Integration on Lefschetz thimble:
(potentially?)
from heavy ion collisions to superconductivity

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FBK - ECT*

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Prologue

In 2011 googling for complex Langevin and analytic continuation
and I found these E. Witten's papers:

Analytic Continuation Of Chern-Simons Theory [arXiv:1001.2933],
A New Look At the Path Integral Of Quantum Mechanics [arXiv:1009.6032].

127 + 78 pages of "geometrical quantum stuff" … too much for me

Let me summarise what I have understood
(mostly from Section 3.1 of the first paper: the Airy function)

Path integral and Morse theory

Start from an oscillating integral $$Z = \int_{\mathbb{R}^n} \mathrm{d}x^n \, g(x) e^{f(x)}$$

Complexify the degrees of freedom $$Z = \int_{\mathcal{C}} \mathrm{d}z^n \, g(z) e^{f(z)}$$

If Re[f(z)] is a Morse function
(real-valued function whose critical point are not degenerate)

Deform appropriately the original integration path (Morse theory)

$$Z = \int_{\mathcal{C}} \mathrm{d}z^n \, g(z) e^{f(z)} = \sum_\sigma n_\sigma \int_{\mathcal{L}_\sigma} \mathrm{d}z^n g(z) e^{f(z)}$$

$\mathcal{L}_\sigma$ for each stationary point p_σ the L_σ (thimble) is the union of the paths of steepest descent that fall in p_σ at ∞

$\mathcal{C} = \sum_\sigma n_\sigma \mathcal{L}_\sigma$ the thimbles provide a basis of the relevant homology group, with integer coefficients

Lefschetz thimble: generalisation of the one dimensional steepest-descent curve to n-dim problems

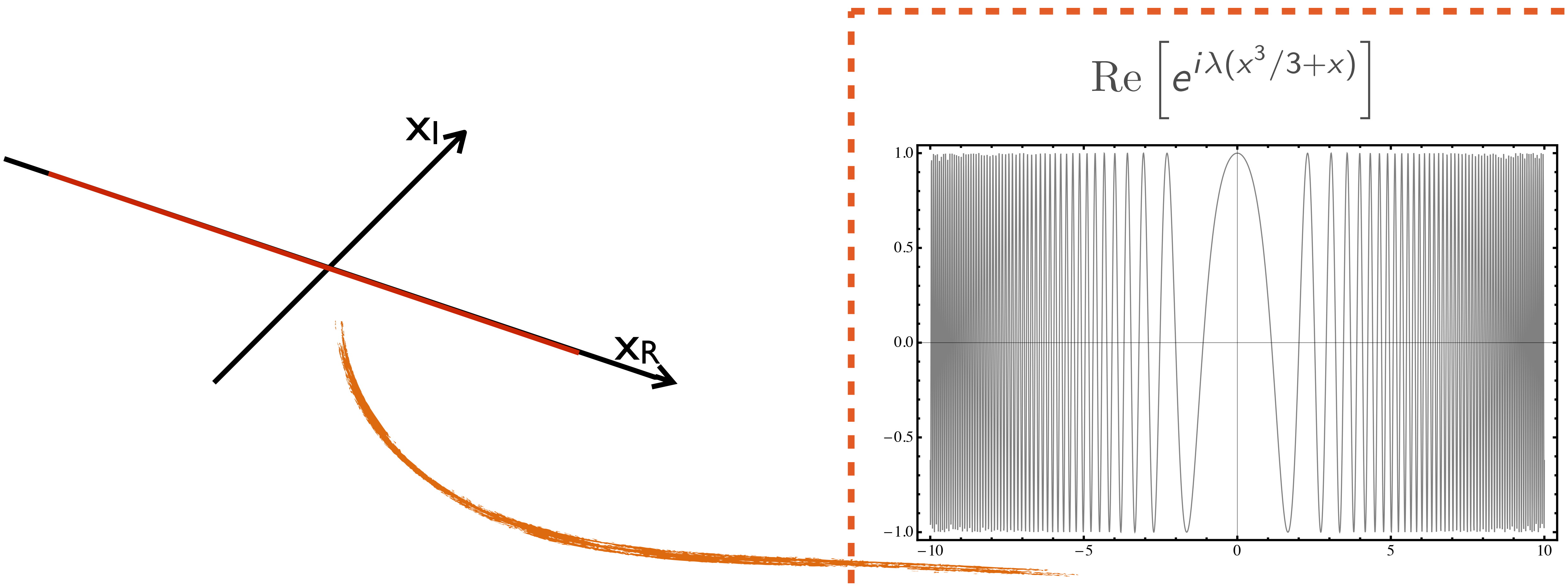
Try with the Airy function

The Airy function

$$\mathrm{Ai}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\left(\frac{t^3}{3}+x\,t\right)}\mathrm{d}t$$

Witten was looking at analytic continuation in λ

→ sign problem integrating with Monte Carlo



The Airy function

Saddle point integration

$$\mathrm{Ai}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\left(\frac{t^3}{3}+x\,t\right)}\mathrm{d}t$$

- Complexify the variable $t \to t_R + it_I = z$ ⇢ $\dfrac{1}{2\pi}\displaystyle\int_\gamma e^{i\left(\frac{z^3}{3}+xz\right)}\mathrm{d}z$

- Consider the real part of the function in the exponent

$$\mathbb{R}[\mathcal{I}] = -t_R^2 t_I + \frac{t_I^3}{3} - x t_I$$

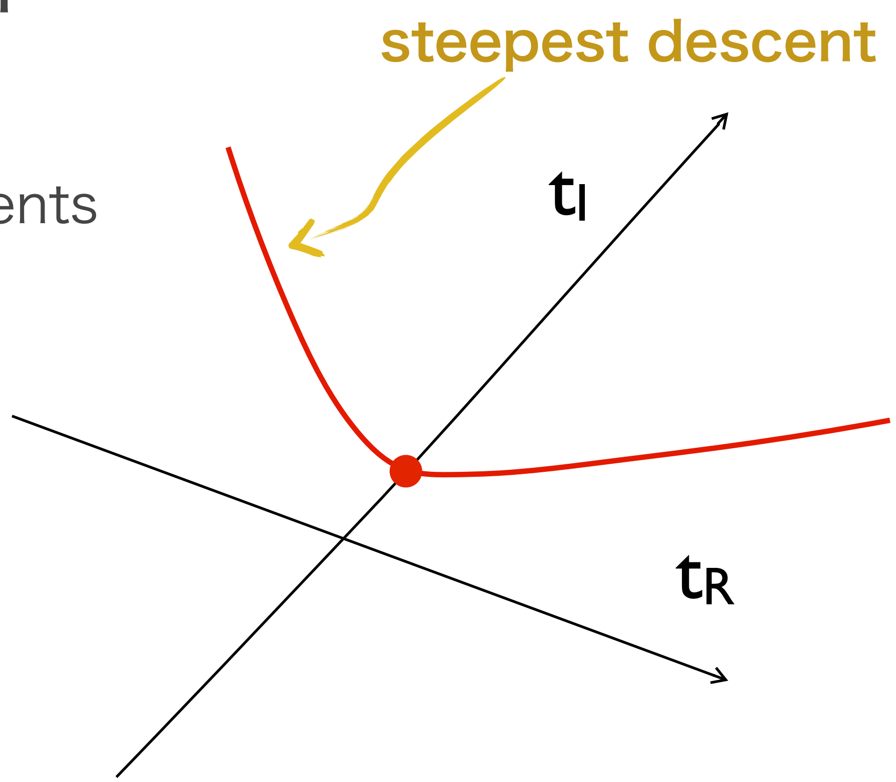
We want a new non-oscillating integration path that fastest converges to the integral

- Find the stationary points

$$\frac{\partial \mathbb{R}[\mathcal{I}(t_R, t_I)]}{\partial t_R} = 0$$
$$\frac{\partial \mathbb{R}[\mathcal{I}(t_R, t_I)]}{\partial t_I} = 0$$

- Integrate along steepest descents

$$\frac{\mathrm{d}t_R}{\mathrm{d}\tau} = -\frac{\partial \mathbb{R}[\mathcal{I}(t_R, t_I)]}{\partial t_R}$$
$$\frac{\mathrm{d}t_I}{\mathrm{d}\tau} = -\frac{\partial \mathbb{R}[\mathcal{I}(t_R, t_I)]}{\partial t_I}$$



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- Integrate along steepest descents

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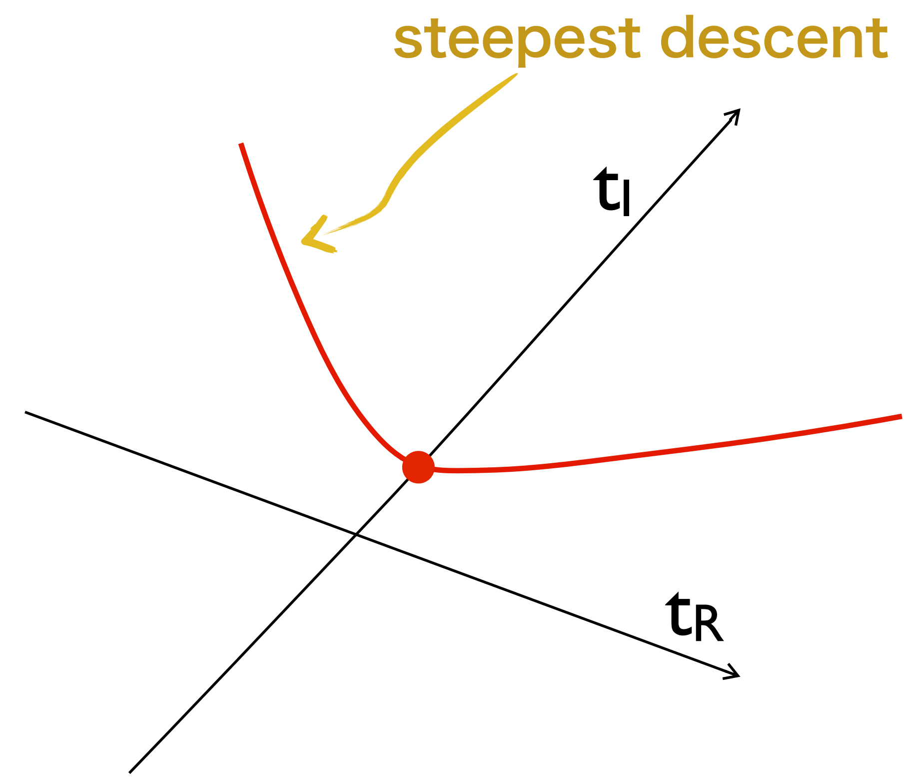
$$\frac{\mathrm{d}t_I}{\mathrm{d}\tau} = -\frac{\partial \mathbb{R}[\mathcal{I}(t_R,t_I)]}{\partial t_I}$$

- Main contribution to the integral from the region surrounding the critical points

