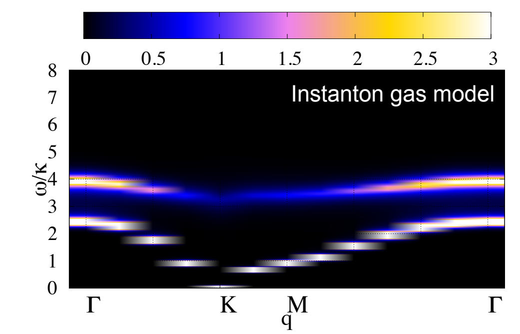


2) No long-range order, but increasing local AFM interactions.

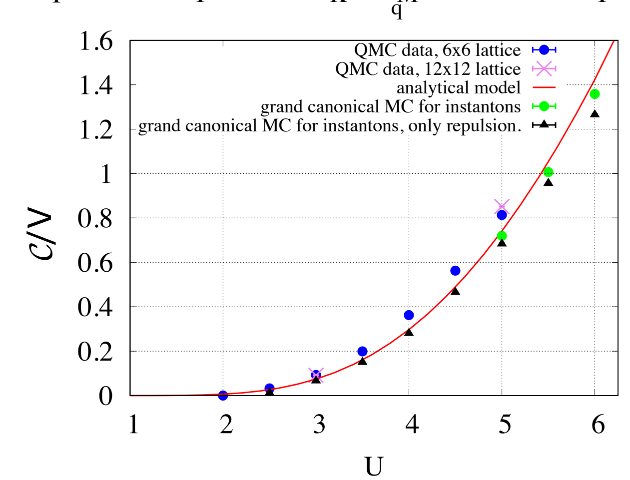


3) Good agreement with exact QMC for the spectral functions everywhere except of the close vicinity of the Dirac point.



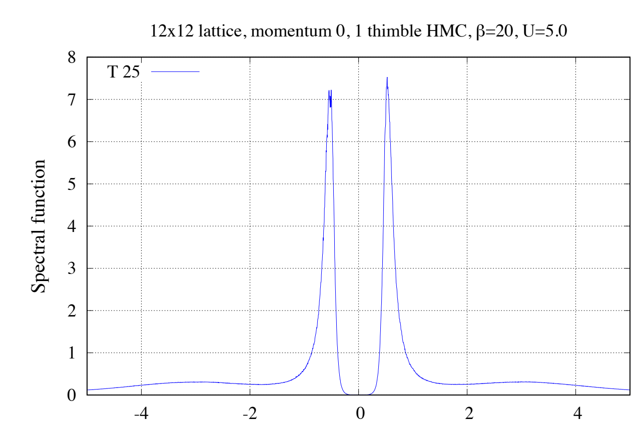


4) Instanton gas approximation provides the high accuracy prediction for the structure of the dominant saddle point.



