Complex Solutions to Sign Problems Henry Lamm

w/ Andrei Alexandru, Gökçe Başar, Paulo Bedaque, Scott Lawrence, Neill Warrington 1709.01971, 1804.00697, 1807.02027, 180x.xxxxx









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• Sign problem: the suffering of stochastic sampling highly oscillatory distributions because results require precise cancellations of positive and negative contributions, generically it is **exponentially** bad in particle number, volume, chemical potential

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Many interesting problems in QCD exist at $\mu \neq 0$



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Complex Solutions

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• For $\mu \neq 0$, S_F is complex \implies sign problem :

$$S_F = \int \mathrm{d}^D x \left[\bar{\psi}^a \left(\partial \!\!\!/ + \mu \gamma_0 + i A \!\!\!/ + m \right) \psi^a \right]$$

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...but analytically, we know ways to deal¹

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$$\int \mathbf{D}\phi e^{-S} = \int_{-\infty}^{+\infty} \mathrm{d}x e^{-(x-i\alpha)^2} = \sqrt{\pi}$$

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CIT guarantees holomorphic f(x) (physics) unchanged
Nonholomorphic f(x), like the average sign, (σ), can change!

$$\langle \sigma \rangle_{\mathcal{M}} = \frac{\int_{\mathbb{R}^N} \mathcal{D}\phi \; e^{-S_{\text{eff}}[\phi;\lambda]}}{\int_{\mathbb{R}^N} \mathcal{D}\phi \; e^{-\text{Re}(S_{\text{eff}}[\phi;\lambda])}} = \frac{\text{holomorphic}}{\text{non-holomorphic}}$$

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• Lefschetz thimbles: steepest descent from *isolated* critical points

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- Thimbles usually unknown; hard to determine correct set.



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Evolve \mathbb{R}^N with holomorphic gradient flow³: $\frac{d\phi_i}{dt} = \overline{\frac{\partial S}{\partial \phi_i}}$

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Manifold under flow is just $\mathcal{M}_g \oplus \mathcal{G}!$

Stokes' phenomenon prevent thimble decomposition



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Stokes' phenomenon prevent thimble decomposition



Effect of Stokes' phenomenon on flow is $\langle \sigma \rangle < 1$ due to "bumps"

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Ain't no thang but a flow thang.



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In the continuum:

$$S = \int \mathrm{d}^2 x \, \left[F_{\mu\nu} F^{\mu\nu} + \bar{\psi}^a (\partial \!\!\!/ + \mu_Q \gamma_0 + m - g Q_a A) \psi^a \right]$$

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which we discretize and integrate out the fermions to obtain:

$$S = \frac{1}{g^2} \sum_{r} (1 - \cos P_r) - \sum_{a} \ln \det D_{xy}^{(a)}$$
$$P_r \equiv A_1(r) + A_0(r + \hat{x}) - A_1(r + \hat{t}) - A_0(r) .$$
$$D_{xy}^{(a)} = m_a \delta_{xy} + \frac{1}{2} \sum_{\nu \in \{0,1\}} \eta_\nu \left[e^{iQ_a A_\nu(x) + \mu \delta_{\nu 0}} \delta_{x + \hat{\nu}, y} - e^{-iQ_a A_\nu(x) - \mu \delta_{\nu 0}} \delta_{x, y + \hat{\nu}} \right].$$

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$$g = 0.50$$
 and $m_a = 0.05$, $Q_1 = Q_+ = +2$ and $Q_{2,3} = Q_- = -1$

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• Baryon with $am_B \approx 0.6$

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QED_{1+1}



 $\langle \sigma \rangle$ and $\langle n \rangle$ as a function of μ for $10,14 \times 10$ for QED_{1+1} with $N_f=3$

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The Jacobian must be flowed as well: $\frac{dJ_{ij}}{dt} =$

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⁴A. Alexandru et al. "Fast estimator of Jacobians in the Monte Carlo integration on Lefschetz thimbles". In: *Phys. Rev.* D93.9 (2016), p. 094514. arXiv: 1604.00956 [hep-lat].