- **Along the steepest descent $\mathbb{I}[\mathcal{I}]$ is constant**
  no sign problem from there

$$\frac{1}{2\pi}e^{i\phi}\int_{\gamma} e^{\mathbb{R}\left[i\left(\frac{z^3}{3}+xz\right)\right]}\mathrm{d}z$$

integrate on SD



The Airy function

Saddle point integration

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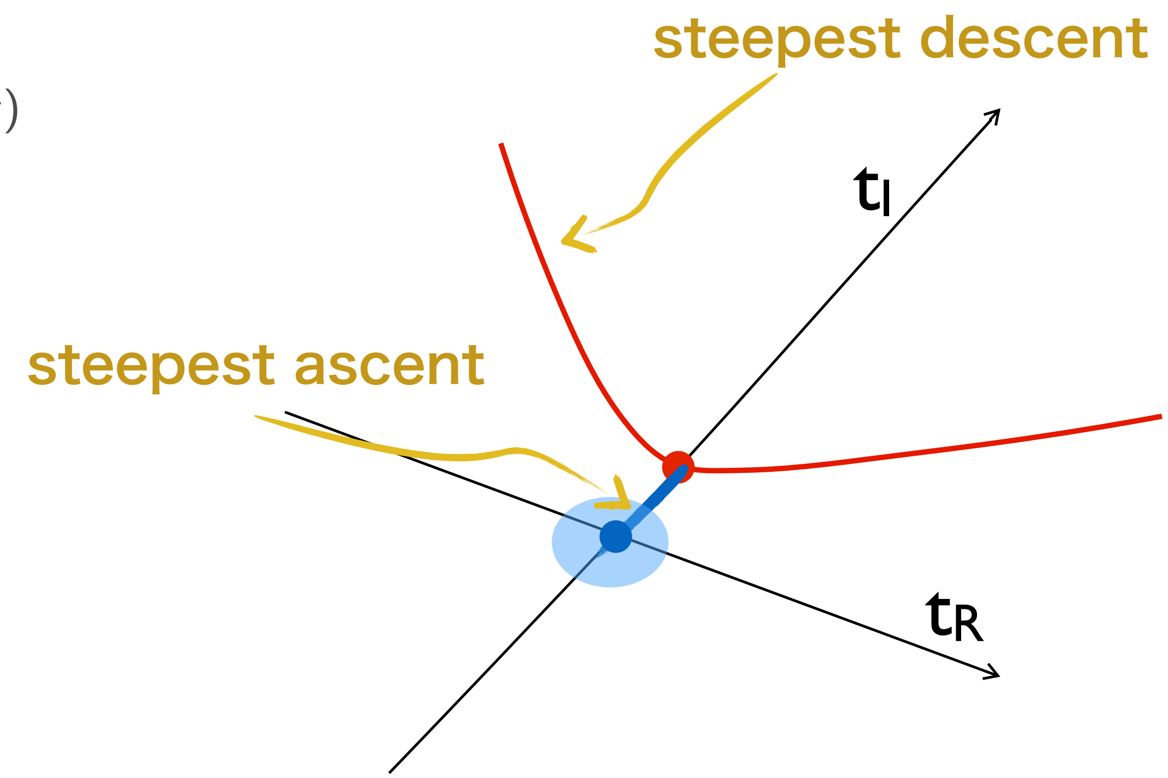
Morse theory

$$Z = \int_{\mathcal{C}} \mathrm{d}z^n\, g(z) e^{f(z)} = \sum_{\sigma} n_\sigma \int_{\mathcal{L}_\sigma} \mathrm{d}z^n g(z) e^{f(z)}$$

# of intersections between steepest ascent and original integration domain



The Airy function

Saddle point integration

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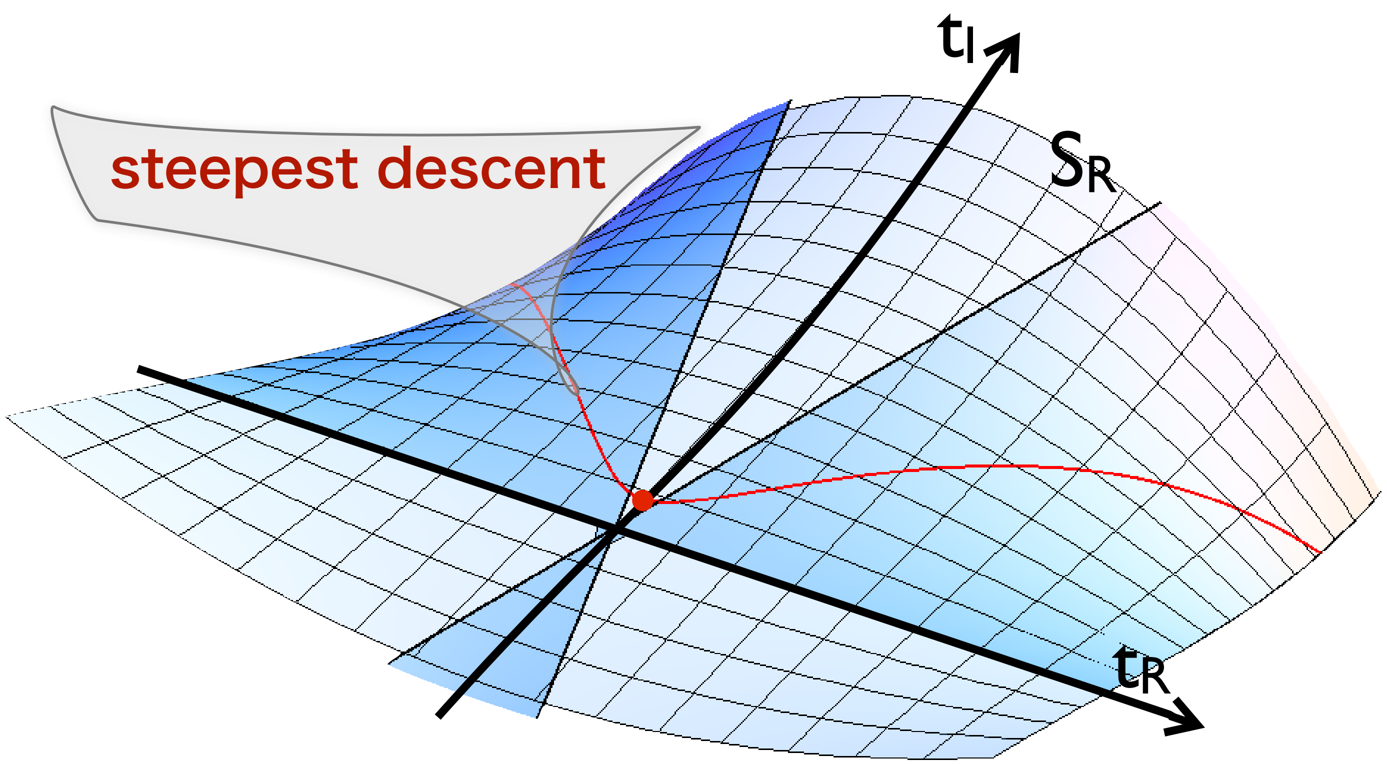
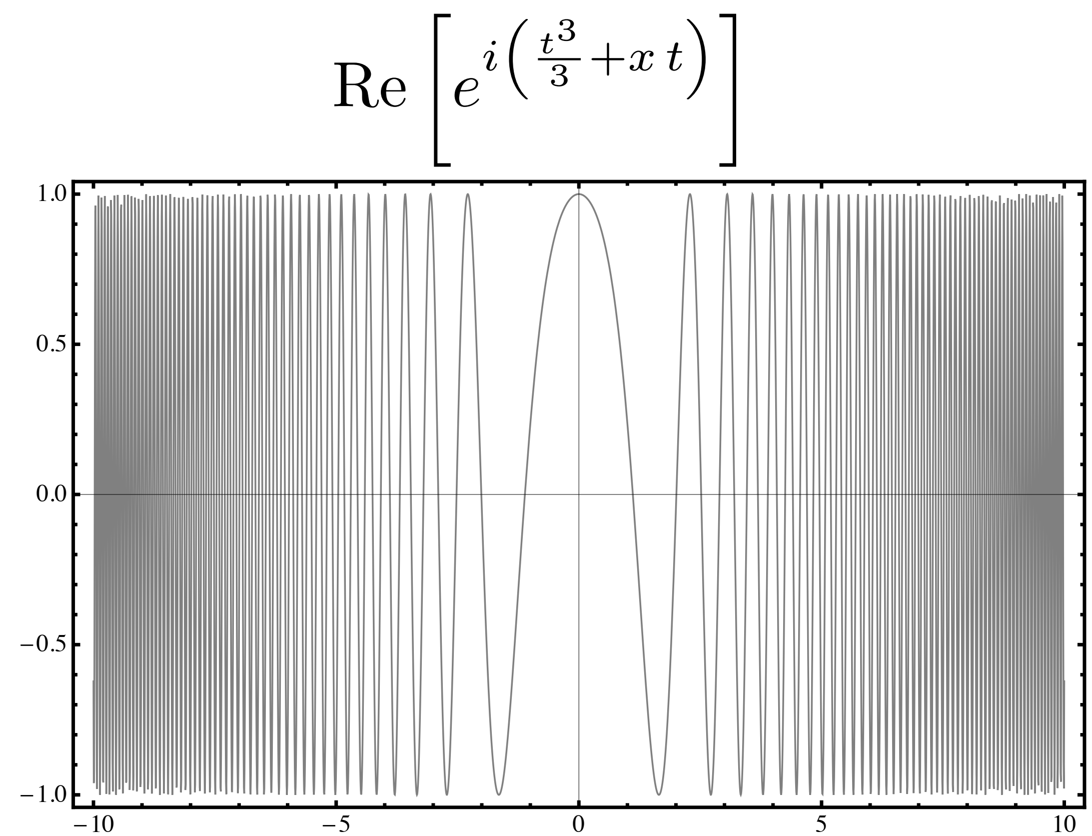
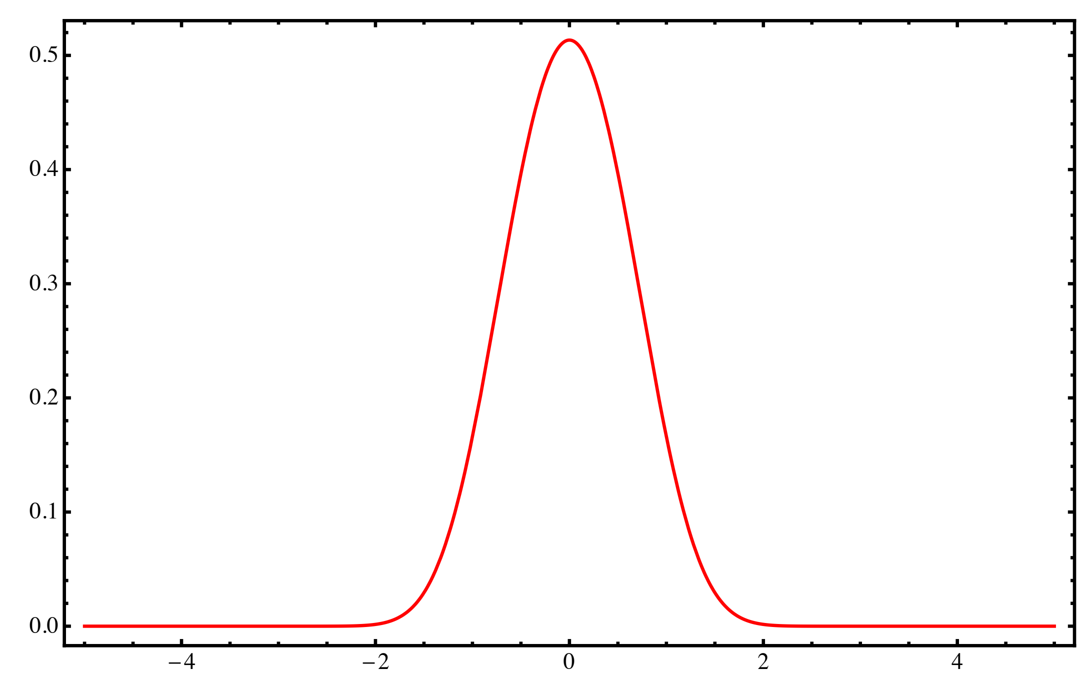




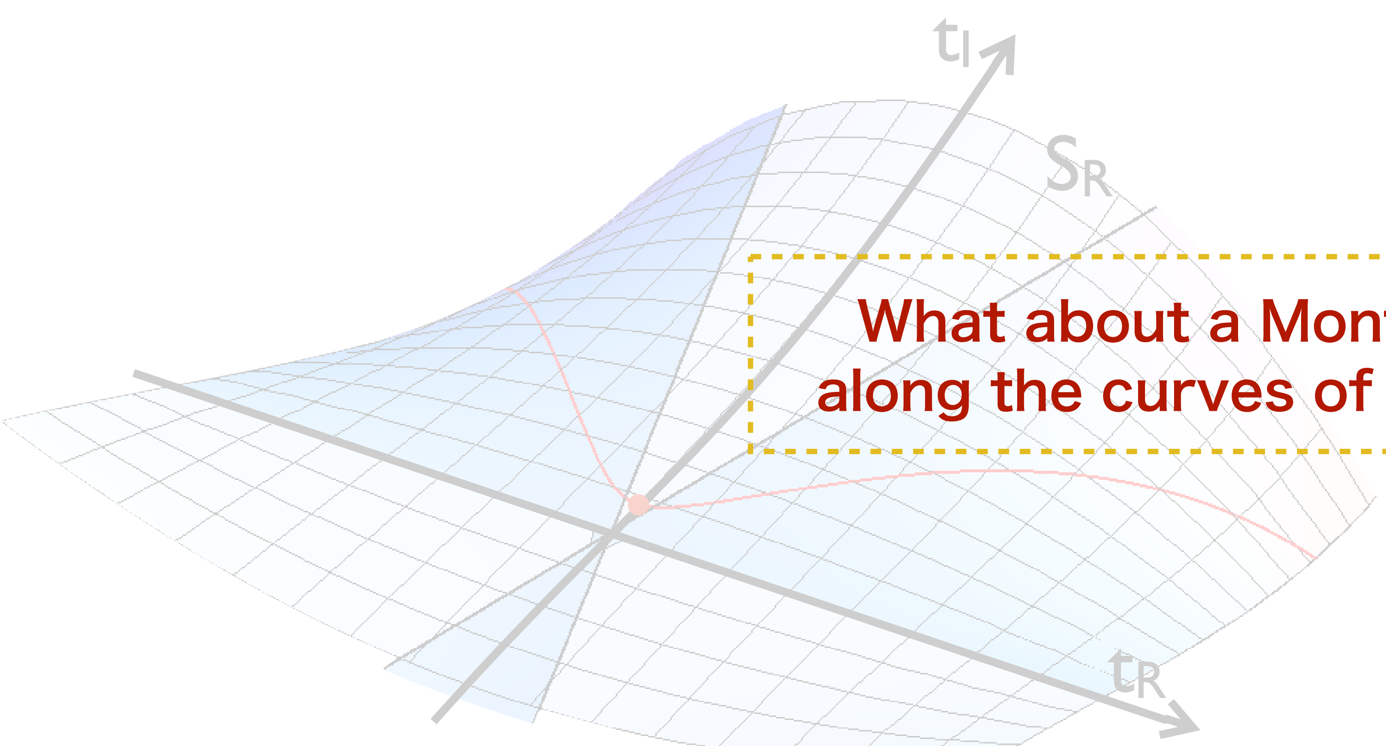


Saddle point integration

Works extremely well for low dimensional oscillating integrals.