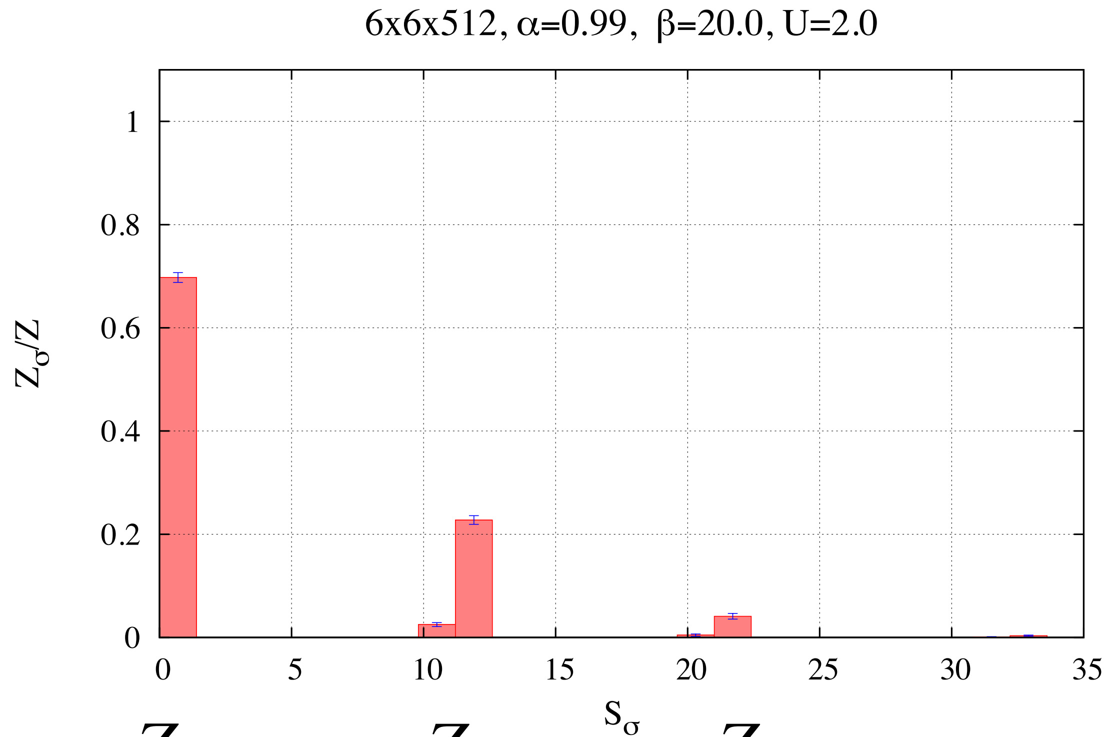
Note: AFM order disappears anyway away of half filling (if chemical potential is larger than the mass gap) thus the accuracy in its description is not that important. However, local AFM correlations remain. Thus it might be a good approximation to study the case of finite chemical potential

5) In order to describe the appearance of the long range AFM order, it is enough to compute the integral over just one dominant thimble, predicted by the instanton gas approximation.



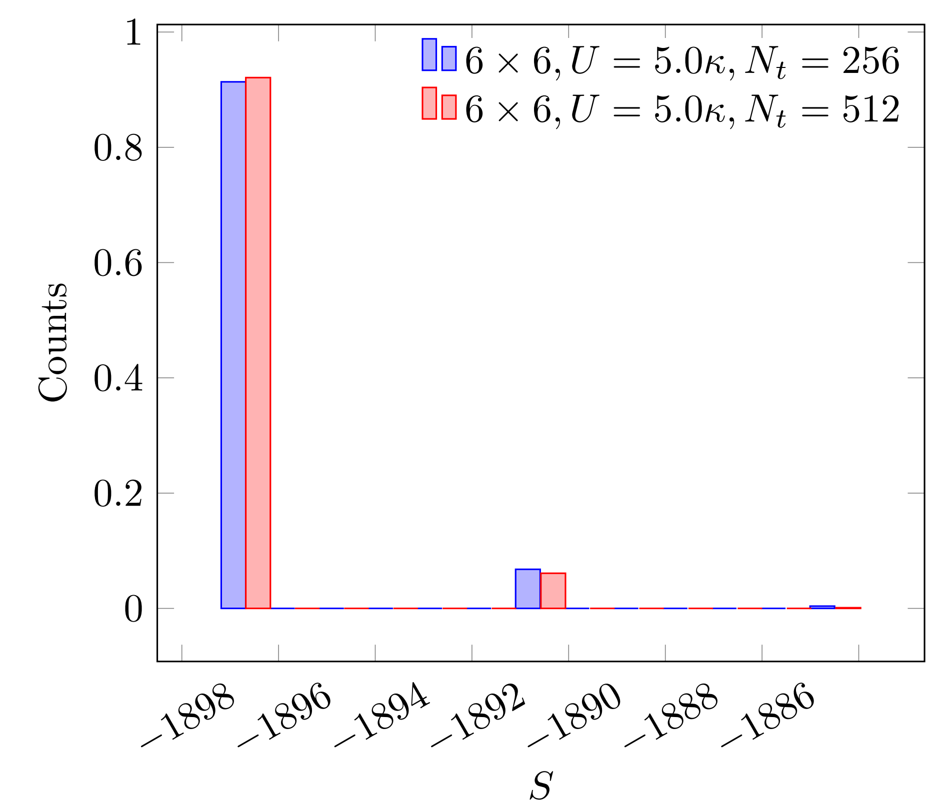
Further perspectives: other models, complex instantons at finite chemical potential

