The sign problem and the Lefschetz thimbles in two dimensional Hubbard model

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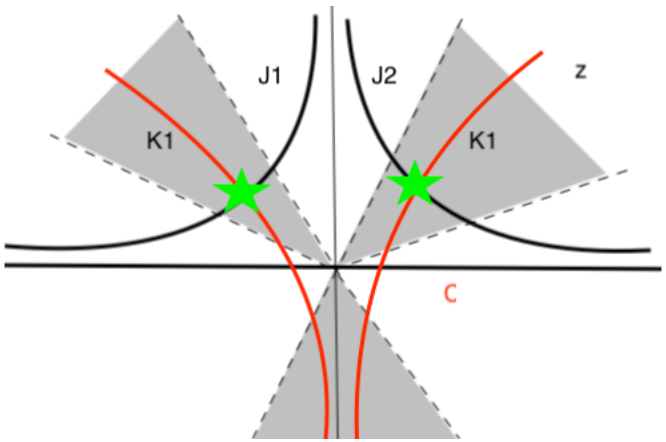
Lefschetz thimbles

Lefschetz-Morse theory: specific construction of suitable integration contour

Thimble: $\mathcal{J}_\sigma : \dfrac{dz(t)}{dt} = -\dfrac{\delta \bar{S}(z)}{\delta \bar{z}}$

Anti-thimble: $\mathcal{K}_\sigma : \dfrac{dz(t)}{dt} = +\dfrac{\delta \bar{S}(z)}{\delta \bar{z}}$



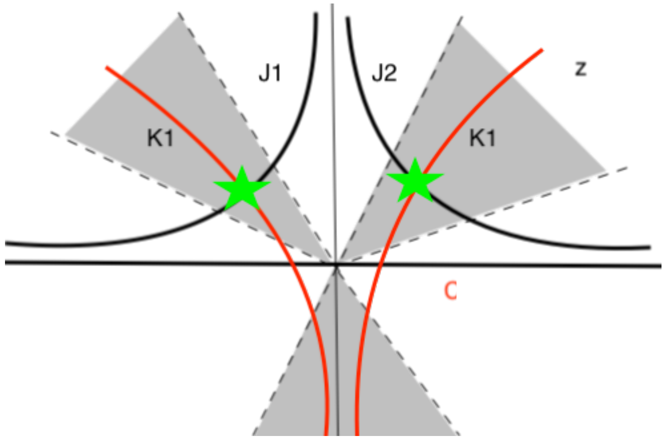
Cauchy theorem: $J_1 + J_2 + C = 0$

$$\mathcal{Z} = \sum_\sigma n_\sigma \mathcal{Z}_\sigma \qquad \mathcal{Z}_\sigma = \int_{\mathcal{J}_\sigma} \mathcal{D}z\, e^{-S(z)} \qquad n_\sigma = \langle \mathcal{K}_\sigma, C \rangle$$

Lefschetz thimbles: sign problem

Thimble: $$\mathcal{J}_\sigma : \frac{dz(t)}{dt} = -\frac{\delta \bar{S}(z)}{\delta \bar{z}}$$

Holomorphic flow



Hamiltonian flow for imaginary part of action:

$$\mathrm{Im} S(J_\sigma) = \mathrm{const}$$

$$\mathcal{Z} = \sum_\sigma n_\sigma \, e^{-i\,\mathrm{Im} S(z_\sigma)} \int_{\mathcal{Z}_\sigma} \mathcal{D}z \, e^{-S(z)}$$

Issues:

- **Numbers n_σ can have both signs: residual sign problem in the sum over thimbles**
- **Thimble is non-trivial manifold: residual sign problem in the thimble integral due to Jacobian**
- **Knowledge of all saddle points and numbers n_σ is needed.**

Lefschetz thimbles: sign problem

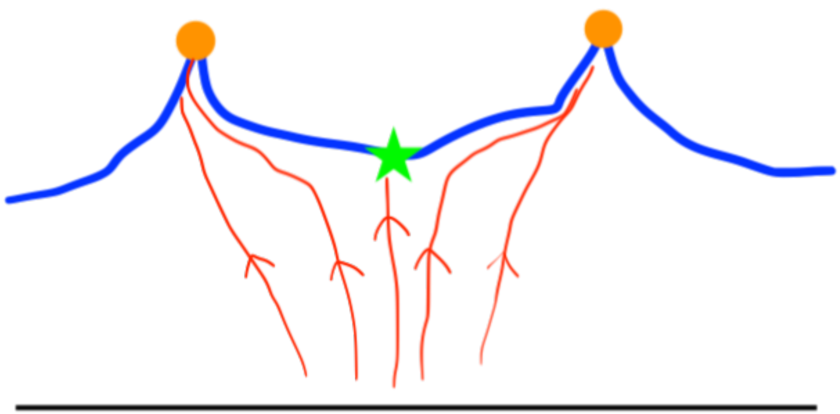
Ideas to avoid these problems:

