Lefschetz Thimbles in (1+1)d QED

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Introduction

- Approach to deal with the sign problem
- Interested in expectation values of observables:

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

- The partition function in lattice qcd looks like:

$$Z = \int \left(\prod_{x,\nu} dU_\nu(x) \right) det[M(U_\nu(x), \mu_B)] e^{-S_G(U_\nu(x))}$$

with: Haar-measure $dU_\nu(x)$, fermionmatrix M, link variable $U \in SU(3)$, baryon chemical potential μ_B, gauge action S_G

- if μ_B is complex, the fermion determinant is not positive definite; cannot be interpreted as a probability density
- no Markov Chain Monte Carlo methods possible

Lefschetz Thimbles

- Lefschetz Thimbles are real manifolds embedded in a complex space (Solomon Lefschetz ca. 1930s)
- Pham:

$$\int_{\mathbb{R}^n} e^{-i\theta(x_1,\ldots,x_n)} f(x_1,\ldots,x_n) dx_1 \ldots dx_n$$
$$= \sum_{\sigma} n_\sigma \int_{J_\sigma} e^{-i\theta(z_1,\ldots,z_n)} f(z_1,\ldots,z_n) dz_1 \ldots dz_n$$

with: Lefschetz Thimbles J_σ, intersection numbers $n_\sigma \in \mathbb{Z}$, a Morse function θ

Lefschetz Thimbles

- Morse function: smooth function g with only nondegenerate critical points p, i.e. $\nabla g(p) = 0$ and $Hess(g(p)) = \left(\frac{\partial^2 g}{\partial x_i \partial x_j}\right)_{ij}$ is regular
- $S_I = const$:

$$\langle \mathcal{O} \rangle = \frac{\sum_\sigma n_\sigma e^{-S_I} \int_{J_\sigma} e^{-S_R(z_1,\ldots,z_n)} \mathcal{O} dz_1 \ldots dz_n}{\sum_\sigma n_\sigma e^{-S_I} \int_{J_\sigma} e^{-S_R(z_1,\ldots,z_n)} dz_1 \ldots dz_n}$$

- Why? Thimble transformation yields an integral similar to a normal distribution, easy to integrate, positive definite, can be interpreted as probability distribution

Lefschetz Thimbles

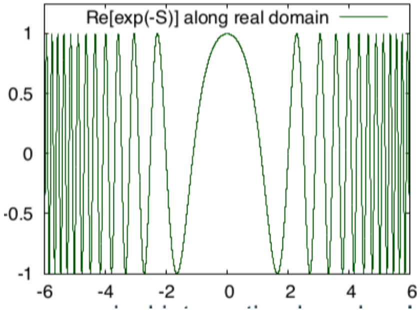
- Problem: how to find thimbles and intersection numbers
- Comprehensive paper by E. Witten
- Thimbles are attached to the critical points of the morse function
- At the critical point, the action is minimal
- Thimble through equation of steepest ascent:

$$\frac{\omega_J}{d\tau} = \frac{\partial \overline{S}}{\partial \overline{\omega_J}}$$

Example: Airy funtion

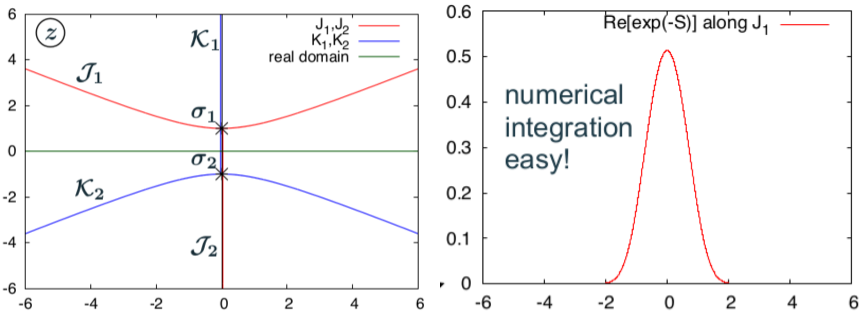
- Airy function:

  $$\mathrm{Ai}(x) = \int_0^\infty \cos(\tfrac{t^3}{3} + xt)dt = e^{\mathrm{Im}((\frac{t^3}{3}+xt))} \int_{-\infty}^{\infty} e^{\mathrm{Re}((\frac{t^3}{3}+xt))} dt$$