Usually combined with an asymptotic expansion around the stationary point (sort of perturbative expansion).

The phase is stationary +
important contributions localized =
good for sign problem



What about a Monte Carlo integral along the curves of steepest descent

QFTs on Lefschetz thimble

- Can we use the thimble basis to compute the path integral for a QFT ?

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathcal{C}} \prod_x \mathrm{d}\phi_x e^{-S[\phi]} \mathcal{O}[\phi]}{\int_{\mathcal{C}} \prod_x \mathrm{d}\phi_x e^{-S[\phi]}} \longrightarrow \langle \mathcal{O} \rangle = \frac{\sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \prod_x \mathrm{d}\phi_x e^{-S[\phi]} \mathcal{O}[\phi]}{\sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \prod_x \mathrm{d}\phi_x e^{-S[\phi]}}$$

$\longrightarrow$ Lot of things to discuss …

QFTs on Lefschetz thimble

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⟶ Lot of things to discuss ...

- ☐ Integrals are of the form $\int \mathrm{d}x\, g(x) e^{-f(x)}$
  what if g(x) is an extensive quantity (e.g. the fermionic determinant)?

- ☐ **On a Lefschetz thimble the imaginary part of the action is constant** but the measure term does introduce a new **residual phase**, due to the curvature of the thimble

- ☐ We should integrate on all the thimbles. Is it feasible? Can we consider just one or a class of thimbles instead?

These are open questions
I do not have final solutions
in particular for QCD

QFTs on Lefschetz thimble

☐ Integrals are of the form $\int \mathrm{d}x\, g(x) e^{-f(x)}$

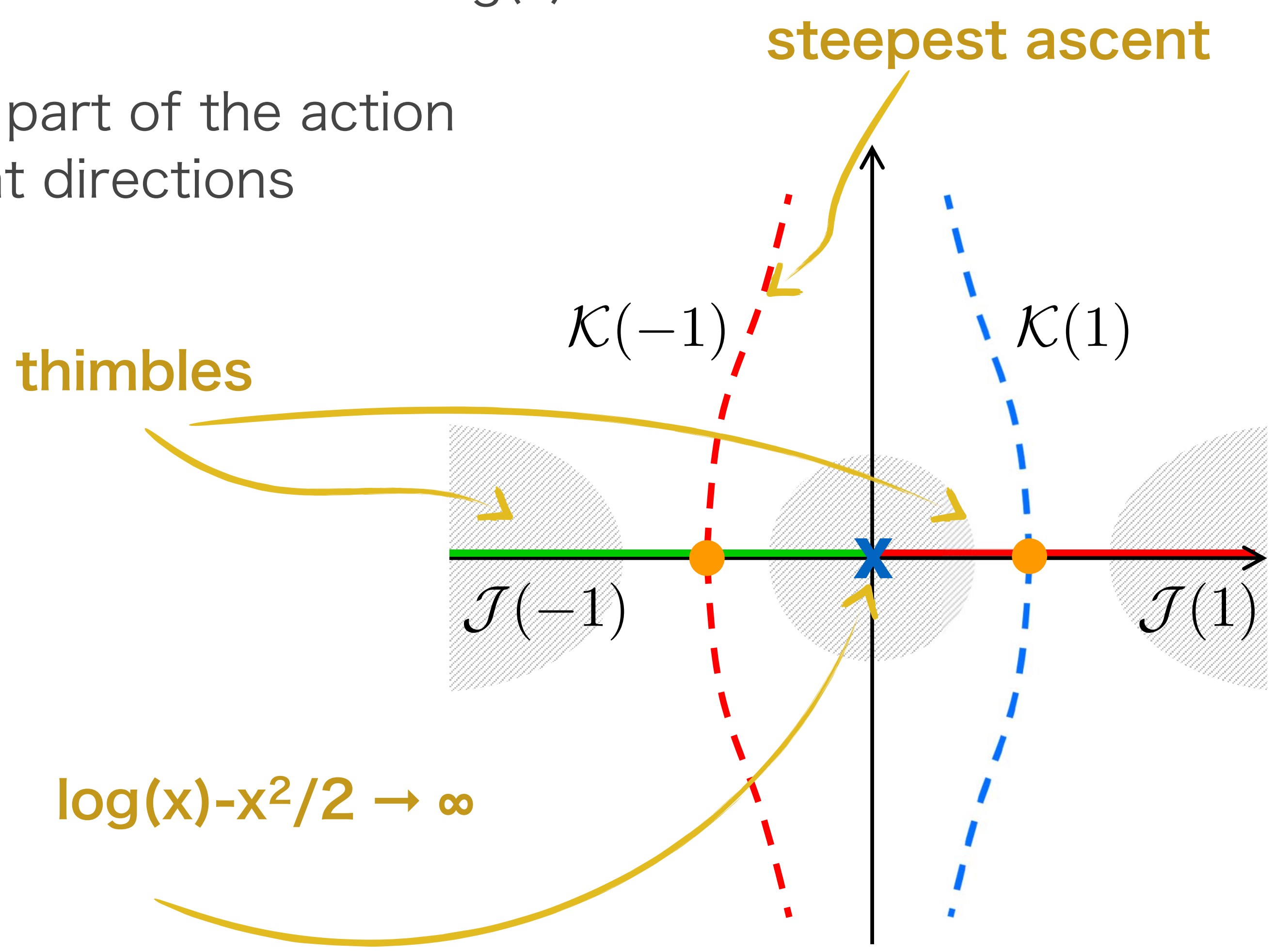
what if g(x) is an extensive quantity (e.g. the fermionic determinant)?

↘ **T. Kanazawa and Y. Tanizaki. arXiv:1412.2802**

If g(x) is holomorphic/meromorphic put log(g(x)) in the exponent
you can still define the thimble and integrate on that

The only thing is that now the thimble can ends in a zero of the g(x)
which is not at infinity of the variable domain.
If this is the case it can be that the imaginary part of the action
changes approaching that point from different directions

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, x\, e^{-x^2/2}$$



QFTs on Lefschetz thimble

- **On a Lefschetz thimble the imaginary part of the action is constant** but the measure term does introduce a new **residual phase**, due to the curvature of the thimble

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathcal{J}_0} \prod_x \mathrm{d}\phi_x e^{-S[\phi]} \mathcal{O}[\phi]}{\int_{\mathcal{J}_0} \prod_x \mathrm{d}\phi_x e^{-S[\phi]}}$$

Additional phase coming from the Jacobian of the transformation between the canonical complex basis and the tangent space to the thimble

↘ **Does it lead to a sign problem?**

Must be checked case by case

It is encouraging that:

- ↘ dΦ=1 at leading order and <dΦ>≪1 are strongly suppressed by e^{-S}
- ↘ there is strong correlation between phase and weight (precisely the lack of such correlation is the origin of the sign problem)
- ↘ In fact this residual phase is completely neglected in the saddle point method

QFTs on Lefschetz thimble

- **On a Lefschetz thimble the imaginary part of the action is constant** but the measure term does introduce a new **residual phase**, due to the curvature of the thimble

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathcal{J}_0} \prod_x \mathrm{d}\phi_x e^{-S[\phi]} \mathcal{O}[\phi]}{\int_{\mathcal{J}_0} \prod_x \mathrm{d}\phi_x e^{-S[\phi]}}$$

Additional phase coming from the Jacobian of the transformation between the canonical complex basis and the tangent space to the thimble

↘ **What to do with the residual phase**

⟶ demanding in terms of computation power but affordable

↘ **HMC:** H. Fujii et al JHEP 1310 (2013) 147

↘ **Stochastic estimators:** M.C. et al. PRD 89,114505 (2014)
Based on Langevin algorithm to stay on the thimble
scales as $\mathcal{O}(n \times N_\tau \times N_R)$
with:
- n the number of lattice sites
- N_τ steps along the gradient flow
- N_R number of stochastic sources

QFTs on Lefschetz thimble

- We should integrate on all the thimbles. Is it feasible? Can we consider just one or a class of thimbles instead?

$$\langle \mathcal{O} \rangle = \frac{\sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \prod_x \mathrm{d}\phi_x e^{-S[\phi]} \mathcal{O}[\phi]}{\sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \prod_x \mathrm{d}\phi_x e^{-S[\phi]}}$$

It is really difficult to establish if we really need to sum all the contribution from the different thimbles

Looking at one dimensional problem often you need to sum all.
But, for example, in a field theory as $\lambda\,\Phi^4$ at finite μ, the correct solution was obtained with only one thimble, so maybe one or two are sufficient for QFTs on a lattice

Must be checked case by case

QFTs on Lefschetz thimble

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Must be checked case by case

You are lucky if:

- The system has a single global minimum
- There are degenerate global minima, that are however connected by symmetries
- There are degenerate global minima, with vanishing probability of tunnelling

You are not so lucky if:

- There is a large number of stationary points that accumulate near the global minimum giving a finite contribution

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Must be checked case by case

It might also be that you are interested in the dynamics around one or a couple of known particular saddle points. In this case integrating on the thimble gives you alle the quantum correction to the classical dynamics associated with those critical points.

