Manifolds of Glory: Complex Contours for Ameliorating the Sign Problem

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Based on 1804.00697 and 1808.09799

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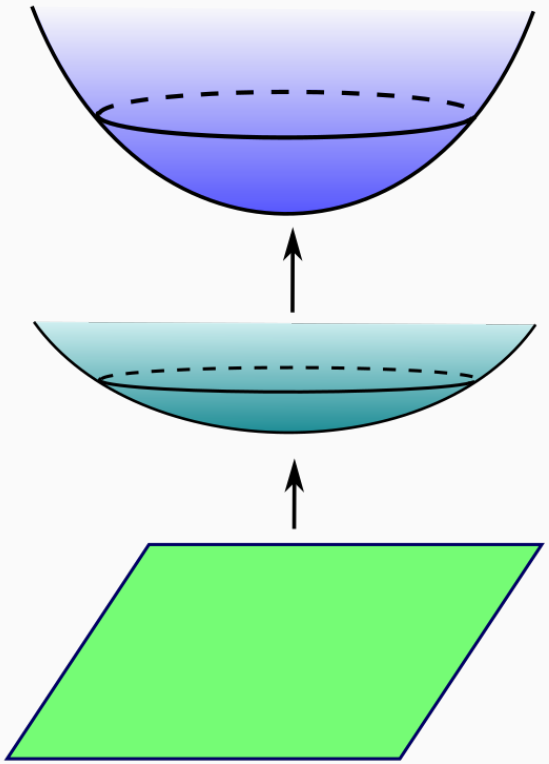
SIGN'18 in Universität Bielefeld



Fermion Sign Problem in a Path Integral

How to calculate a thermodynamic expectation value?

$$\langle \mathcal{O} \rangle \equiv \frac{1}{Z} \int \mathcal{D}\phi \, \mathcal{O} e^{-S(\phi)}$$

Importance sampling: draw N samples ϕ_n from $p(\phi) \propto e^{-S(\phi)}$.

What if S isn't real?

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}\phi \, \mathcal{O} \, e^{-iS_I} e^{-S_R} \Big/ \int \mathcal{D}\phi \, e^{-S_R}}{\int \mathcal{D}\phi \, e^{-iS_I} e^{-S_R} \Big/ \int \mathcal{D}\phi \, e^{-S_R}} = \frac{\left\langle \mathcal{O} e^{-iS_I} \right\rangle_{S_R}}{\left\langle e^{-iS_I} \right\rangle_{S_R}}$$

The **average phase** $\langle \sigma \rangle$ may be **small**.

QCD (finite density), Hubbard model (away from half-filling)
Thirring model, *QED* (both at finite density)

The Gaussian Sign Problem

$$Z = \int_{-\infty}^{\infty} \mathrm{d}x \; e^{-(x - i\mu)^2}$$

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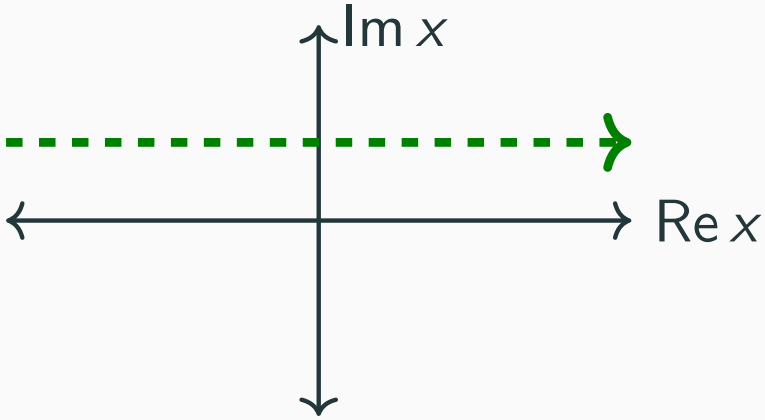
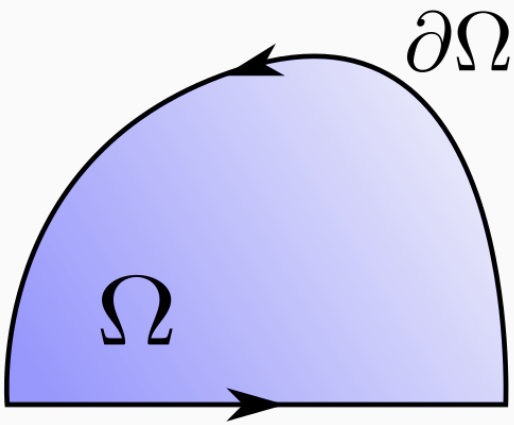
Invoke Cauchy's theorem!