Highly oscillating integrand, not positive definite *[C. Schmidt]*

Example: Airy funtion



left: original integration domain and Thimble structure, Anti-Thimbles also connected to the critical points *[C. Schmidt]*
right: integrand along the Thimble, resembling a normal distribution *[C. Schmidt]*

Lefschetz Thimbles

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- easy to compute intersection number in the case of an Airy-function
- in general not easy or even clear, how to compute the intersection numbers
- if possible: manifolds near Lefschetz Thimbles with a significantly reduced sign problem, e.g. contraction algorithm *[Alexandru et. al.]*, tangential space *[F. Ziesché]*

Lefschetz Thimbles of the local action

- Idea:

  Path optimization with Lefschetz Thimbles *[priv. comm. C. Schmidt]*
- find the critical configuration structure
- look at one single link as if it was isolated
- use the local action, which is generated by this link, to calculate the new integration path

Lefschetz Thimbles of the local action

- Action: $S = -\log\det M$
- the fermionmatrix can be decomposed into: $M = A_{x,\nu} + u_{x,\nu} v_{x,\nu}^T$,

with: $$u_j = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ -U_{x,\nu}^{-1} \\ 0 \\ \vdots \\ 0 \end{pmatrix},\ v_j = \begin{pmatrix} 0 & \dots & 0 & 1 & U_{x,\nu} & 0 & \dots & 0 \end{pmatrix}$$

- Now consider a change in the action, generated by updating one link (local action)

Lefschetz Thimbles of the local action

$$\begin{aligned}\Delta S &= S_{x,\nu}(U') - S_{x,\nu}(U)\\ &= -\ln\det(A_{x,\nu} + u'_{x,\nu} v'^{T}_{x,\nu}) + \ln\det(A_{x,\nu} + u_{x,\nu} v^{T}_{x,\nu})\\ &= -\ln[(1 + v'^{T}_{x,\nu} A^{-1}_{x,\nu} u'_{x,\nu}) \det(A_{x,\nu})] + [\ln(1 + v^{T}_{x,\nu} A^{-1}_{x,\nu} u_{x,\nu}) \det(A_{x,\nu})]\\ &= -\ln(1 + v'^{T}_{x,\nu} A^{-1}_{x,\nu} u'_{x,\nu}) + \ln(1 + v^{T}_{x,\nu} A^{-1}_{x,\nu} u_{x,\nu})\end{aligned}$$

- u, v are sparse vectors with only two entries
- this saves a lot of computation time, because we only need to now four entries of each $A^{-1}_{x,\nu}$

Lefschetz Thimbles of the local action

- Complexification of the variables:
  $e^{i\phi} = U \to U' = R \cdot e^{i\phi}$
- domain not a unit circle any more
- assume that the modulus of the link is a function of the phase:
  $U' = U \cdot \Delta U = U \cdot |\Delta U| e^{-i\phi}$
- To find a rule, apply necessary condition for the action on the Lefschetz Thimble: $S_I = const.$
- This yields:

$$|\Delta U|(\phi) = \frac{-b \pm \sqrt{b^2 4ac}}{2a}$$

with:

$$a = \mathrm{Im}[a_{21} U_{x,\nu} e^{i\phi} / S_{loc}(U_{x,\nu})]$$
$$b = \mathrm{Im}[(1 + a_{11} - a_{22}) / S_{loc}(U_{x,\nu})]$$
$$c = \mathrm{Im}[-a_{12} U_{x,\nu}^{-1} e^{-i\phi} / S_{loc}(U_{x,\nu})]$$

- First model: compact QED_2, (1+1)d, U(1) symmetry, with staggered fermions, in the strong coupling limit
- lattice regularized partition function:

$$Z = \int_{\bigoplus^{2V} U(1)} \left(\prod_{x,\nu} dU_\nu(x) \right) det[M(U_\nu(x))]$$

with: lattice volume $V = N_\tau \cdot N_\sigma$, link variables $U_\nu(x)$, Haar-measure $dU_\nu(x)$