I'll show you later 1 and 1/2 example

How to stay on the thimble

Langevin

PRD Rapid 88, 051501 (2013)

$$\frac{\mathrm{d}\phi_i^R(\tau)}{\mathrm{d}\tau} = -\frac{\delta S^R(\phi(\tau))}{\delta\phi_i^R(\tau)} + \eta_i^R(\tau)$$

$$\frac{\mathrm{d}\phi_i^I(\tau)}{\mathrm{d}\tau} = -\frac{\delta S^R(\phi(\tau))}{\delta\phi_i^I(\tau)} + \eta_i^I(\tau)$$

$$\frac{\mathrm{d}\eta_i(\tau)}{\mathrm{d}\tau} = \sum_k \eta(\tau)_k \partial_k \partial_j S_R$$

projection of the noise on the tangent space

Metropolis

PRD Rapid 88, 051502 (2013)

$$\frac{\mathrm{d}\phi_i(r)}{\mathrm{d}r} = \frac{1}{r}\overline{\frac{\delta S}{\delta\phi_i(r)}} \dashrightarrow \phi_i(n+1) = \phi_i(n) + \delta r \overline{\frac{\delta S}{\delta\phi_i}}$$

Other methods

- **HMC:** H. Fujii et al JHEP 1310 (2013) 147
- **another one:** F. Di Renzo and G. Eruzzi Lattice2014

How to stay on the thimble

Langevin
PRD Rapid 88, 051501 (2013)

We want to compute this:

boundend from below on J_0

$$\langle \mathcal{O} \rangle = \frac{1}{Z_0} e^{-iS_I} \int_{\mathcal{J}_0} \prod_x \mathrm{d}\phi_x e^{-S_R[\phi]} \mathcal{O}[\phi]$$

constant on J_0

$$\frac{\mathrm{d}\phi}{\mathrm{d}\tau} = -\frac{\overline{\delta S}}{\delta \phi} \dashrightarrow \frac{\mathrm{d}S_R}{\mathrm{d}\tau} = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\tau}\left(S + \overline{S}\right) = -\frac{1}{2}(\nabla_x S \cdot \overline{\nabla}_x \overline{S} - \overline{\nabla}_x \overline{S} \cdot \nabla_x S) = -||\partial S||^2$$

We can use a Langevin algorithm but **how can we stay on the thimble?**

preserve J_0 by construction

$$\frac{\mathrm{d}\phi_i^R(\tau)}{\mathrm{d}\tau} = -\frac{\delta S^R(\phi(\tau))}{\delta \phi_i^R(\tau)} + \eta_i^R(\tau)$$

$$\frac{\mathrm{d}\phi_i^I(\tau)}{\mathrm{d}\tau} = -\frac{\delta S^R(\phi(\tau))}{\delta \phi_i^I(\tau)} + \eta_i^I(\tau)$$

Need to be projected on the tangent space to J_0

How to stay on the thimble

Langevin

PRD Rapid 88, 051501 (2013)

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Need to be projected on the tangent space to J_0

The tangent space at the stationary point is easy to compute (given by the hessian)

We can get tangent vectors at any point if we can transport the noise along the gradient flow so that it remains tangent to the thimble

$$\mathcal{L}_{\partial S_R}(\eta) = 0 \quad \leftrightarrow \quad [\partial S_R, \eta] = 0 \quad \leftrightarrow \quad \frac{\mathrm{d}\eta_i(\tau)}{\mathrm{d}\tau} = \sum_k \eta(\tau)_k \partial_k \partial_j S_R$$

projection of the noise on the tangent space

How to stay on the thimble

Langevin

PRD Rapid 88, 051501 (2013)

$$\langle \mathcal{O} \rangle = \frac{1}{Z_0} e^{-iS_I} \int_{\mathcal{J}_0} \prod_x \mathrm{d}\phi_x e^{-S_R[\phi]} \mathcal{O}[\phi]$$

$$\frac{\mathrm{d}\phi_i^R(\tau)}{\mathrm{d}\tau} = -\frac{\delta S^R(\phi(\tau))}{\delta \phi_i^R(\tau)} + \eta_i^R(\tau)$$

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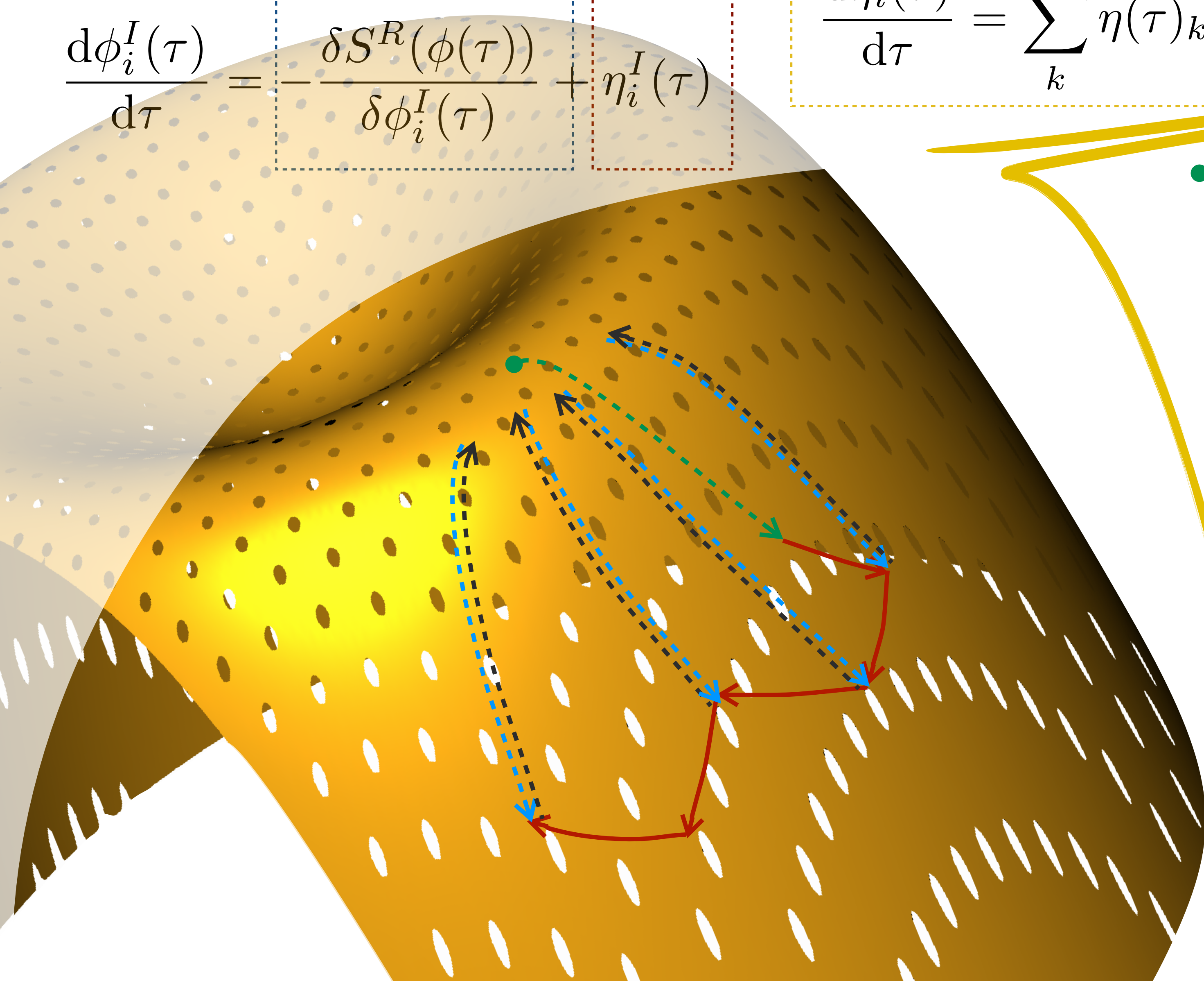


Start from the global minimum of the real part of the action, generate a noise vector projected on the thimble and follow the steepest descent

Perform a Langevin step using the noise evolved along the steepest descent and compute the observables

Go back along the steepest ascent until you are in a region where quadratic approx. is valid and then project the configuration on the thimble

Generate a new noise and go back along the steepest descent

How to stay on the thimble

Langevin on the Lefschetz thimble
vs Complex Langevin

Lefschetz Langevin

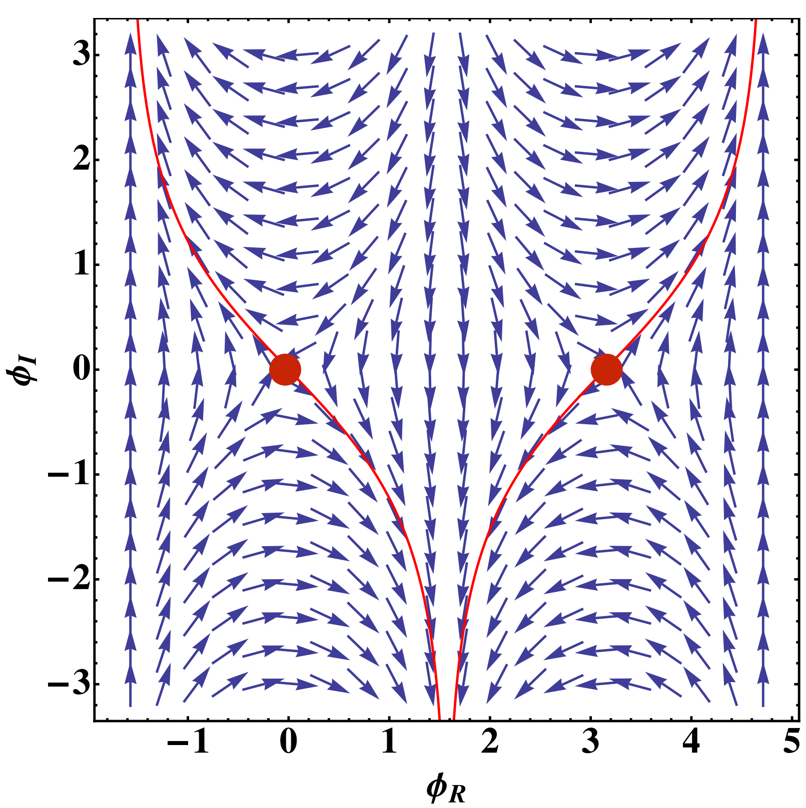
$$\frac{\mathrm{d}\phi_i^R(\tau)}{\mathrm{d}\tau} = -\frac{\delta S^R(\phi(\tau))}{\delta \phi_i^R(\tau)} + \eta_i^R(\tau)$$

$$\frac{\mathrm{d}\phi_i^I(\tau)}{\mathrm{d}\tau} = -\frac{\delta S^R(\phi(\tau))}{\delta \phi_i^I(\tau)} + \eta_i^I(\tau)$$

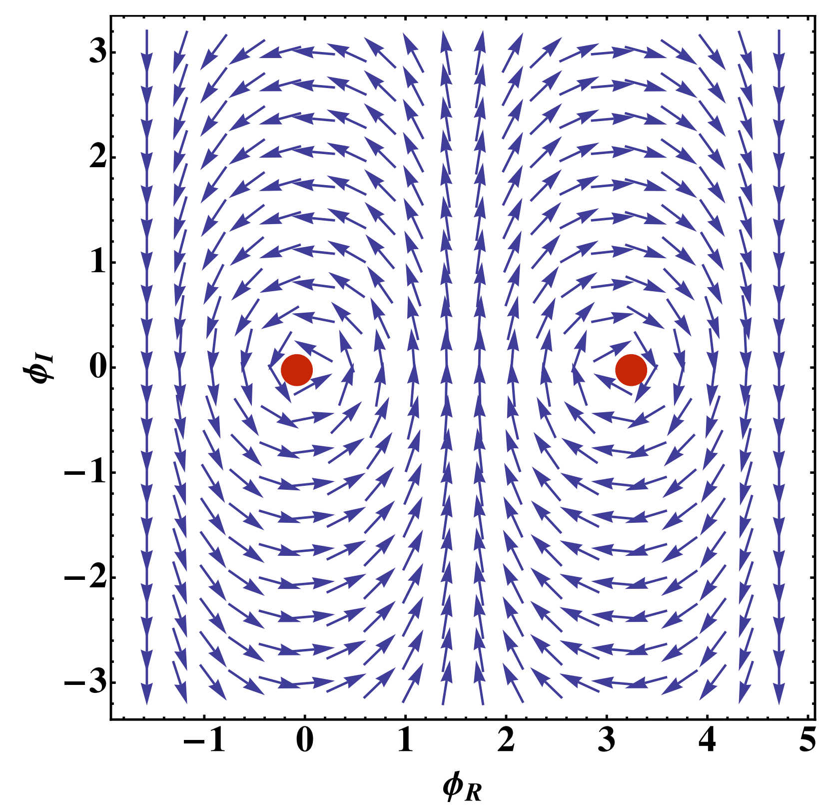
Complex Langevin

$$\frac{\mathrm{d}\phi_i^R(\tau)}{\mathrm{d}\tau} = -\frac{\delta S^R(\phi(\tau))}{\delta \phi_i^R(\tau)} + \eta_i^R(\tau)$$

$$\frac{\mathrm{d}\phi_i^I(\tau)}{\mathrm{d}\tau} = +\frac{\delta S^R(\phi(\tau))}{\delta \phi_i^I(\tau)} + \eta_i^I(\tau)$$



I think the relation between the two approaches has to be studied carefully.
See for example
G. Aarts et al. JHEP 1410 (2014) 159



How to stay on the thimble

Metropolis

PRD Rapid 88, 051502 (2013)