- **Map integration contour into complex space via holomorphic flow: Cauchy theorem is guaranteed, no need to know saddle points and intersection numbers**

$$\mathcal{J}_\sigma : \frac{dz(t)}{dt} = -\frac{\delta \bar{S}(z)}{\delta \bar{z}}$$

Holomorphic flow

Invertible change of integration variables



- **Find any contour satisfying ImS = const and Cauchy theorem**

Remaining issues:

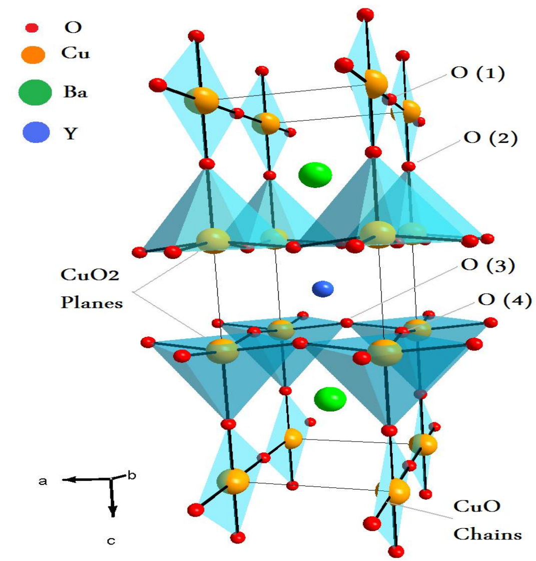
- **This work: Numbers n_σ can have both signs: residual sign problem in the sum over thimbles**
- **Avoided: Knowledge of all saddle points and numbers n_σ is needed.**
- **Thimble is non-trivial manifold: residual sign problem in the thimble integral due to Jacobian**

Two dimensional Hubbard model

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

- **Strongly correlated electrons in two dimensions**
- **Often considered in the context of high-Tc superconductivity**
- **Technical developments can be transferred to gauge theory with fermions**

Based on ArXiv:1712.02188
M. Ulybyshev, S.V.



Cuprate high-Tc superconductor

Fig. taken from Wikipedia

Four-fermion interaction term

1) Hubbard-Stratonovich transformation:

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

OR

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

2) Discrete auxiliary variables:

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

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

Four-fermion interaction term

One can represent Hubbard-Stratonovich transformation in more general way:

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

S.R. White, R.L. Sugar, and R.T. Scalettar, Phys. Rev. B 38:11665, 1988.

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

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

$$M_{h.} = I + \prod_{t=1}^{N_t} \left(e^{-\delta(h-\mu)} \mathrm{diag}\left(e^{-i\phi_{x,t} + \chi_{x,t}}\right)\right)$$

$e^{i\sum_x \phi_x \hat{n}_x}$ $\qquad$ α $\qquad$ $e^{\sum_x \chi_x \hat{n}_x}$

1 $\qquad$ 0

Sign problem

$$e^{i\sum_x \phi_x \hat{n}_x} \qquad \alpha \qquad e^{\sum_x \chi_x \hat{n}_x}$$

1 $\longleftrightarrow$ 0

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

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

$$M_{el.} = I + \prod_{t=1}^{N_t}\left(e^{-\delta(h+\mu)}\mathrm{diag}\left(e^{\chi_{x,t}}\right)\right)$$

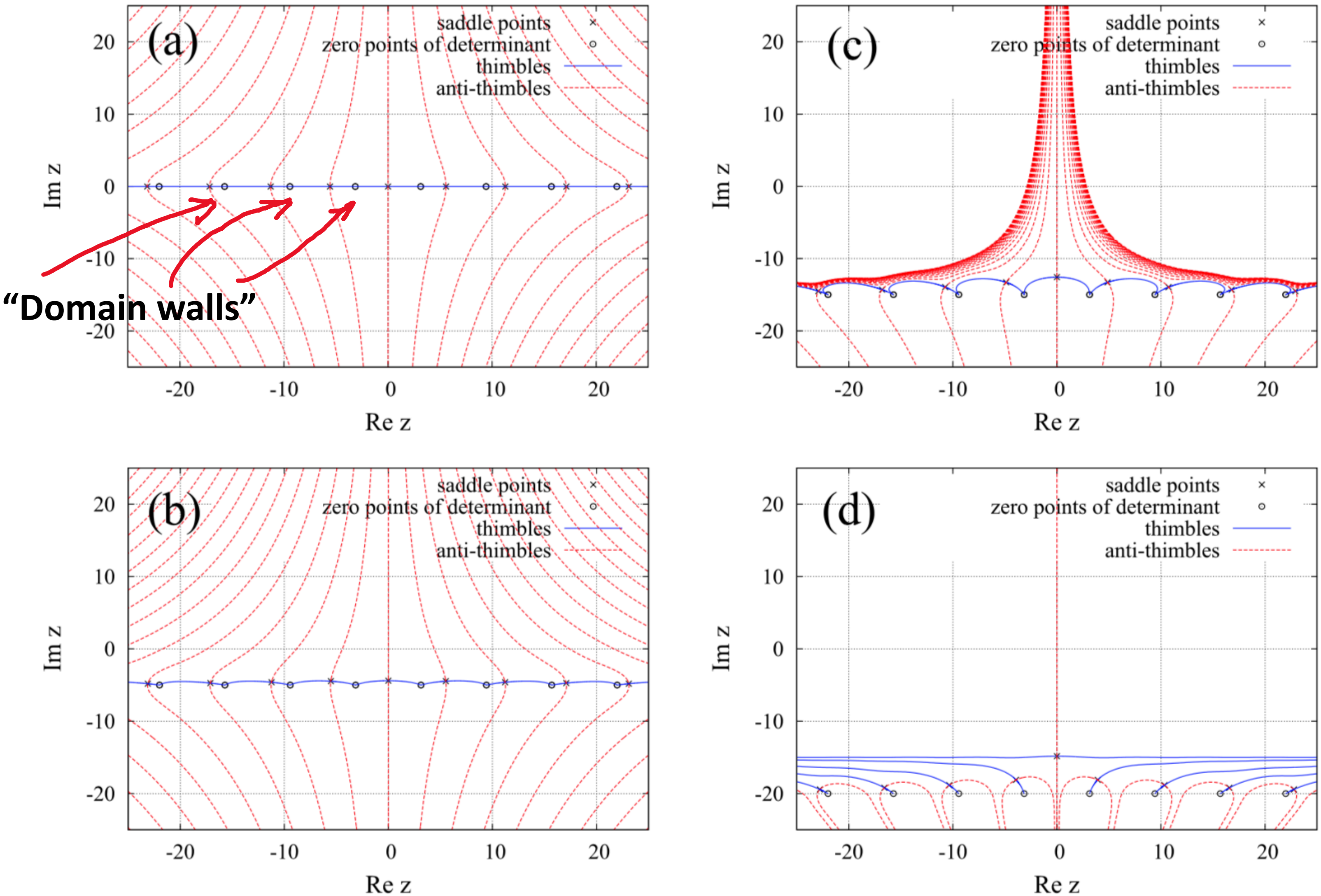
$$M_{h.} = I + \prod_{t=1}^{N_t}\left(e^{-\delta(h-\mu)}\mathrm{diag}\left(e^{\chi_{x,t}}\right)\right)$$

$$\mu = 0: \quad M_{el.} = M_{h.}^{\dagger} \qquad\qquad M_{el.} = M_{h.}$$

$$\mu \neq 0: \quad \det(M_{el.}M_{h.}) \in \mathbb{C} \qquad\qquad \det(M_{el.}M_{h.}) \in \mathbb{R}$$