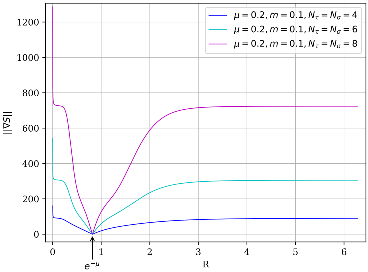
- Fermion Matrix:

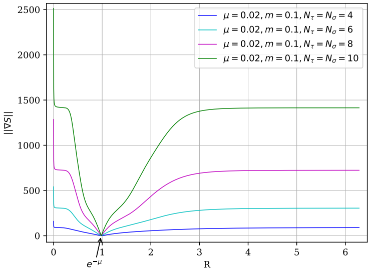
$$M_{x,y} = \frac{1}{2} \sum_{x,\nu} \eta_\nu(x) \left(e^{\mu\delta_{\nu,0}} U_\nu(x) \delta_{x+\hat{\nu},y} - e^{-\mu\delta_{\nu,0}} U_\nu^{-1}(x-\hat{\nu}) \delta_{x-\hat{\nu},y} \right) + \sum_x m\delta_{x,y}$$

with: staggered phases $\eta_\nu(x)$, chemical potential μ, fermion mass m

QED_2 1 flavour

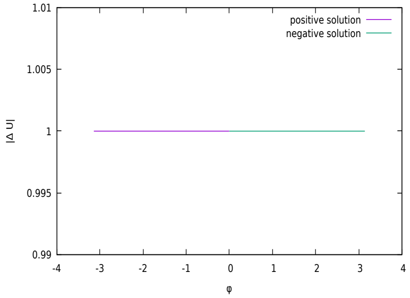
- find critical configurations
- start from unit config, check if $\nabla S = 0 \implies ||\nabla S|| = 0$
- if not, scale time links (they 'carry' the mu)





$||\nabla S||$ depending on the scaling of the time links for different lattice sizes, $\mu = 0.2$ (left), $\mu = 0.02$ (right). The graphs reach zero for $R = e^{-\mu}$

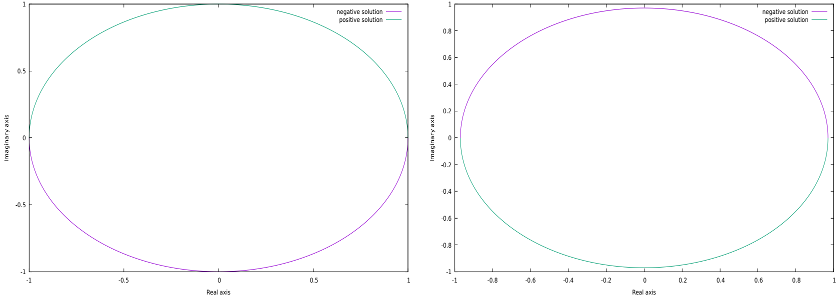
QED_2 1 flavour



$|\Delta U|(\phi)$ for a space link (left) and a time link (right)

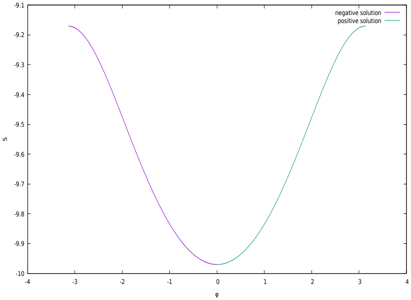
- each graph is a combination of the two solutions of the polynomial root equation
- gained: parameterization of the thimble without solving flow equation

Proceedings, Results 1 flavour



Complex plane and thimble composed of the positive and negative solution according to $|\Delta U|(\phi)$ for a space link (left) and a time link (right)

QED_2 1 flavour



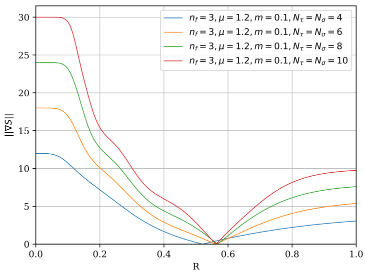
Action $S(\phi)$ on the local thimble for the space link (left)