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The Jacobian must be flowed as well: $\frac{dJ_{ij}}{dt} = \frac{\partial}{\partial \theta}$



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The Jacobian must be flowed as well: $\frac{dJ_{ij}}{dt} = \frac{\partial^2 S}{\partial \zeta_i \partial \zeta_j}$

Wrongians: $J \approx 1$ or $\text{Im}(J) = 0 \implies \text{Speed up but reweighting}^4$



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Prohibitive reweighting from W - J from **exceptional** configurations when T is large

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Gets worse in: $d > 1, g \to \infty$, gauge theories, and at transition⁵

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A sufficiently good learnifold avoids all these issues

learnifold: $\mathcal{M} \subset \mathbb{C}^N$ obtained by supervised machine learning⁶



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$$\tilde{\phi}_i(\phi) = \phi_i + if(T_i\phi) \tag{1}$$

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Use $\cos A_{\mu}$, $\sin A_{\mu}$ to insure that \mathcal{L}_T obeys CIT

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Use $\cos A_{\mu}, \sin A_{\mu}$ to insure that \mathcal{L}_T obeys CIT $v_j = \sigma \left(b_j + \sum_i w_{ij} v_i \right)$

Perform a backward propagate with gradient descent to adjust b_j, w_{ij}

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1+1 Thirring model with Wilson fermions

$$S = \sum_{x,\nu} \frac{N_F}{g^2} (1 - \cos A_\nu(x)) + \sum_{x,y} \bar{\psi}^\alpha(x) D^W_{xy}(A) \psi^\alpha(y), \qquad (2)$$

and with the hopping parameter $\kappa = 1/(2m+4)$,

$$D_{xy}^{W} = \delta_{xy} - \kappa \sum_{\nu=0,1} \left[(1 - \gamma_{\nu}) e^{iA_{\nu}(x) + \mu\delta_{\nu}0} \delta_{x+\nu,y} + (1 + \gamma_{\nu}) e^{-iA_{\nu}(x) - \mu\delta_{\nu}0} \delta_{x,y+\nu} \right],$$
(3)

The integration over the fermion fields leads to

$$S = N_F \left(\frac{1}{g^2} \sum_{x,\nu} (1 - \cos A_\nu(x)) - \log \det D(A) \right) \,. \tag{4}$$

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• The parameters used: $g = 1.0, m = -0.25, N_F = 2$

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• $am_f = 0.30(1)$ and $am_b = 0.44(1) \implies m_b/m_f = 1.5(2)$

1+1 Thirring 40×10



 $\langle e^{-iS_I+i\operatorname{Im}\log \det J}\rangle$ and $\langle n \rangle/m_f$ as a function of μ/m_f for 40×10 with $am_f = 0.30(1)$. The dashed curve represents the free fermion gas with the same mass.

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• Perhaps we don't try and reach thimbles at all!



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• What if thimbles aren't optimal? Perhaps we instead seek the exact surface of maximal $\langle \sigma \rangle^{78}$

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Sign-optimized manifold methods: Find $\mathcal{M}_S \subset \mathcal{M}_{\lambda}^{9^{\circ}}$



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What \mathcal{M}_{λ} should one choose?

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 $^{^{10}{\}rm F}.$ Bursa and M. Kroyter. "A simple approach towards the sign problem using path optimisation". In: (2018). arXiv: 1805.04941 [hep-lat].

• For fermionic theories, we find a useful \mathcal{M}_{λ} to be

$$\tilde{A}_0(A_0, A_i 1) = A_0 + i \left(\lambda_0 + \lambda_1 \cos A_0 + \lambda_2 \cos 2A_0\right)$$
$$\tilde{A}_i(A_0, A_i) = A_i$$

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• For bosonic theories, other groups have shown that nearest-neighbor correlations are important¹⁰

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$$H(\pi, A) = \frac{1}{2} \sum_{x} \pi_{x} [J(A)J^{\dagger}(A)]_{xy}^{-1} \pi_{y} + S_{R}(\tilde{A}(A))$$

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$$H(\pi, A) = \frac{1}{2} \sum_{x} \pi_{x} [J(A)J^{\dagger}(A)]_{xy}^{-1} \pi_{y} + S_{R}(\tilde{A}(A))$$
$$P(\pi, A) \propto e^{-H(\pi, A)} \xrightarrow{\text{marginalize}}_{\text{over}} \sum_{\pi} P(\pi, A) \propto |\det J| e^{-S(A)}$$

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Within our \mathcal{M}_{λ} , we can analytically compute $[J(A)J^{\dagger}(A)]_{xy}^{-1}$ \Rightarrow so \mathcal{M}_{S} as fast as \mathbb{R}^{N}

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Prelim. 2+1 Thirring with Staggered Fermions



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Prelim. 2+1 Thirring with Staggered Fermions $N_S = 6^2$



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Questions?