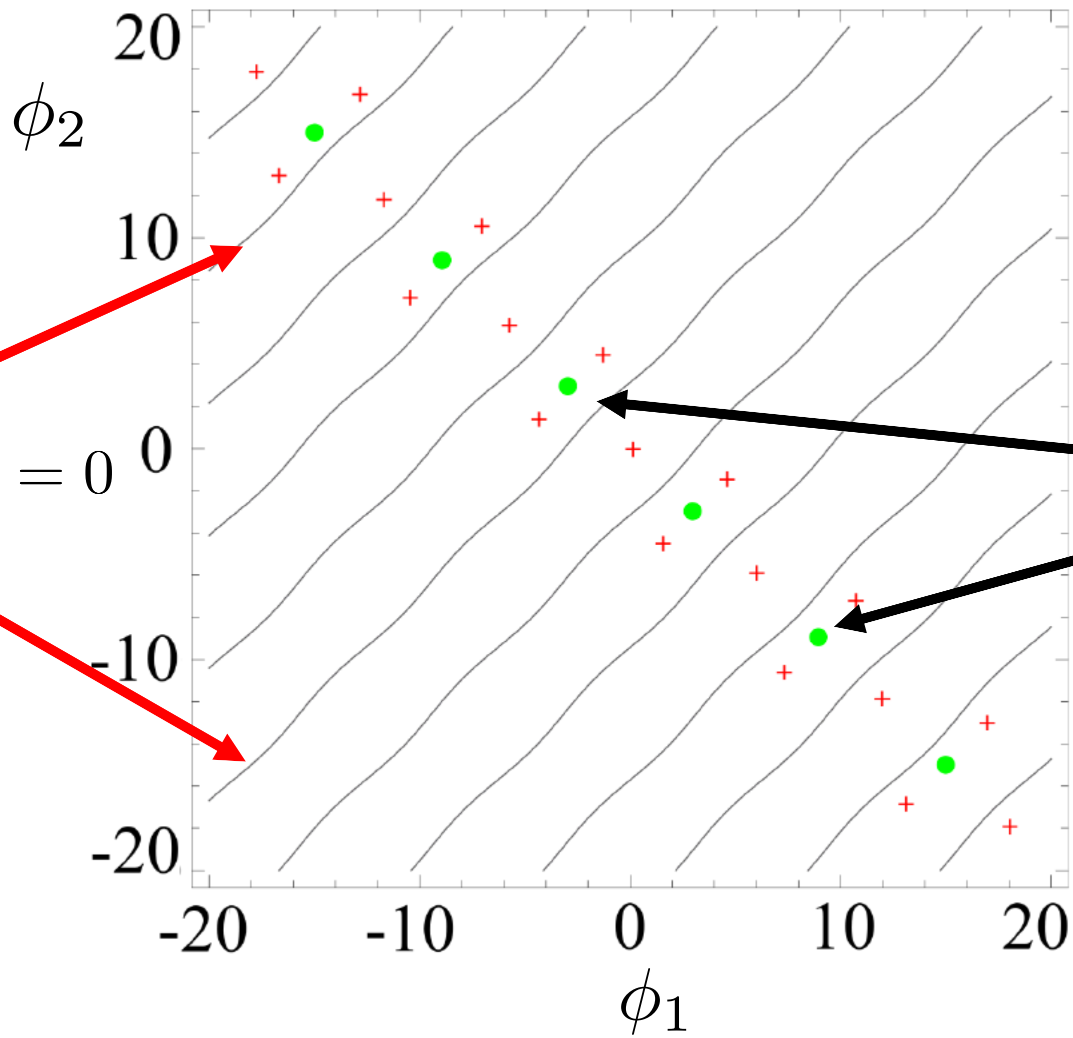
Non-semipositive definite

Multimodal problem: one-site model $\alpha = 1$



”Domain walls”: $S_{ferm} = \mathrm{Tr}\ln\left[M_{el.}M_{h.}\right]$ $\boxed{\det(M_{el.}M_{h.}) = 0}$

Multimodal problem: two-site model $\alpha = 1$



$\det(M_{el.} M_{h.}) = 0$

Relevant $n_\sigma \neq 0$

saddle points

$$\frac{\partial S(\chi)}{\partial \chi} = 0$$

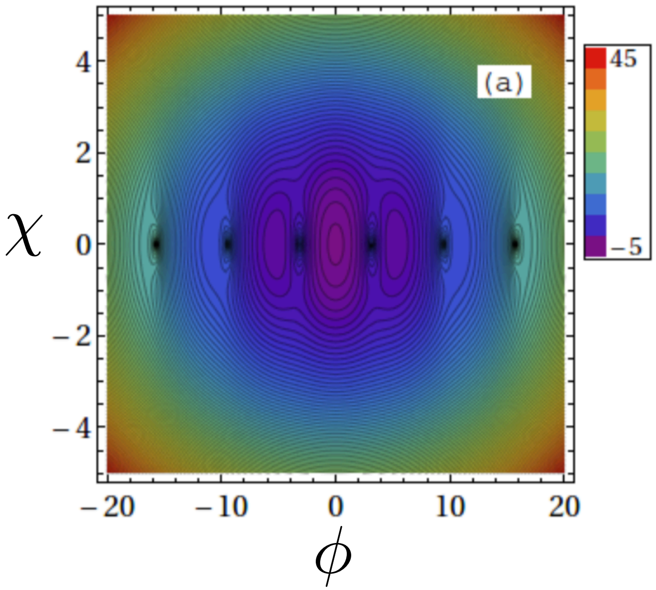
$\mu = 0$

Multiple integration "domains"