$$Z(\mu) = \int_{-\infty+i\mu}^{\infty+i\mu} \mathrm{d}x \; e^{-(x-i\mu)^2} = \int_{-\infty}^{\infty} \mathrm{d}x \; e^{-x^2}$$

No sign problem!

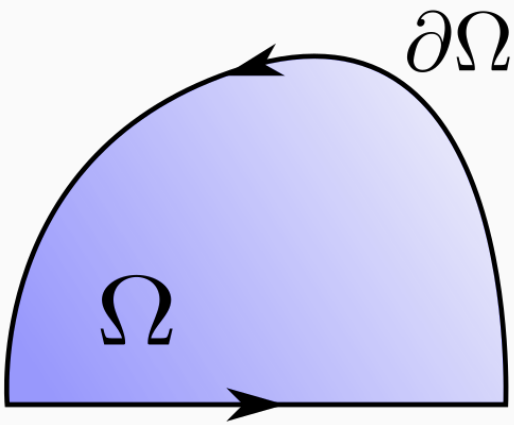
Cauchy's Integral Theorem



For any holomorphic function $f(z)$:

$$0 = \int_{\partial\Omega} f \, \mathrm{d}z$$

Cauchy's Integral Theorem

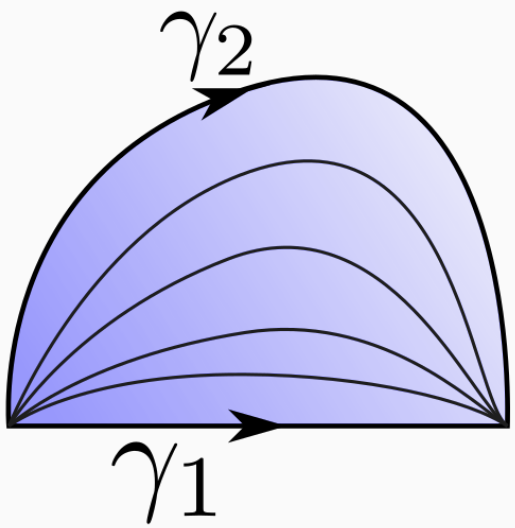


For any holomorphic function $f(z)$:

$$0 = \int_{\partial\Omega} f \, \mathrm{d}z$$

$$\int_{\gamma_1} f \, \mathrm{d}z = \int_{\gamma_2} f \, \mathrm{d}z$$

If we can continuously deform γ_1 to γ_2, "tracing out" Ω.



Testbed: Thirring Model

Fermions (2 flavors) with a repulsive $(\bar{\psi}\gamma_\mu\psi)^2$ interaction.

$$S_{\text{eff}}[A] = -\frac{N_F}{g^2}\sum_{x,\mu}\cos A_\mu(x) - N_F \log\det D[A]$$

with Kogut-Susskind staggered fermions

$$D_{xy}[A] = m\delta_{xy} + \frac{1}{2}\sum_{\nu}\Big[e^{iA_\nu(x)+\mu\delta_{\nu 0}}\delta_{x,(y+\hat{\mu})}(-1)^{x_0+\cdots+x_{\nu-1}} - e^{-iA_\nu(x)-\mu\delta_{\nu 0}}\delta_{(x+\hat{\mu}),y}(-1)^{x_0+\cdots+x_{\nu-1}}\Big]$$