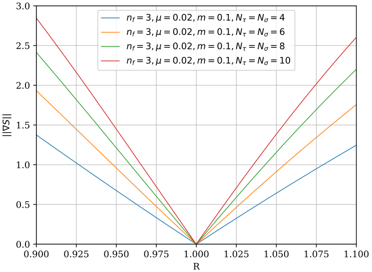
- now 3 flavours, to get a harder sign problem
- Fermionmatrix *[collaboration C. Schmidt, A. Lindemeier, P. Hegde, S. Singh]*:

$$M^{(i)}_{x,y} = \frac{1}{2}\sum_{x,\nu}\eta_\nu(x)\left(e^{q_i\mu\delta_{\nu,0}}U_\nu(x)\delta_{x+\hat{\nu},y} - e^{-q_i\mu\delta_{\nu,0}}U^{-1}_\nu(x-\hat{\nu})\delta_{x-\hat{\nu},y}\right) + \sum_x m\delta_{x,y}$$

  with: staggered phases $\eta_\nu(x)$, chemical potential μ, fermion mass m, $q_1 = -1,\ q_2 = -1,\ q_3 = +2$
- Action: $S = -\sum_i \ln\det(M^{(i)}_{x,\nu})$

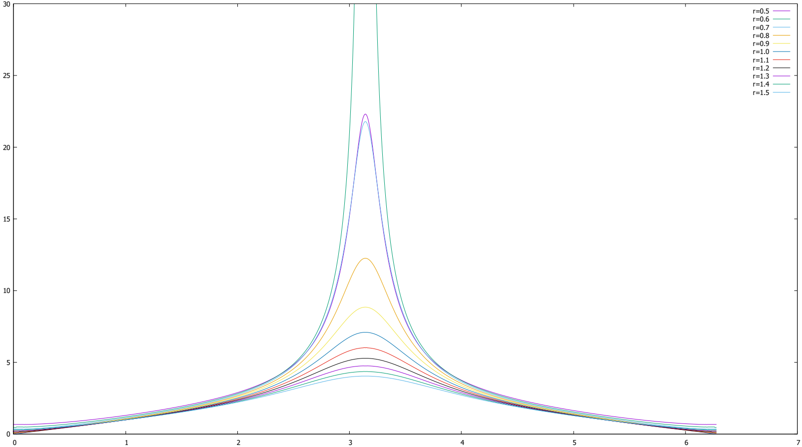
- Again: find the critical configurations and calculate thimbles from there
- To find $|\Delta U|(\phi)$, now need to find roots of 6th order polynomial
- numerical solver, still cheaper than matrix inversion





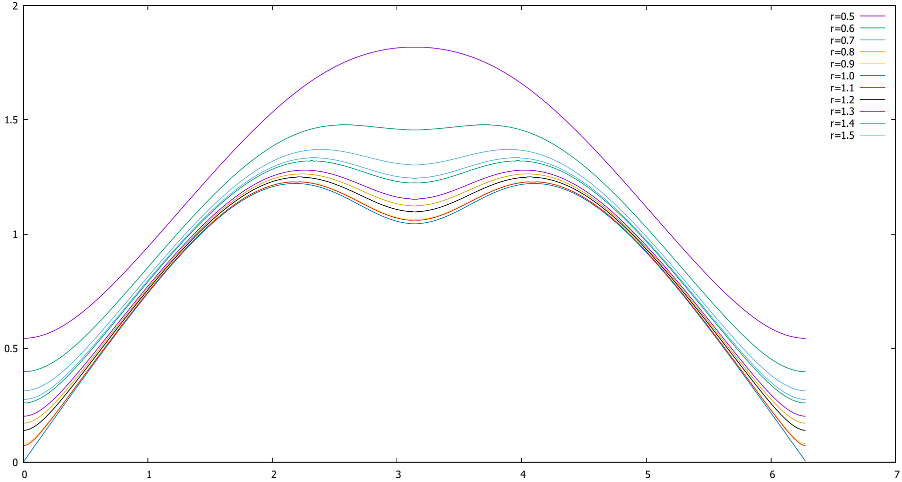
Scaling of time links for different lattice sizes for $\mu = 1.2$ (left) and $\mu = 0.02$ (right)