In the neighbourhood of a critical point →

$$S[\phi] = S[\phi_0] + S_G[\eta] + \mathcal{O}(|\eta|^3)$$

$$S_G = \frac{1}{2}\sum_k \lambda_k \eta_k^2$$

$$\phi_i = \phi_i^0 + \sum_k w_{ki}\eta_k$$

G is the flat thimble associated to the gaussian action S_G

The $\boldsymbol{\lambda}$ and **w** are solutions of

$$\boxed{H w_k = \lambda_k \bar{w}_k}$$

where **H** is the Hessian

$\boldsymbol{\eta}$ real are the direction of steepest descent of S_R and the equations of steepest descent of η for the Gaussian action can be explicitly solved in term of a new parameter $r=e^{-\tau}$

$$\rightarrow \quad \frac{\mathrm{d}\eta_k}{\mathrm{d}r} = \frac{1}{r}\frac{\partial \bar{S}_G}{\partial \eta_k} = \frac{1}{r}\lambda_k\eta_k \quad \rightarrow \quad \eta_k \propto r^{\lambda_k}$$

How to stay on the thimble

Metropolis
PRD Rapid 88, 051502 (2013)

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⇒

$$\phi_i = \phi_i^0 + \sum_k w_{ki}\eta_k$$

G is the flat thimble associated to the gaussian action S_G

$$\rightarrow \quad \frac{d\eta_k}{dr} = \frac{1}{r}\frac{\partial \bar{S}_G}{\partial \eta_k} = \frac{1}{r}\lambda_k\eta_k \quad \rightarrow \quad \eta_k \propto r^{\lambda_k}$$

but for r= ε infinitesimal the Lefschetz and Gaussian thimbles coincide ⇒

$$\phi_i(\epsilon) = \phi_i^0 + \sum_k w_{ki}\xi_k = \phi_i^0 + \sum_k \epsilon^{\lambda_k} w_{ki}\eta_k$$

$$\frac{d\phi_i}{dr} = \frac{1}{r}\frac{\partial \bar{S}}{\partial \phi_i} \qquad r \in [\epsilon, 1]$$

Start with a random real η vector, compute Φ(ε) and evolve using steepest descent

How to stay on the thimble

Metropolis
PRD Rapid 88, 051502 (2013)

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G is the flat thimble associated to the gaussian action S_G

$$\phi_i(\epsilon) = \phi_i^0 + \sum_k w_{ki}\xi_k = \phi_i^0 + \sum_k \epsilon^{\lambda_k} w_{ki}\eta_k$$

Integration measure →

$$\int_{\mathcal{I}} \mathrm{d}\phi = \int_{\mathbb{R}^n} \det[J_\eta^\phi]\mathrm{d}\eta = \int_{\mathbb{R}^n} \left(\prod_k \epsilon^{\lambda_k}\right) \det[J_\xi^\phi]\mathrm{d}\eta$$

Jacobian of the transformation between ξ and Φ

residual phase along the steepest descent →

$$\frac{d[\mathbf{J}_\xi^\phi]_{ik}}{dr} = \frac{1}{r}\overline{\frac{\partial^2 S}{\partial\phi_i\partial\phi_j}}\overline{[\mathbf{J}_\xi^\phi]_{jk}}$$

$$[\mathbf{J}_\xi^\phi]_{ik}(r=\epsilon) = \mathbf{w}_{ki}.$$

How to stay on the thimble

Metropolis

PRD Rapid 88, 051502 (2013)

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$$S[\phi] = S[\phi_0] + S_G[\eta] + \mathcal{O}(|\eta|^3)$$

$$S_G = \frac{1}{2}\sum_k \lambda_k \eta_k^2$$

$$\phi_i = \phi_i^0 + \sum_k w_{ki}\eta_k$$

G_0 is the flat thimble associated to the gaussian action S_G

η → n-dim random vector living on the manifold defined by the eigenvectors of the Hessian computed at the critical point with positive eigenvalues

$|\eta|$ → distance along the thimble

$|\eta|/\delta r$ → number of steps along the steepest descent

$$\frac{\mathrm{d}\phi_i(r)}{\mathrm{d}r} = \frac{1}{r}\overline{\frac{\delta S}{\delta\phi_i(r)}}$$

$$\dashrightarrow \quad \phi_i(n+1) = \phi_i(n) + \delta r\,\overline{\frac{\delta S}{\delta\phi_i}}$$

How to stay on the thimble

Metropolis

PRD Rapid 88, 051502 (2013)

In the neighbourhood of a critical point →

$$S[\phi] = S[\phi_0] + S_G[\eta] + \mathcal{O}(|\eta|^3)$$

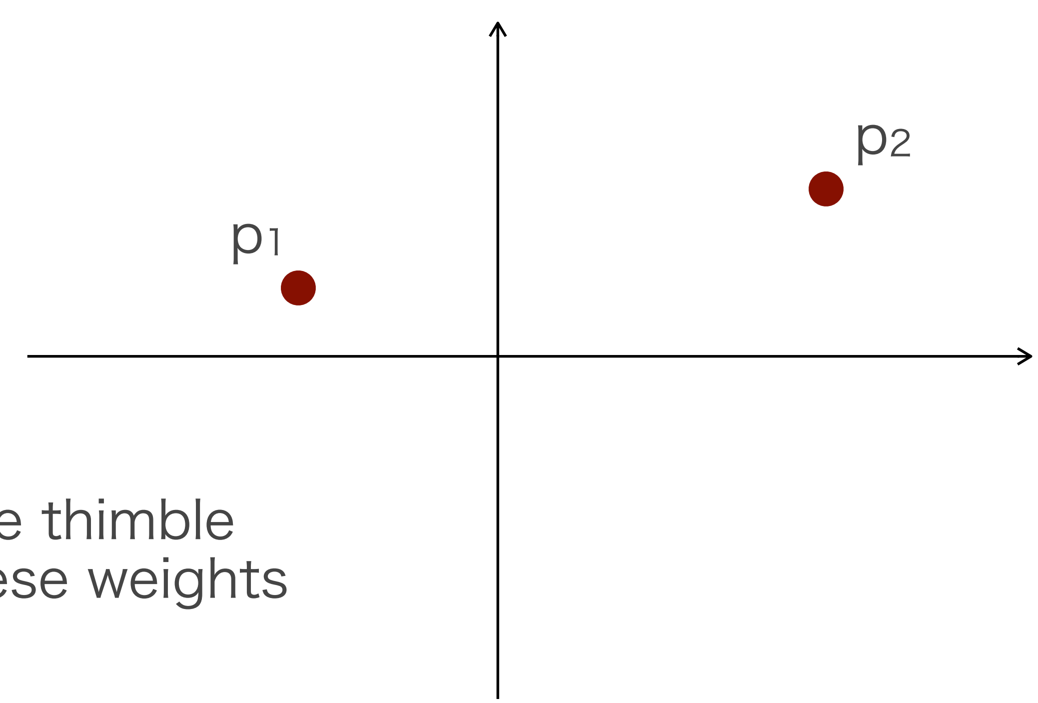
$$S_G = \frac{1}{2}\sum_k \lambda_k \eta_k^2$$

⇒

$$\phi_i = \phi_i^0 + \sum_k w_{ki}\eta_k$$

G_0 is the flat thimble associated to the gaussian action S_G

η → n-dim random vector living on the manifold defined by the eigenvectors of the Hessian computed at the critical point with positive eigenvalues



η →

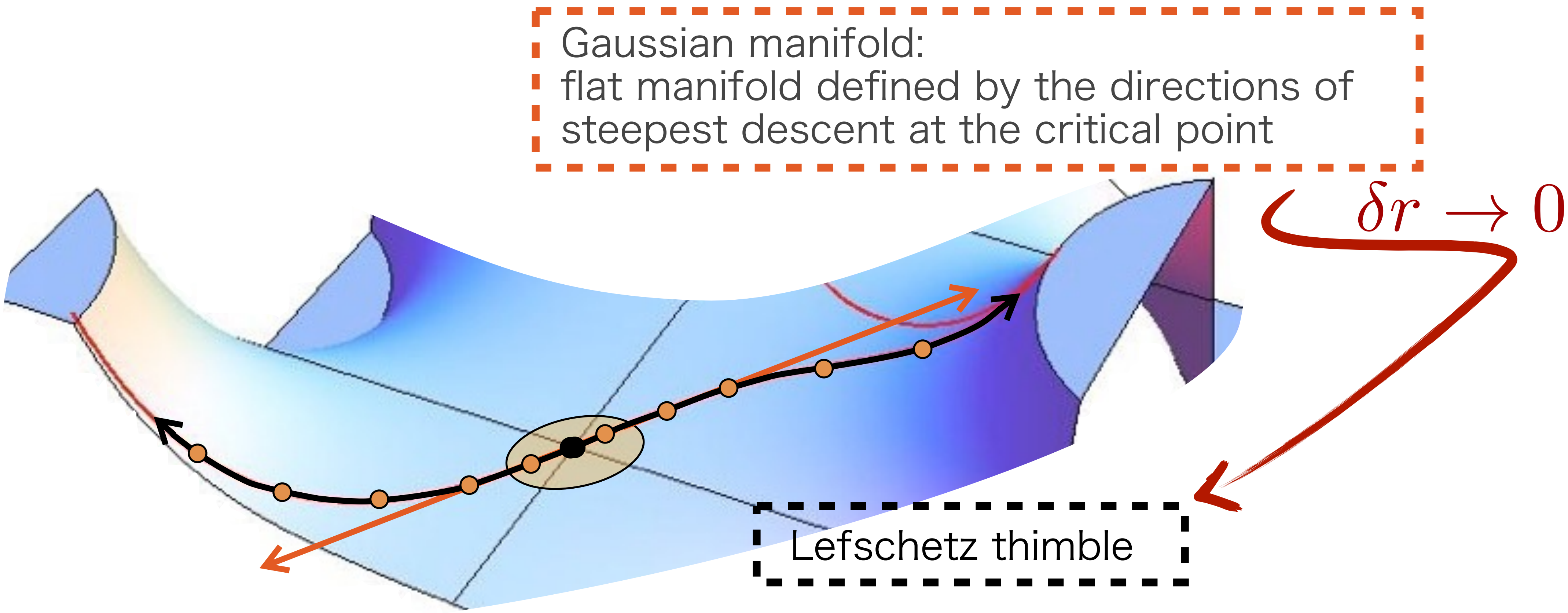
Φ(p1) → $n_{p_1} e^{-S[\phi_{p_1}]}$

Φ(p2) → $n_{p_2} e^{-S[\phi_{p_2}]}$

← select the thimble using these weights

How to stay on the thimble

Gaussian thimble



$|\eta|/\delta r = N$ → number of steps along the steepest descent

Decreasing δr your manifold get closer and closer to the Lefschetz thimble

If the action decreases fast away from the stationary point
integrating on the Gaussian thimble can be sufficient

How to stay on the thimble

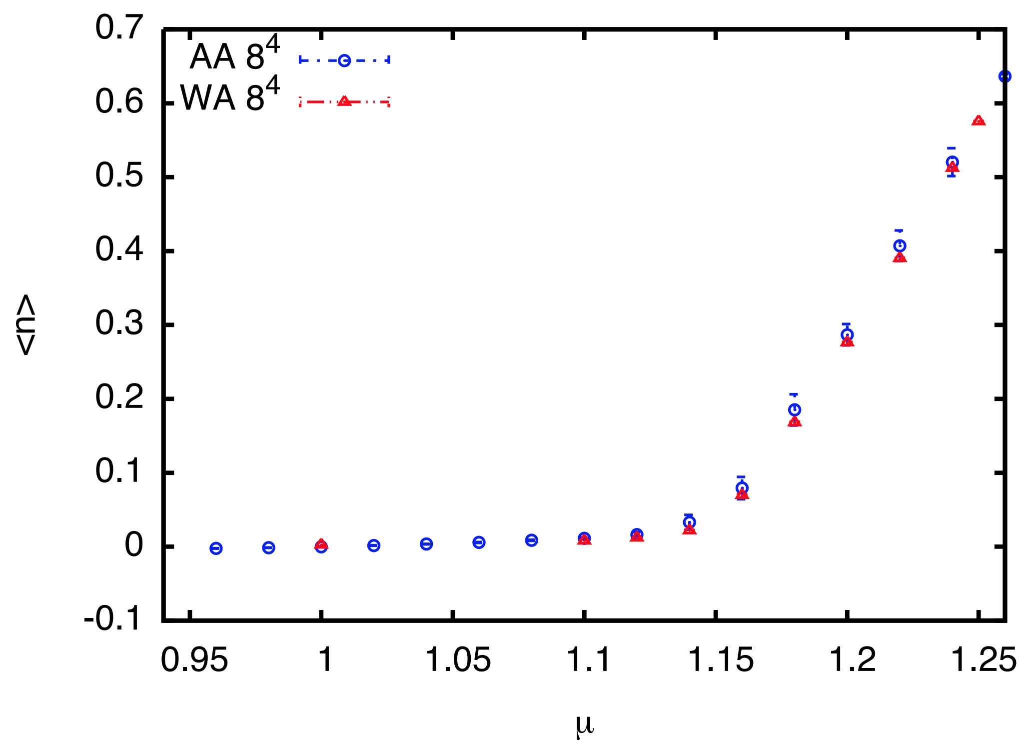
Gaussian thimble

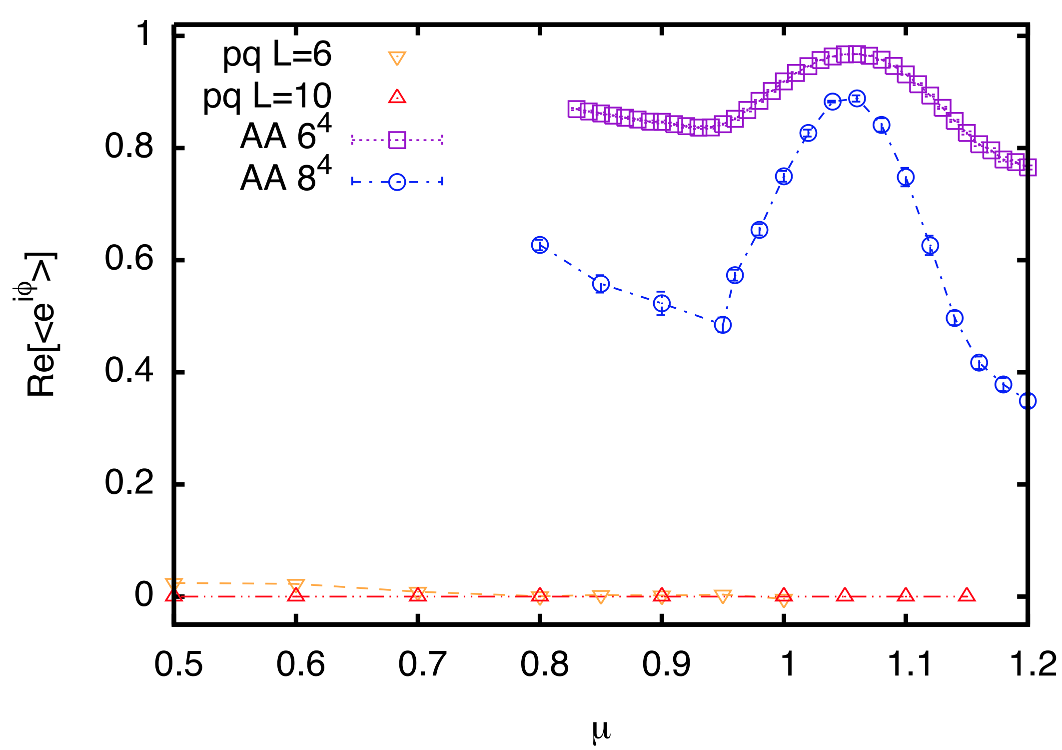
It works PRD Rapid 88, 051501 (2013)

λ Φ⁴ theory

$$S[\phi,\phi^*]=\sum_x[(2d+m^2)\phi_x^*\phi_x+\lambda(\phi_x^*\phi_x)^2\;-\sum_{\nu=0}^{4}(\phi_x^*e^{-\mu\delta_{\nu,0}}\phi_{x+\hat\nu}+\phi_{x+\hat\nu}^*e^{\mu\delta_{\nu,0}}\phi_x))$$

$$\langle n\rangle=\frac{1}{V}\frac{\partial\ln Z}{\partial\mu}$$

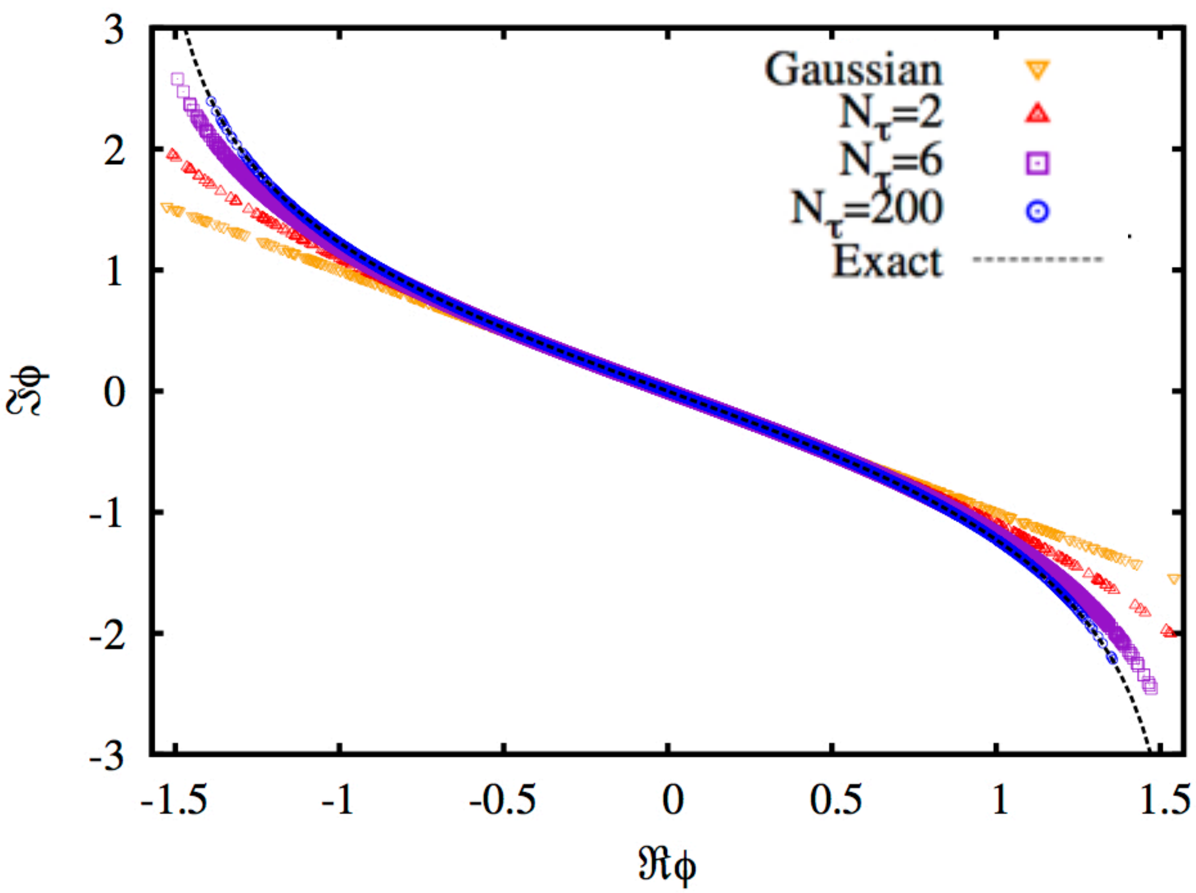




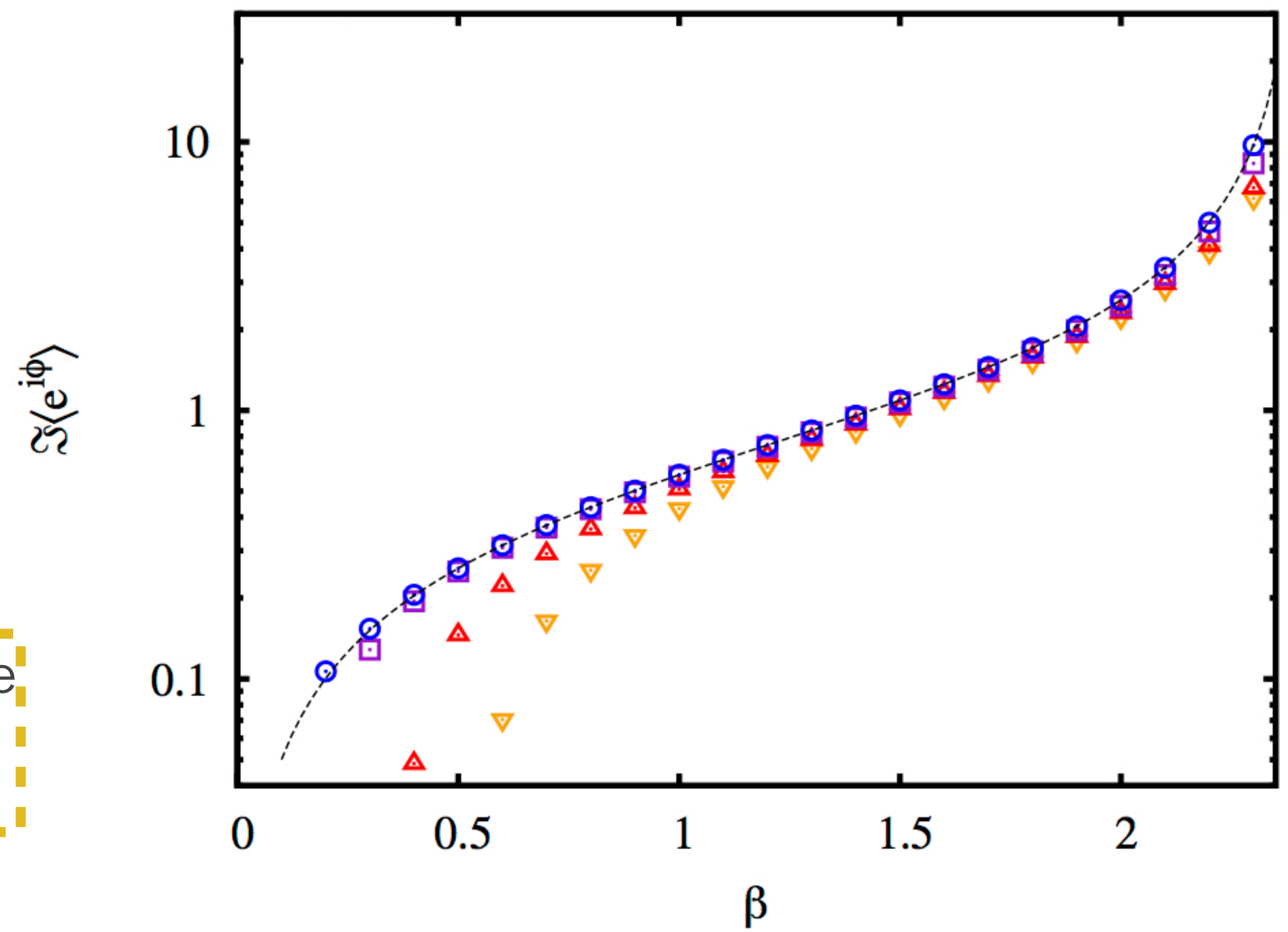
How to stay on the thimble

Gaussian thimble
may not work PRD Rapid 88, 051502 (2013)

U(1) one plaquette model $S = -i\frac{\beta}{2}\left(U + U^{-}1\right) = -i\beta\cos\phi$



$$\langle e^{i\phi}\rangle = i\frac{J_1(\beta)}{J_0(\beta)}$$



There are parameter regions where integration on the Gaussian manifold is sufficiently accurate

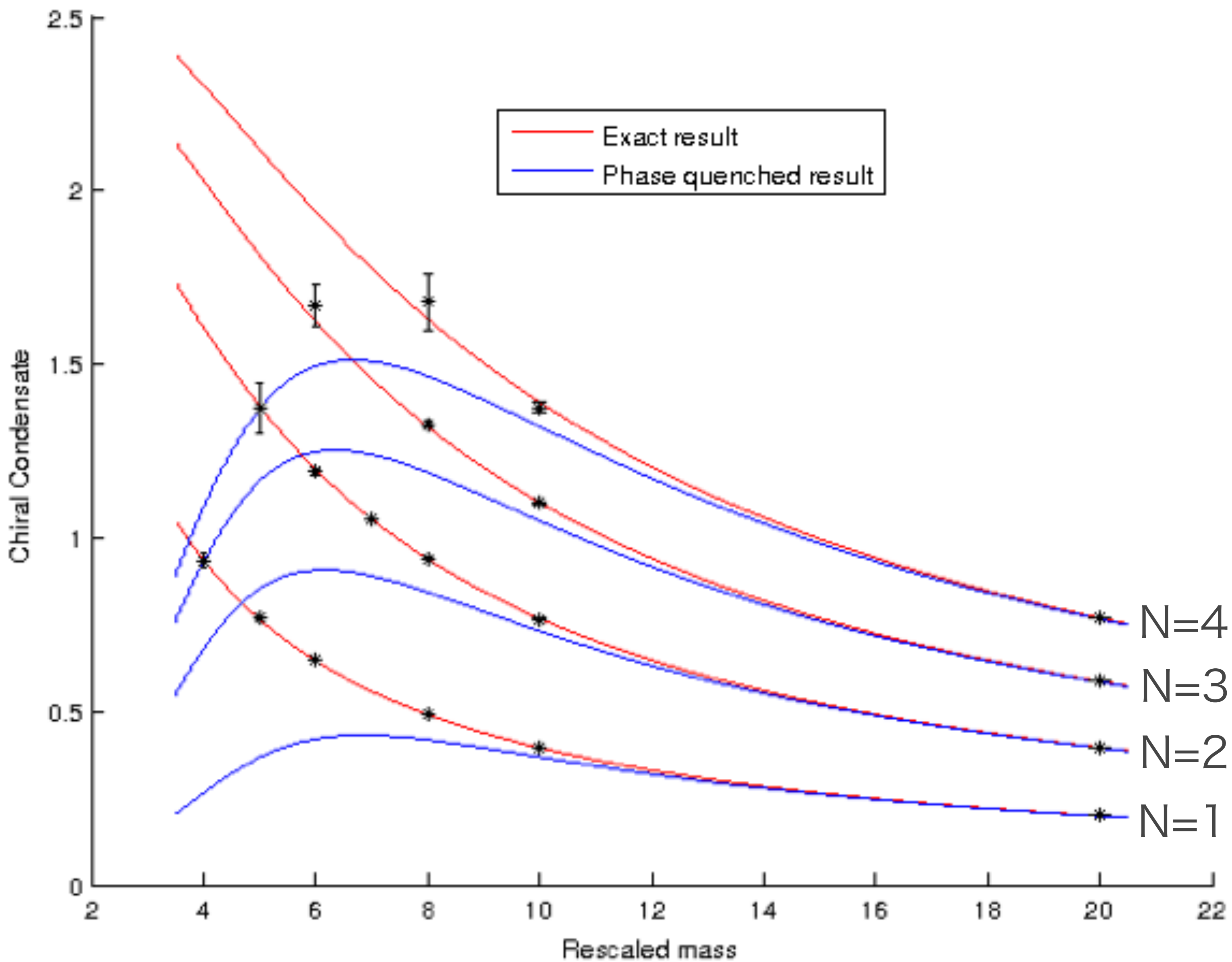
Chiral random matrix model on the thimble

G. Eruzzi and F. Di Renzo

Example of thimble calculation with a fermionic log[Det] in the action

$$Z_N^{N_f}(m) = \int d\Phi_1 d\Phi_2 \det{}^{N_f}\left(D_\mu + m\right) e^{-2N\mathrm{Tr}[\Phi_1^\dagger\Phi_1+\Phi_2^\dagger\Phi_2]}$$

$$D_\mu + m = \begin{pmatrix} m & e^{\mu}\Phi_1 - e^{-\mu}\Phi_2^\dagger \\ -e^{-\mu}\Phi_1^\dagger + e^{\mu}\Phi_2 & m \end{pmatrix}$$



→ Obtained with a new algorithm to stay on the thimble
F. Di Renzo Lattice2014

→ Integration done on one thimble (the trivial stationary point)

QFTs on selected Lefschetz thimbles

- We should integrate on all the thimbles. Is it feasible? Can we consider just one or a class of thimbles instead?

$$\langle \mathcal{O} \rangle = \frac{\sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \prod_x \mathrm{d}\phi_x e^{-S[\phi]} \mathcal{O}[\phi]}{\sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \prod_x \mathrm{d}\phi_x e^{-S[\phi]}}$$

Must be checked case by case

It might also be that you are interested in the dynamics around **one or a couple of known particular saddle points**. In this case integrating on the thimble gives you alle the quantum correction to the classical dynamics associated with those critical points.

I'll show you NOW 1 and 1/2 example

Hubbard model on the Lefschetz thimble

A. Mukherjee and M.C. PRB 90, 025134 (2014)

- Two-dim Hubbard model, probably the most famous model in the condensed matter community.
- It has been hypothesised to contain the essential physics of high-temperature superconductivity.
- **Has sign problem**

Hamiltonian

$$\mathcal{H} = -t \sum_{\langle ij\rangle\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) - \sum_{i\sigma} \mu_\sigma n_{i\sigma} + U \sum_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right)$$

t → hopping parameter

U → on-site interaction strength

μ_σ → chemical potential for spin σ

Interaction term

$$n_{i\uparrow} n_{i\downarrow} = \tfrac{1}{2}\xi_i[(e^{i\theta_i} n_{i\uparrow} + e^{-i\theta_i} n_{i\downarrow})^2 - (e^{2i\theta_i} n_{i\uparrow} + e^{-2i\theta_i} n_{i\downarrow})] + \tfrac{1}{2}(1-\xi_i)(e^{i\theta_i'}\Delta_i^\dagger + e^{-\theta_i'}\Delta_i)^2,$$

$$\Delta_i = c_{i\uparrow} c_{i\downarrow}$$

Hubbard model on the Lefschetz thimble

A. **Mukherjee** and M.C. PRB 90, 025134 (2014)

→ Two-dim
conden
→ It has b
temper
→ **Has sig**

Hami

$\mathcal{H} = -$ $\quad {}^{i\theta_i} n_{i\downarrow})^2 - (e^{2i\theta_i} n_{i\uparrow} + e^{-2i\theta_i} n_{i\downarrow})]$

${}_i^{\dagger} + e^{-\theta_i'} \Delta_i)^2,$

t →

U →

μ_σ →

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$$\Delta_i = c_{i\uparrow} c_{i\downarrow}$$

Hubbard model on the Lefschetz thimble

A. Mukherjee and M.C. PRB 90, 025134 (2014)

Through Hubbard-Stratonovich

Introduce auxiliary bosonic field and integrate the fermionic degrees of freedom

$$n_{i\uparrow}n_{i\downarrow} = \tfrac{1}{2}\xi_i[(e^{i\theta_i}n_{i\uparrow} + e^{-i\theta_i}n_{i\downarrow})^2 - (e^{2i\theta_i}n_{i\uparrow} + e^{-2i\theta_i}n_{i\downarrow})] + \tfrac{1}{2}(1-\xi_i)(e^{i\theta_i'}\Delta_i^\dagger + e^{-\theta_i'}\Delta_i)^2,$$

$$\Delta_i = c_{i\uparrow}c_{i\downarrow}$$

$\theta_i,\ \theta_i'$ and ξ_i → arbitrary

$$\langle \mathcal{X} \rangle = \frac{\int_{\mathbb{R}^n} \mathcal{D}\boldsymbol{\phi}\, \mathcal{X}[\boldsymbol{\phi}] e^{-\mathcal{S}[\boldsymbol{\phi}]}}{\int_{\mathbb{R}^n} \mathcal{D}\boldsymbol{\phi}\, e^{-\mathcal{S}[\boldsymbol{\phi}]}}$$

$$\mathcal{S}[\boldsymbol{\phi}] = \sum_{\alpha\nu} \frac{\phi_{\alpha\nu}^2}{2} - \log\det \boldsymbol{M}[\boldsymbol{\phi}]$$

sign problem

We use $\xi_i = 1$ and $\theta_i = \pi/2$

→ $\det M[\phi] \in \mathbb{R}$ **not positive definite!**

We study repulsive Hubbard model (U>0) away from half-filling (μ<0)

→ Intermediate to strong coupling regime (U/t =4 and 8)

→ For each set of parameters we consider a **SINGLE PHASE** associated with **uniform time-independent real mean-field solutions**

quantum fluctuations are attached to the usually studied mean-field solution

Hubbard model on the Lefschetz thimble

A. Mukherjee and M.C. PRB 90, 025134 (2014)

Real saddle-point $\longrightarrow$ $\partial^2_\phi \mathcal{S}$ real matrix

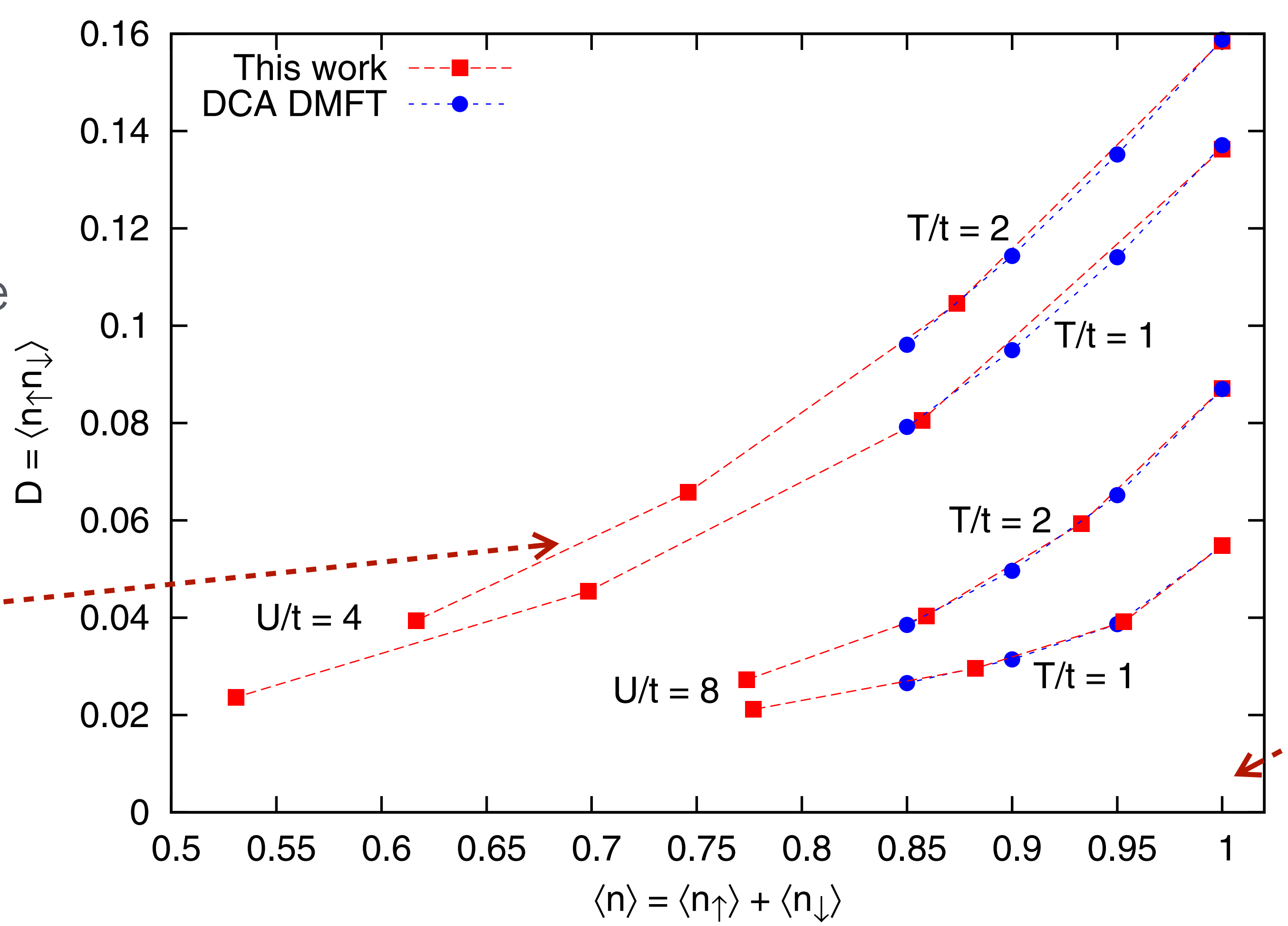
Steepest descent are in $\mathbb{R}^n$

$\longrightarrow$ Lefschetz thimble is a subsector of initial domain of integration region around the saddle point bounded by det[M]=0

$\longrightarrow$ We can use hybrid Monte Carlo with a stepsize small enough to prevent the trajectories from crossing the zero of det[M] (usually non-ergodicity is bad but in this case is what we want)

Double occupancy
extremely local, thermodynamic limit reached very quickly as a function of the lattice size

Away from half filling
no other method is able to perform calculation in this region



Half filling
perfect agreement with Quantum Monte Carlo calculations

Real time dynamics on the Lefschetz thimble

speculations

This is the 1/2 example because I only have results on, more or less, trivial cases

The idea is the following:

assume you have a system in some initial condition at time $\mathbf{t_0}$
and you want to know the expectation value of some observable at time $\mathbf{t_f}$
If you can solve in some way the associated **classical** equation of motions
I will give you all the quantum correction attached to that solution

How?