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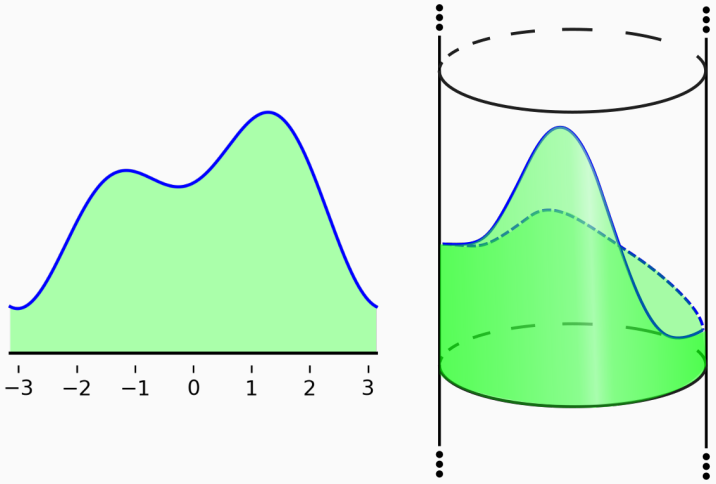
Fields are periodic.

Contour Integration Rules!



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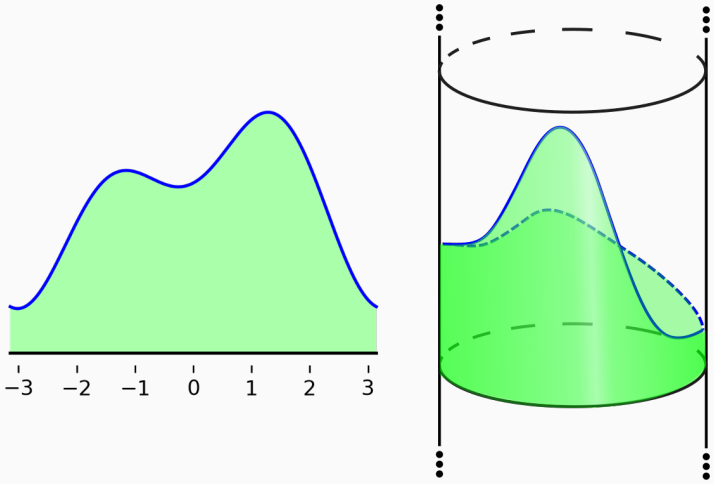

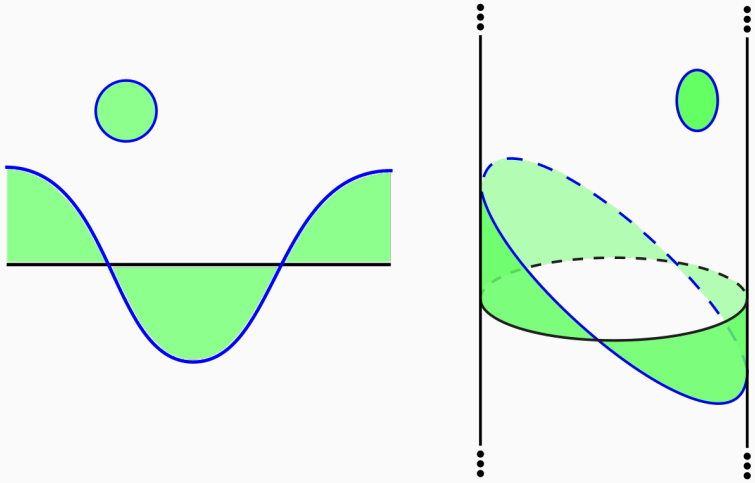

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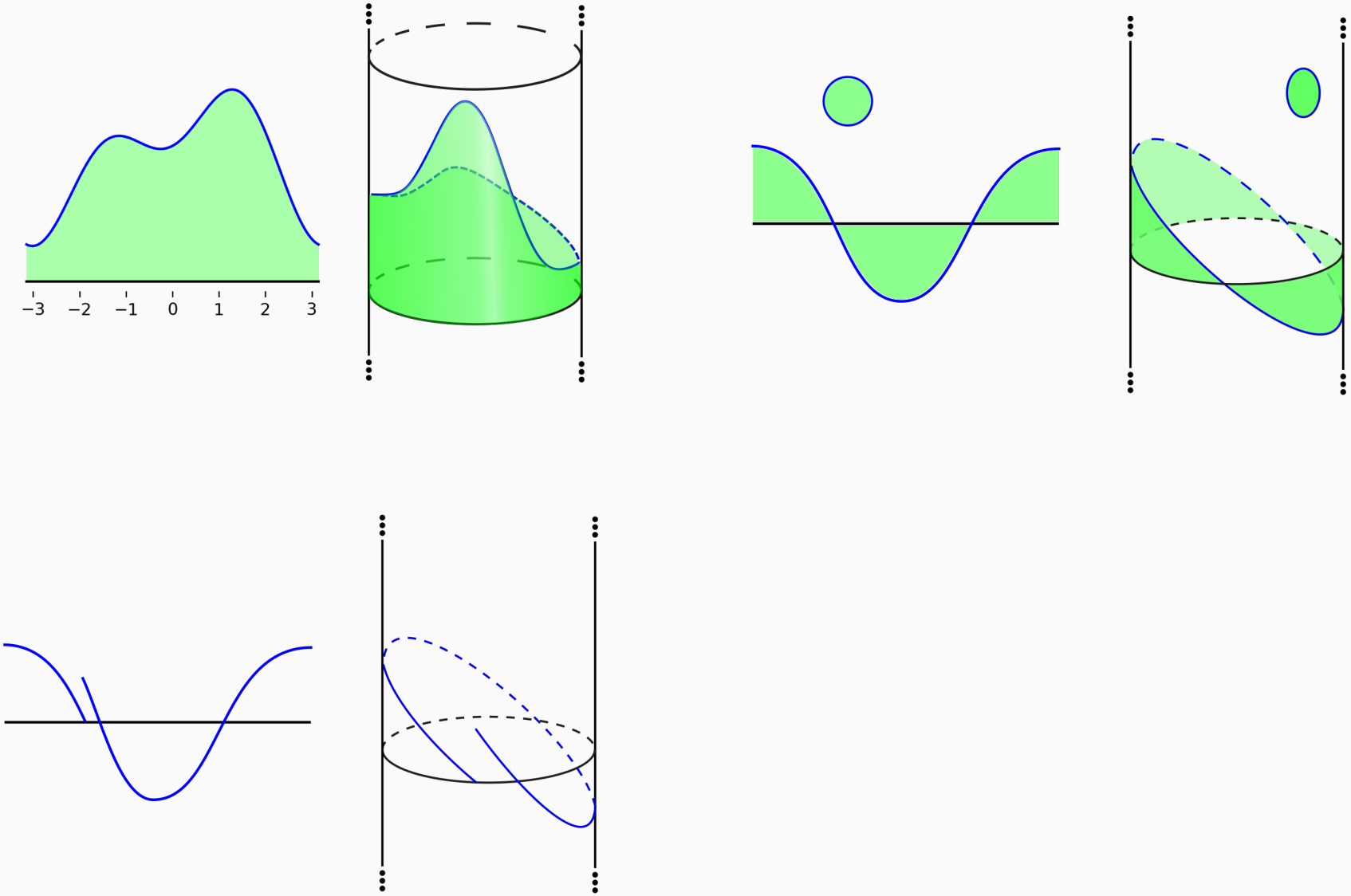

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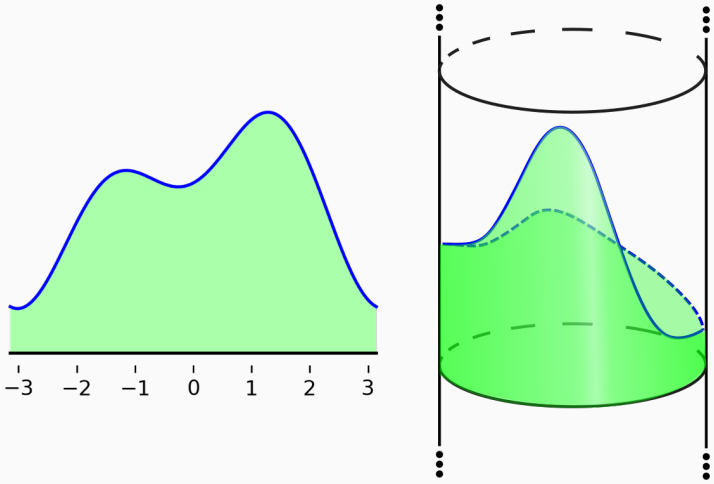

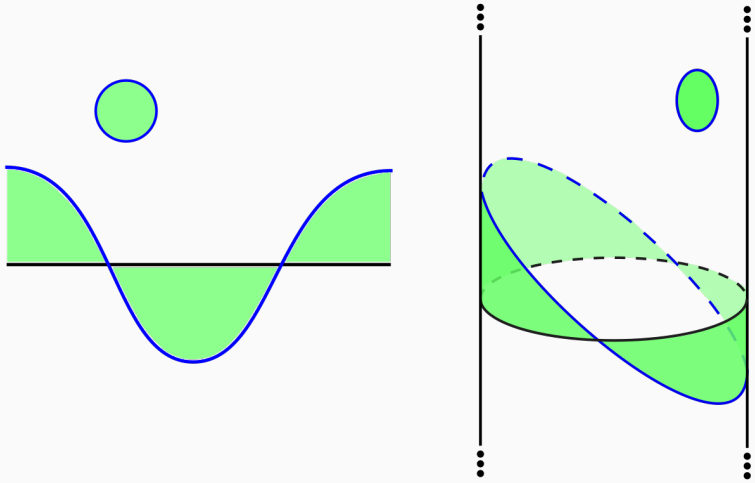

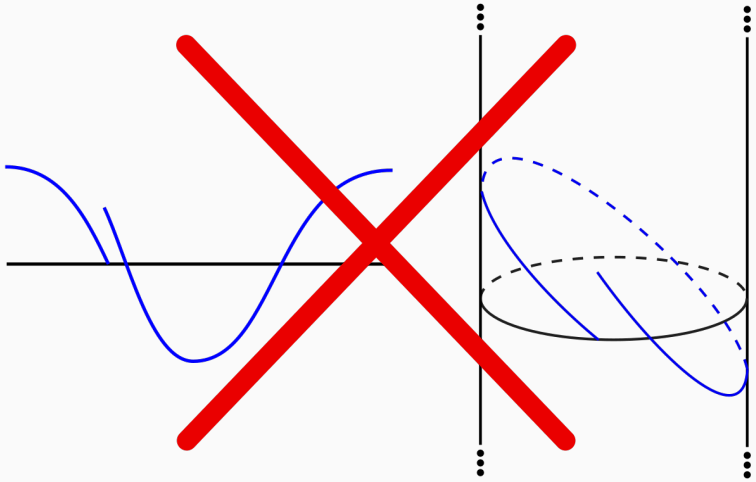

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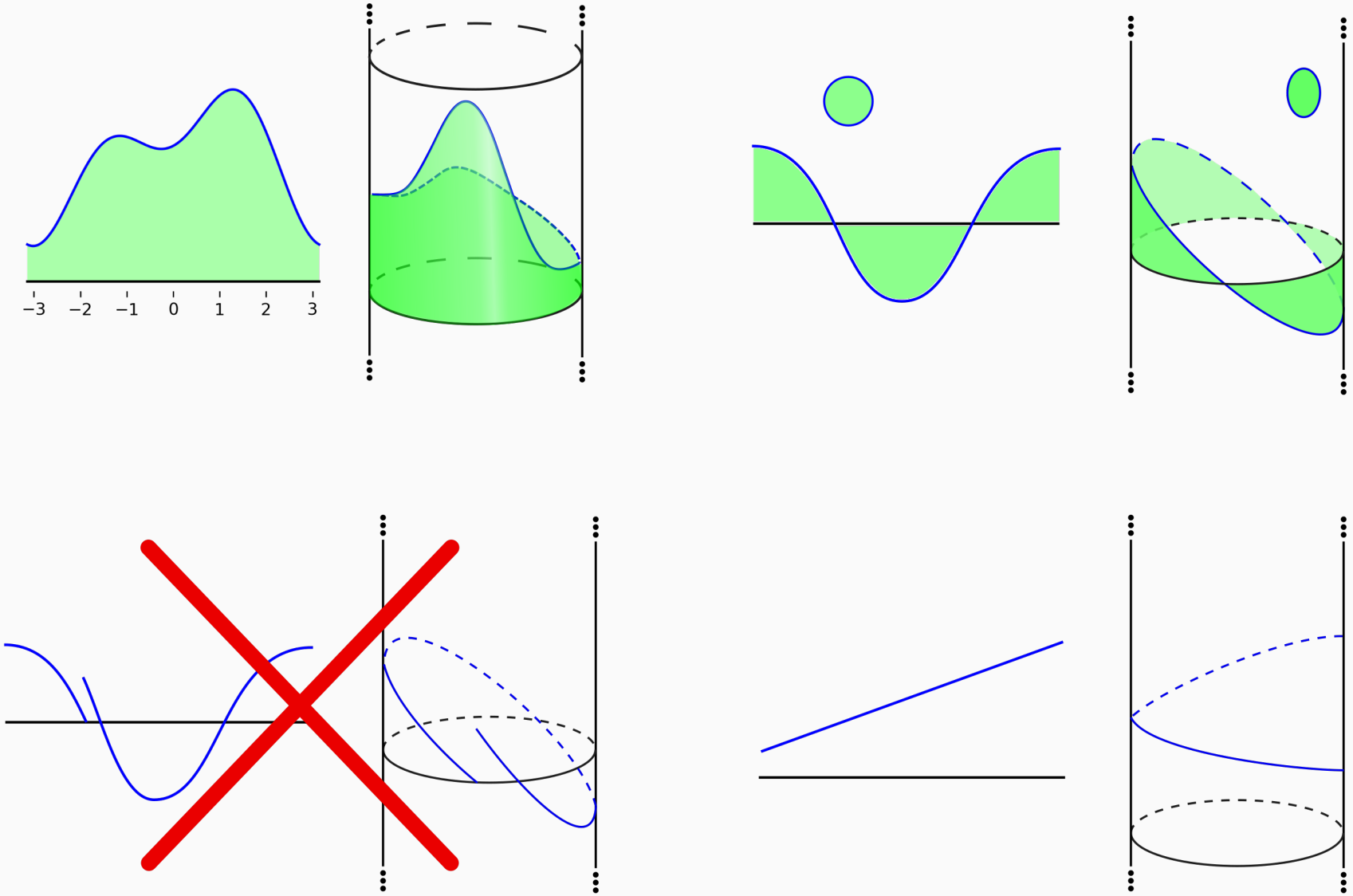