QED_2 3 flavours



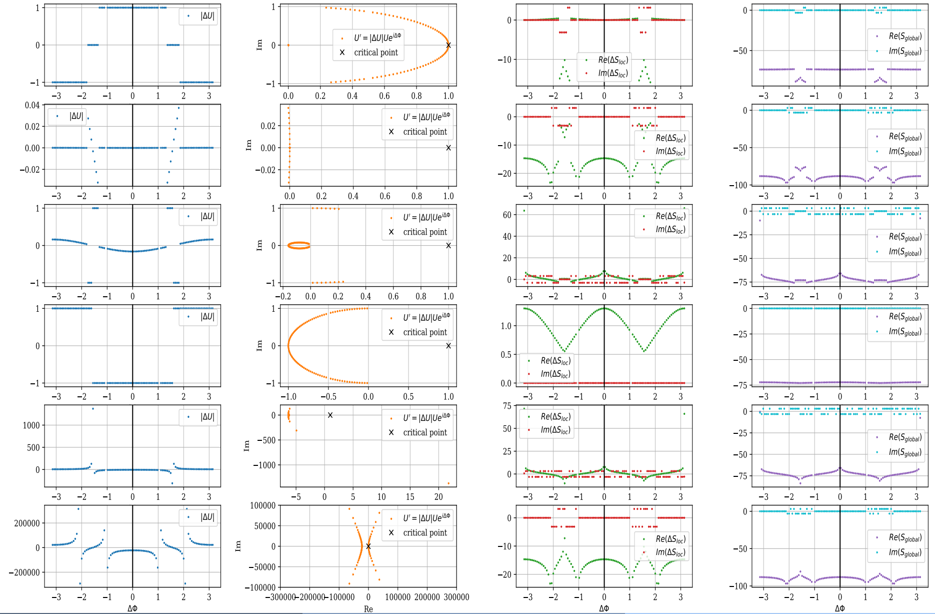
- rotate one link in hope of finding another critical point at $\phi = \pi$
- unfortunately that is not the case, only for all links rotated for $\phi = \pi$
- Plot: One space link rotated with different radii

QED_2 3 flavours



- Plot: One time link rotated with different radii

QED_2 3 flavours



Summary and outlook

- found critical points for 1 flavour/3 flavour
- complete critical point structure for QED_2 3 flavour (analytic, otherwise brute force)
- compute observables
- merge results with gauge action

Thank you for your attention!

Tensorproduct

$$\otimes : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^{n \times m},$$

$$x \otimes y = xy^T = (x_i y_j)_{ij} = \begin{pmatrix} x_1 y_1 & \dots & x_1 y_m \\ \vdots & & \vdots \\ x_n y_1 & \dots & x_n y_m \end{pmatrix}$$

Matrix determinant lemma

Let A be a regular square matrix of dimension m and u, v vectors of length m, then:

$$\det(A + uv^T) = (1 + v^T A^{-1} u) \det(A)$$

Derivation of the polynomial

$$\begin{aligned} \mathrm{Im}(\Delta S) &= 0 \\ \Longrightarrow \ \mathrm{Im}\ln[(1+v'^{T}_{x,\nu}A^{-1}_{x,\nu}u'_{x,\nu})/(1+v^{T}_{x,\nu}A^{-1}_{x,\nu}u_{x,\nu})] &= 0 \\ \Longrightarrow \ \mathrm{Arg}[(1+v'^{T}_{x,\nu}A^{-1}_{x,\nu}u'_{x,\nu})/(1+v^{T}_{x,\nu}A^{-1}_{x,\nu}u_{x,\nu})] &= 0 \ mod \ 2\pi \\ \Longrightarrow \ \mathrm{Im}[(1+v'^{T}_{x,\nu}A^{-1}_{x,\nu}u'_{x,\nu})/(1+v^{T}_{x,\nu}A^{-1}_{x,\nu}u_{x,\nu})] &= 0 \\ \Longrightarrow \ \mathrm{Im}[(1+a_{11}-a_{22}-a_{21}U'_{x,\nu}+a_{12})-a_{21}U'^{-1}_{x,\nu}/(S_{loc})] &= 0 \end{aligned}$$

Derivation of the polynomial

If we solve this for $U^{'}$ and enter the assumption for $U^{'}$ from above, we get:

$$|\Delta U| = \frac{-b \pm \sqrt{b^2 4ac}}{2a}$$

with:

$$a = \mathrm{Im}[a_{21} U_{x,\nu} e^{i\phi} / S_{loc}(U_{x,\nu})]$$
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