Backup slide: numerical check of the validity of the instanton gas model

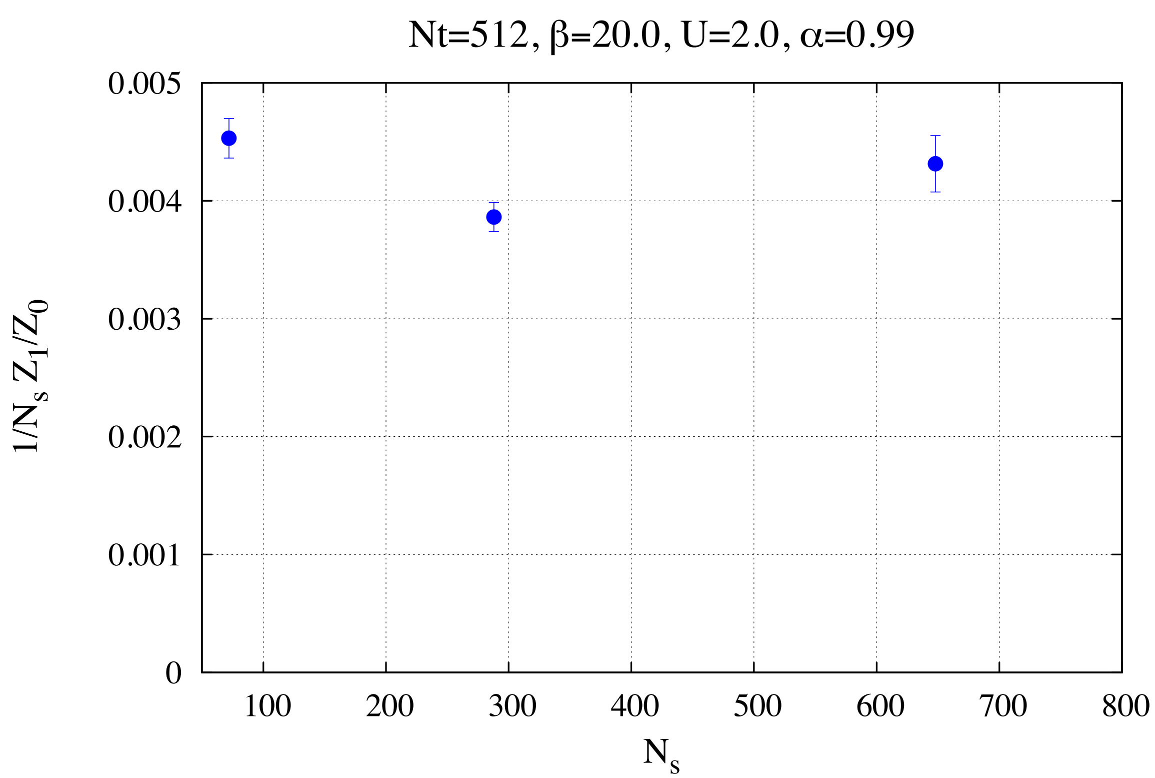


Z_0 Vacuum Z_1 1 instanton Z_2 2 instantons

Dependence on the step in Euclidean time:



Dependence on the system size:



Dependence on the inverse temperature: