Is it worth the effort to find Lefschetz thimbles?

Dávid Pesznyák

in collaboration with

Attila Pásztor

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partition function as a path integral

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- Minkowskian time evolution in any quantum system

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- severity of the sign problem:

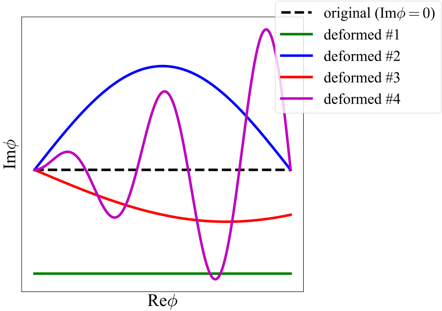
$$\left\langle \frac{w}{r} \right\rangle_r = \frac{\mathcal{Z}_w}{\mathcal{Z}_r} = \sigma \qquad \Longrightarrow \qquad \begin{cases} 1 & \sim \text{perfect!} \\ \approx 0 & \sim \text{not so much...} \end{cases}$$

Fighting the sign problem?

N-dimensinal integral over real fields to

- $2N$-dimensional stochastic dynamics in the real and imaginary parts of complexified fields (i.e. *Complex Langevin Dynamics*)

- N-dimensional integral with deformed integration contour/manifold into the complexified field space



Contour deformations

assuming that $\mathcal{M}$ and $\mathcal{M}'$ are in the same homology class

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$$\mathcal{Z} = \int_{\mathcal{M}} \mathcal{D}\phi \, \det\mathcal{J}(\phi) w[\phi'(\phi)] = \int_{\mathcal{M}} \mathcal{D}\phi \, e^{-S^{\text{eff}}[\phi]}$$

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phase-quenched partition function

$$\mathcal{Z}_{\text{PQ}}^{\text{def}} = \int_{\mathcal{M}} \mathcal{D}\phi \left| \det\mathcal{J}(\phi) w[\phi'(\phi)] \right| = \int_{\mathcal{M}} \mathcal{D}\phi \, e^{-S_{\text{PQ}}^{\text{eff}}[\phi]}$$

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finding a good manifold $\mathcal{M}'$ leads to a milder sign problem

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Is the thimble limit numerically optimal?

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critical points ϕ_{c} solve

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such that $\phi'(t \to \infty) = \phi_{\mathrm{c}}$

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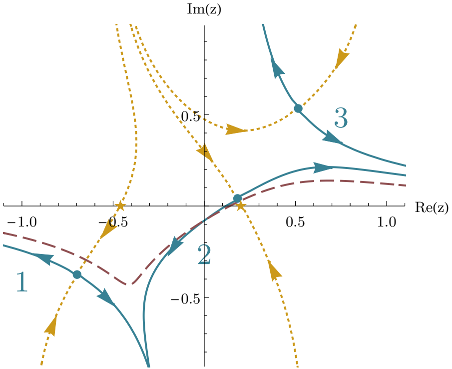
on a given thimble, $\mathrm{Im} S$ is constant $\implies$ no phase fluctuations from e^{-S}

Method I: Lefschetz thimble (example)

- example with action from [arXiv:hep-lat/2007.05436]

$$S(z) = \frac{1}{G} z^2 - \log[(p^2 + i\mu)^2 + (z+m)^2]$$



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1. thimbles are clean analytically, but not necessarily optimal numerically
2. thimble decomposition can solve the sign problem only if a single thimble contributes (or all contributing thimbles have the same phase), *and* the Jacobian can be ignored

Method II: holomorphic flow

holomorphic (upward) flow equations

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with initial conditions $\phi'(t=0) = \phi$

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separate equation for the Jacobian

$$\frac{\mathrm{d}\mathcal{J}}{\mathrm{d}t} = (\mathcal{H}\mathcal{J})^*\,, \qquad \mathcal{J}(t=0) = \mathbb{1}$$

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evolution of

$$\sigma(t) = \langle e^{i\theta} \rangle^{\text{def}}_{\text{PQ}}(t) = \frac{\mathcal{Z}}{\mathcal{Z}^{\text{def}}_{\text{PQ}}(t)}$$

is not necessarily monotonic!

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gradient of the cost function

$$\nabla_p \mathcal{F}(\{p\}) = \nabla_p \log \mathcal{Z}_{\mathrm{PQ}}^{\mathrm{def}}(\{p\}) = -\left\langle \nabla_p \operatorname{Re} S_{\mathrm{PQ}}^{\mathrm{eff}}(\{p\}) \right\rangle_{\mathrm{PQ}}^{\mathrm{def}}$$

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- optimization can be done with standard gradient-based methods

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choose nodes x_i, $i = 1, 2, \ldots, M$, with f linearly interpolating between them,

$$f(\phi, x_{j(\phi)}, x_{j(\phi)+1}, y_{j(\phi)}, y_{j(\phi)+1}) = \frac{y_{j(\phi)}(x_{j(\phi)+1} - \phi)}{x_{j(\phi)+1} - x_{j(\phi)}} + \frac{y_{j(\phi)+1}(\phi - x_{j(\phi)})}{x_{j(\phi)+1} - x_{j(\phi)}}$$

- parameters are simply $\{p\} = \{y_0, \ldots, y_M\}$
- Jacobian is cheap

$$\mathcal{J}(\phi) = 1 + i\frac{y_{j(\phi)+1} - y_{j(\phi)}}{\Delta}$$

- index function $j(\phi) = \text{floor}[(\phi - x_1)/\Delta]$ with $\Delta = x_{i+1} - x_i (= \text{const.})$
- optimization can be done with standard gradient-based methods
- by increasing M and decreasing Δ one can approximate any continuous function, so piecewise linearity is not an assumption, however continuity and being single-valued are

Toy models - 1D integrals

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we monitor improvement with the average phase

$$\sigma = \frac{\mathcal{Z}}{\mathcal{Z}_{\mathrm{PQ}}^{\mathrm{def}}}$$

Model 1: One-site Hubbard-like integral

$$\mathcal{Z}_H = \sqrt{\frac{1}{2\pi U}} \int_{-\infty}^{\infty} \mathrm{d}\phi \left(1 + e^{\mu + U/2 + i\phi}\right)^2 e^{-\phi^2/(2U)}$$

- integration domain: $\phi \in \mathbb{R}$ (noncompact)
- infinitely many critical points ϕ_c
- (dimensionless) parameters: chemical potential μ and interaction U
- sign problem away from half filling ($\mu/U = 1/2$)

Model 2: Gross-Neveu-like (0+1D) integral

$$\mathcal{Z}_{\mathrm{GN}} = \sqrt{\frac{N}{\pi G}} \int_{-\infty}^{\infty} \mathrm{d}\phi \left(p^2 + (m+\phi)^2\right)^N \exp\left(-\frac{N}{G}\phi^2\right)$$

- integration domain $\phi \in \mathbb{R}$ (noncompact)
- finite number of critical points
- parameters: number of flavors N, coupling G, momentum p and mass m
- sign problem induced by complex coupling G

Model 3: heavy-dense Thirring-like integral

$$\mathcal{Z}_{\mathrm{T}} = \int_{-\pi}^{\pi} \mathrm{d}\phi \; \exp\left(\frac{N}{g^2} \cos\phi + \mathrm{i}\phi + \mu \right)$$

- integration domain $\phi \in [-\pi, \pi]$ (compact),
- single critical point at $z_{\mathrm{c}} = i\mathrm{arsinh}(g^2/N)$
- action becomes singular at $\mathrm{Re}z = \pm\pi$
- parameters: number of flavors N, coupling g and chemical potential μ

Model 4: Chern–Simons–like with fermions (compact)

$$\mathcal{Z}_{\text{CS}} = \frac{e^{-ik\pi}}{2^N} \int_{-\pi}^{\pi} \mathrm{d}\phi \, \big(\cosh m - \cos\phi \big)^N \, e^{ik\phi}$$

- integration domain $\phi \in [-\pi, \pi]$ (compact)
- interesting case: $k < N$ (for $k > N$ $\mathcal{Z} = 0$ and $k = N$ critical points are imaginary infinity)
- parameters: number of flavors N, topological charge k and mass m
- sign problem from topological term $e^{ik\phi}$

Summary of toy models

model	Hubbard	Gross-Neveu	Thirring	Chern-Simons
$\int$ domain	noncompact	noncompact	compact	compact
# of CPs	infinite	finite	1	finite
sign problem	μ	complex G	μ	θ term
Im-thimble	finite	finite	divergent	finite

Figure: Flow time evolution (Hubbard)

$$\mathcal{Z}_H = \sqrt{\frac{1}{2\pi U}} \int_{-\infty}^{\infty} \mathrm{d}\phi \left(1 + e^{\mu + U/2 + i\phi}\right)^2 e^{-\phi^2/(2U)}$$

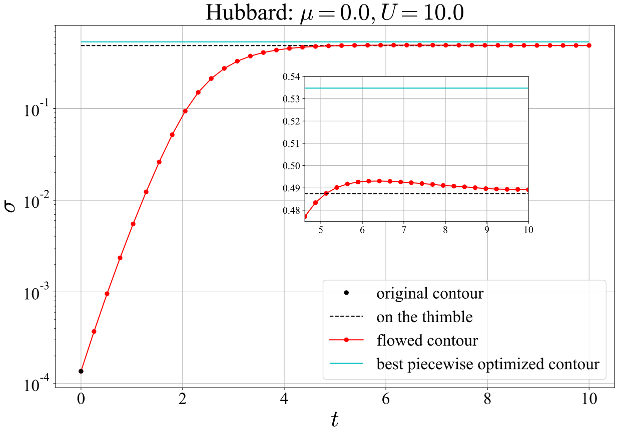

Figure: Contours in the complex plane (Hubbard)

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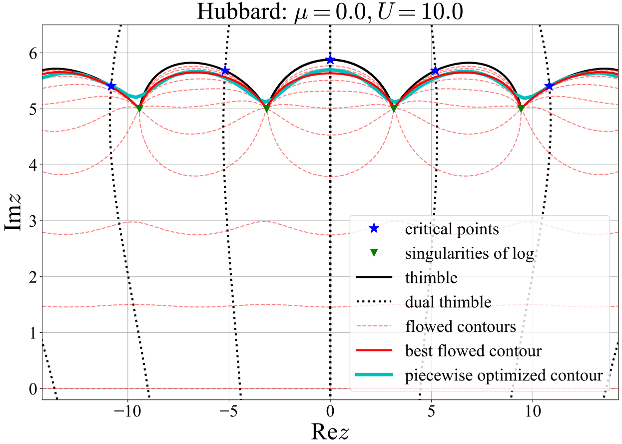

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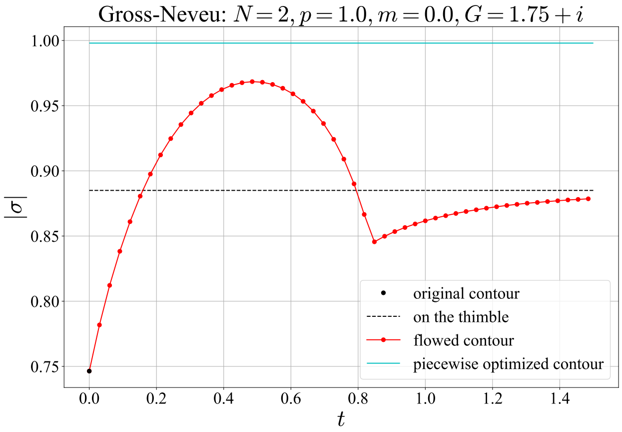

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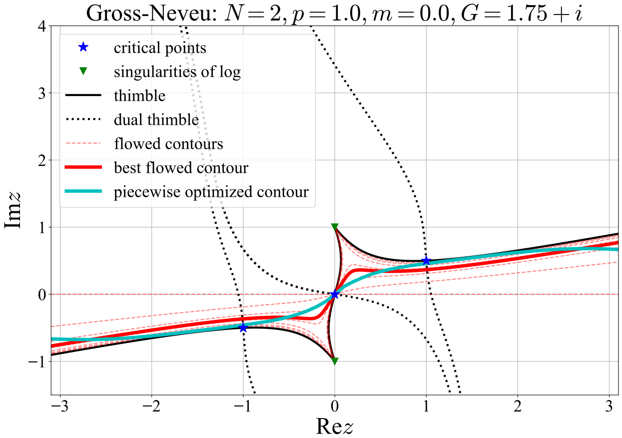