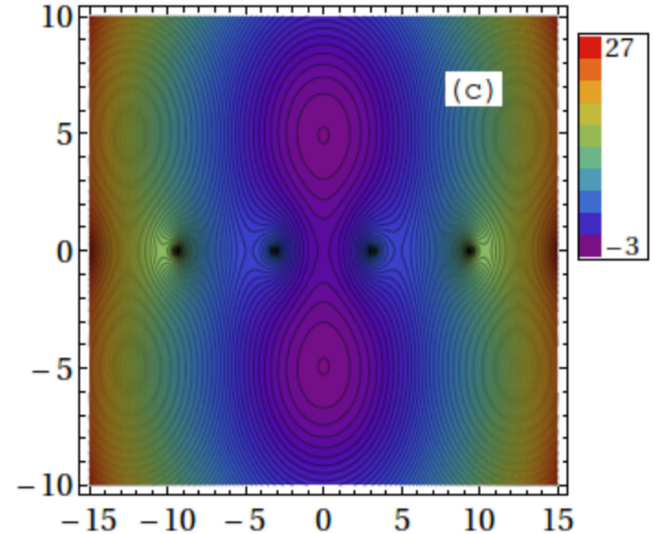
One-site model: general α

Contour plots of ReS

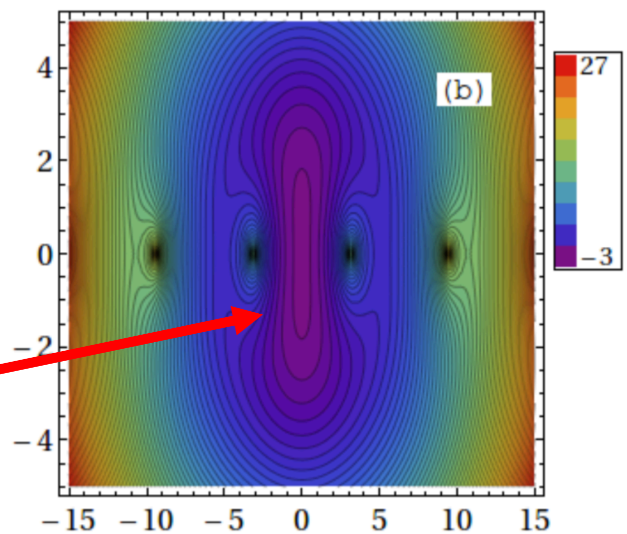
a = 0.95



a = 0.5



a = 0.8



Single thimble?

$$\mu = 0$$

Larger volumes, Monte-Carlo simulations

Taming the sign problem of the finite density Hubbard model via Lefschetz thimbles

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We study the sign problem in the Hubbard model on the hexagonal lattice away from half-filling using the Lefschetz thimbles method. We identify the saddle points, reduce their amount, and perform quantum Monte Carlo (QMC) simulations using the holomorphic gradient flow to deform the integration contour in complex space. Finally, the results are compared against exact diagonalization (ED). We show that the sign problem can be substantially weakened, even in the regime with low temperature and large chemical potential, where standard QMC techniques exhibit an exponential decay of the average sign.

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Keywords: Hubbard model, sign problem, Lefschetz thimbles

M. Ulybyshev et al. ArXiv: 1906.02726

- Hexagonal lattice 2 x 2 (Ns = 8), Nt = 256
- HMC with Gradient flow
- Schur complement solver for fermion force
- Low T, large μ regime
- Observables match exact diagonalization

$$\alpha = 0.8$$

Single thimble regime!

$${N_s}^4 {N_t}^2$$

Computational cost

Conclusions

- **We find representation of the two dimensional Hubburd model favorable for Monte-Carlo simulations on complex manifolds**
- **Proof of concept: HMC by M. Ulybyshev et. al.**
- **Open questions: gauge theory with fermions?**