Start from Schwinger-Keldysh formulation to non-equilibrium QFT

Real time dynamics on the Lefschetz thimble

speculations

Schwinger-Keldish contour

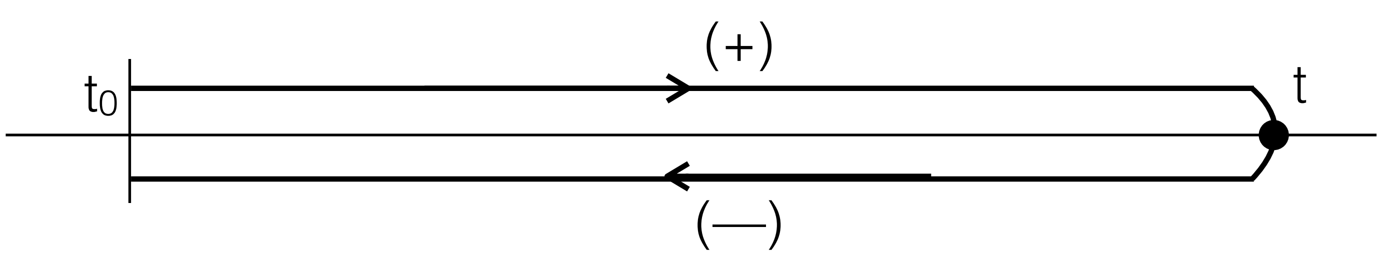
Given an initial state the evolution in time of an operator is given by

$$\langle \mathcal{O} \rangle_t = \mathrm{Tr}[\rho(t)\mathcal{O}] \qquad \rho(t) \longrightarrow \text{Time dependent density matrix}$$

In the Hisemberg picture we can write it as

$$\langle \mathcal{O} \rangle_t = \mathrm{Tr}[\rho(t_0)\mathcal{U}^\dagger(t,t_0)\mathcal{O}(t)\mathcal{U}(t,t_0)] \qquad \rho(t_0) \longrightarrow \text{state at initial time } t_0$$

forward backward



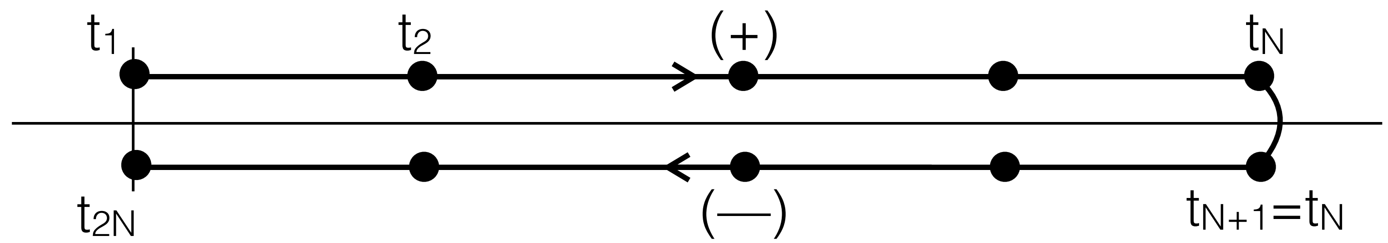
In the same way we can compute correlation functions

$$\langle \mathcal{O}(t)\mathcal{O}(t') \rangle_{t_0} = \mathrm{Tr}[\rho(t_0)\mathcal{U}^\dagger(t,t_0)\mathcal{O}(t)\mathcal{U}(t,t')\mathcal{O}(t')\mathcal{U}(t',t_0)]$$

Real time dynamics on the Lefschetz thimble

speculations

Schwinger-Keldish contour



$$\langle \mathcal{O} \rangle_t = \mathrm{Tr}[\rho(t_0)\mathcal{U}^\dagger(t, t_0)\mathcal{O}(t)\mathcal{U}(t, t_0)]$$

can be expressed in term of a path integral

$$\langle \mathcal{O}(\phi) \rangle = \int \mathrm{d}\phi_1 \mathrm{d}\phi_2 \rho(\phi_1, \phi_2) \int_{\phi_+(0)=\phi_1}^{\phi_-(0)=\phi_2} \mathcal{D}'\phi_- \mathcal{D}\phi_+ e^{iS[\phi_+]-iS[\phi_-]} \mathcal{O}(\phi_+)$$

How we compute this?

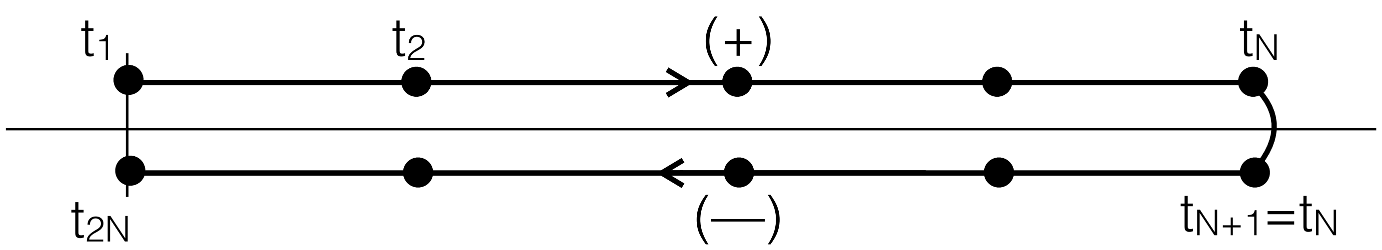
As a first step we consider the case in equilibrium case

$$\rho(\phi_1, \phi_2) = \delta(\phi_1, \phi_2)$$

Real time dynamics on the Lefschetz thimble

speculations

Schwinger-Keldish contour



$$\langle \mathcal{O}(\phi)\rangle = \int \mathrm{d}\phi_1 \mathrm{d}\phi_2 \rho(\phi_1,\phi_2) \int_{\phi_+(0)=\phi_1}^{\phi_-(0)=\phi_2} \mathcal{D}'\phi_- \mathcal{D}\phi_+ e^{iS[\phi_+]-iS[\phi_-]} \mathcal{O}(\phi_+)$$

How we compute this?

I have an idea for the case:

$$\rho(\phi_1,\phi_2) = \delta(\phi_1,\phi_2)$$

→ Solve numerically or analytically the classical equation of motions

→ This classical solution is a stationary point for the action

→ now we can evaluate the expectation value integrating on the thimble attached to that critical point

→ in this way we have included all the quantum fluctuations around the classical solution

the initial conditions fix the UNIQUE thimble on which you have to integrate

Real time dynamics on the Lefschetz thimble

speculations

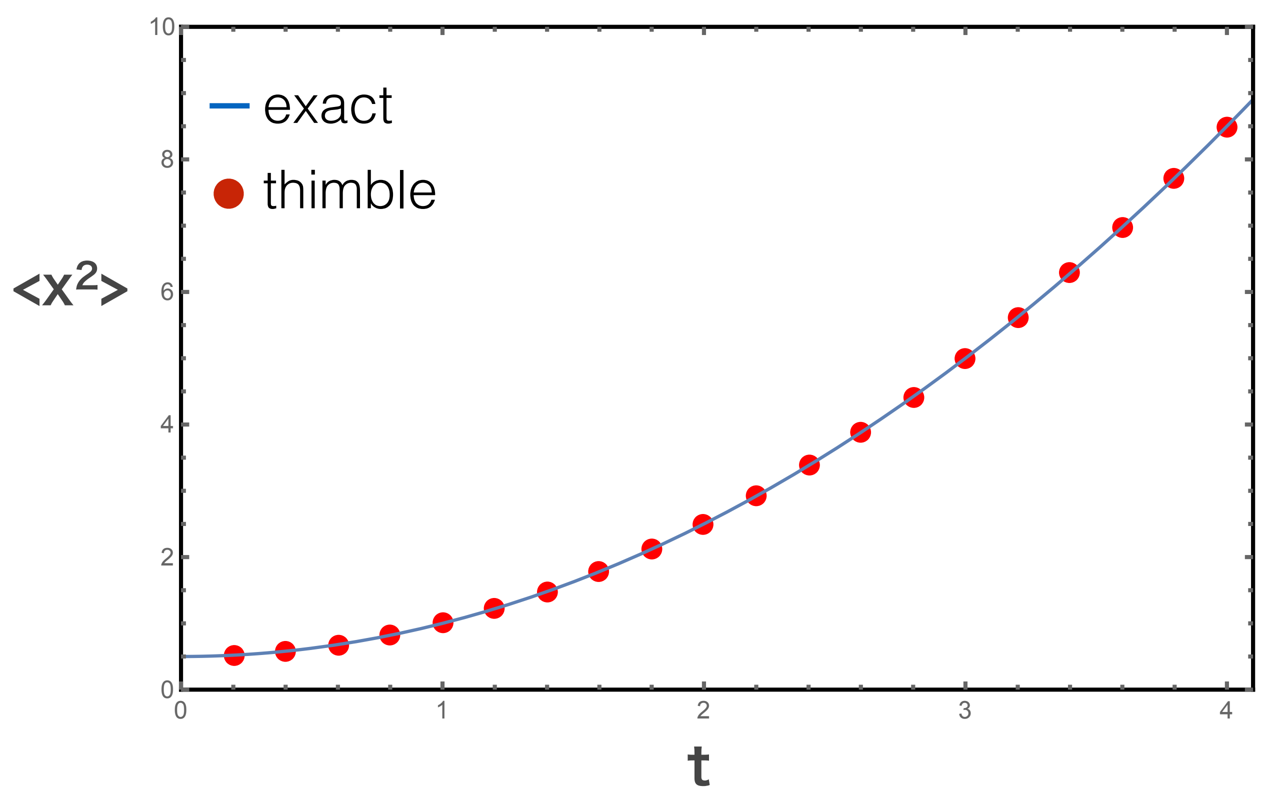
Schwinger-Keldish contour

Since now I have tried with the **free particle** → works

and

the 0+1 dim. non-interacting non-relativistic scalar field theory = **Harmonic oscillator**

→ **works**
less trivial than previous case
but still the thimble is flat so you can do it semi-analytically



QCD (just one slide)

- Complexification: $A_\nu^a(x) \to A_\nu^{a,R}(x) + iA_\nu^{a,R}(x)$

$$SU(3)^{4V} \to SL(3,\mathbb{C})^{4V}$$

- Covariant derivative: $\nabla_{x,\nu,a} F[U] := \dfrac{\partial}{\partial\alpha} F[e^{i\alpha T_a} U_\nu(x)]_{|\alpha=0}$

$$\nabla_{x,\nu,a} = \nabla^R_{x,\nu,a} - i\nabla^I_{x,\nu,a}$$

$$\overline{\nabla}_{x,\nu,a} = \nabla^R_{x,\nu,a} + i\nabla^I_{x,\nu,a}$$

- Equation of steepest descent: $\dfrac{\mathrm{d}}{\mathrm{d}\tau} U_\nu(x;\tau) = (-iT_a \overline{\nabla}_{x,\nu,a} \overline{S}[U]) U_\nu(x;\tau)$

- Defining the thimble for gauge theories is possible: substitute the concept of non-degenerate critical point with that of non-degenerate critical manifold

- **First thing to try:** consider the stationary point with the lower value of the real part of the action and with $n_\sigma \neq 0$
  Define a QFT on the thimble attached to this point.
  - In lattice QCD this should be the trivial vacuum

Conclusions

There are a lot of thing that one can try to study
in the framework of the Lefschetz thimbles

There are a lot of thing that one need to clarify
in order to have all the details under control

Hope that some of you would like to try playing with this!

thank you