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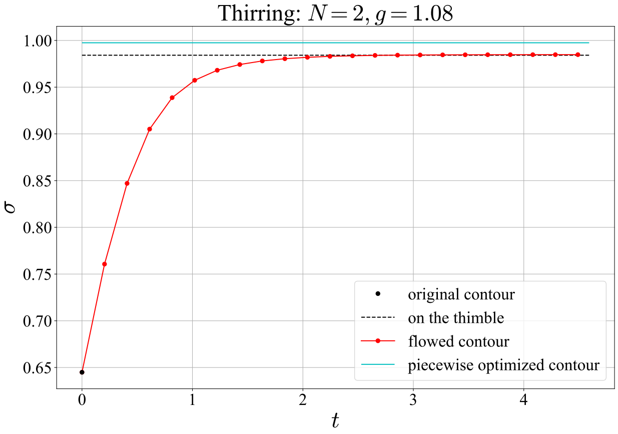

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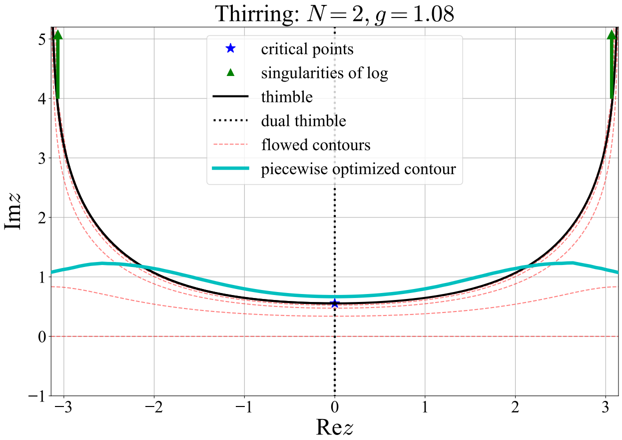

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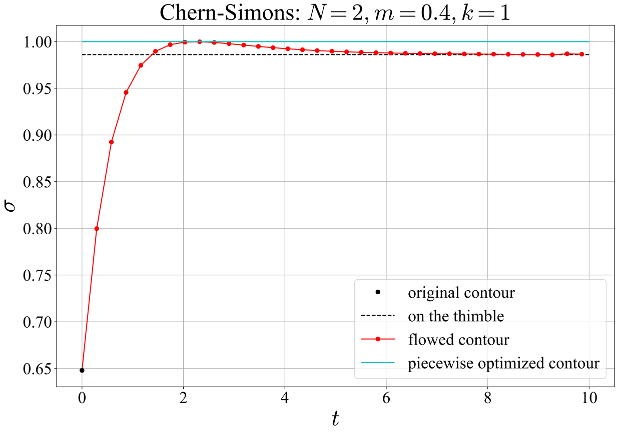

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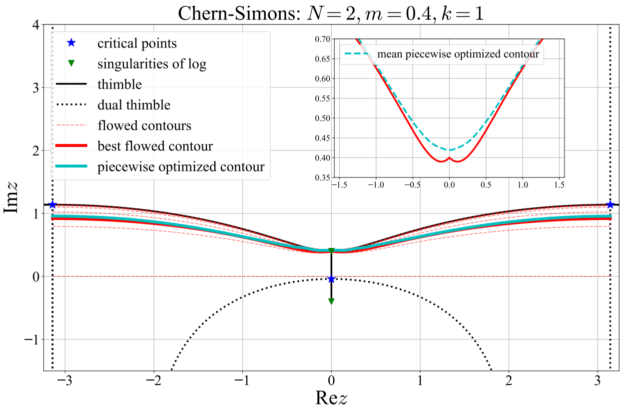

Summary and outlook

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- for not-too-large dimensional integrals this interpolant ansatz can be generalized via simplices
- higher dimensional integrals have further important features (spacetime and internal symmetries) that could be used in constructing a good ansatz for optimization

Thank you!

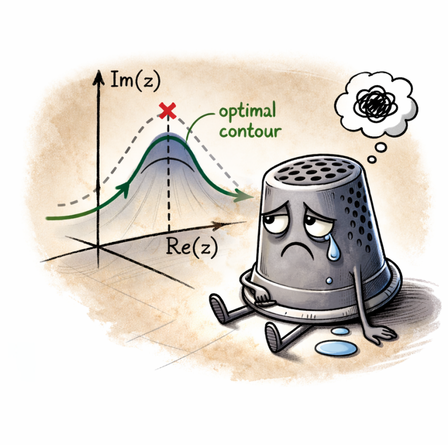

Figure: via ChatGPT