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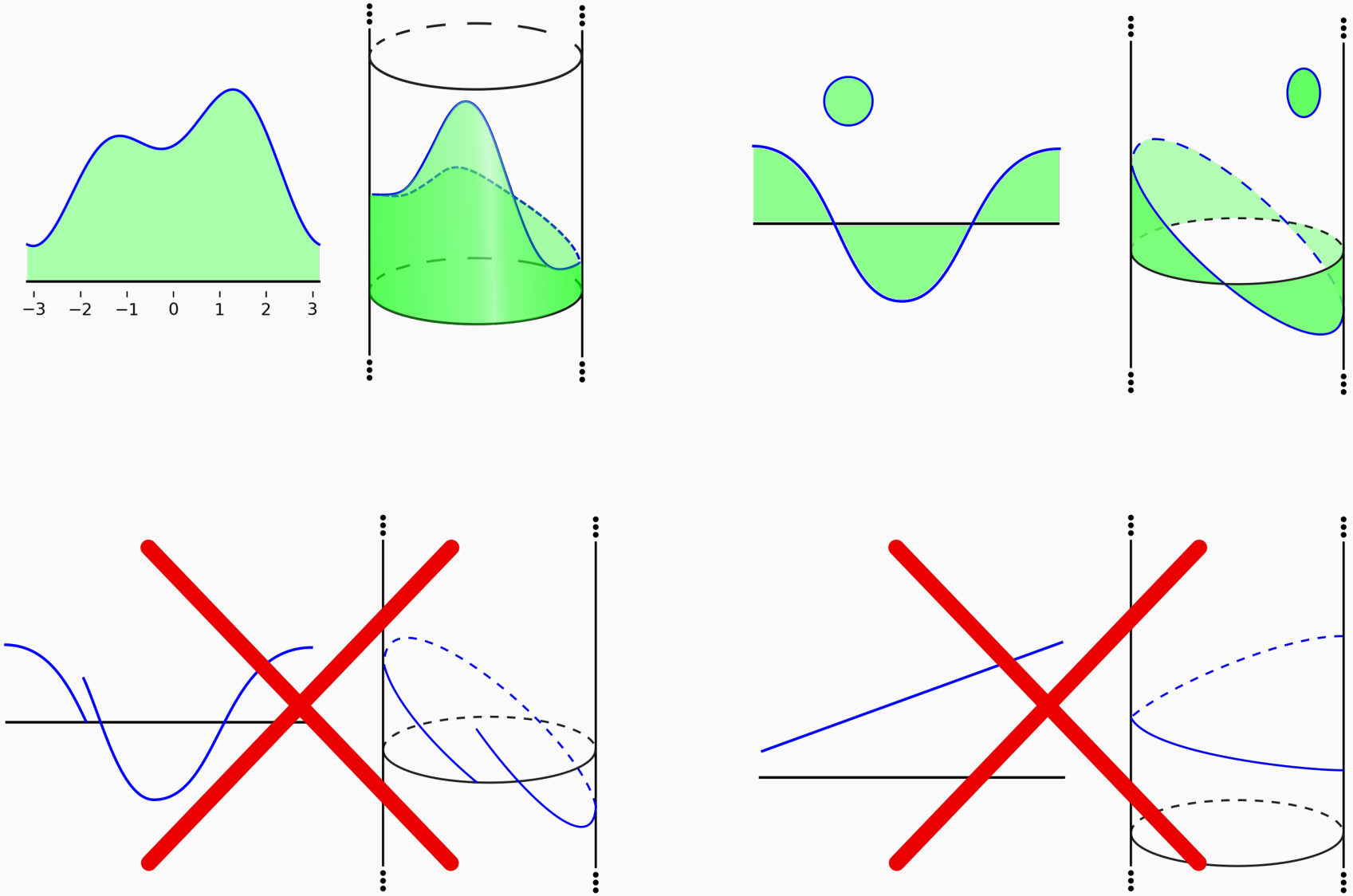

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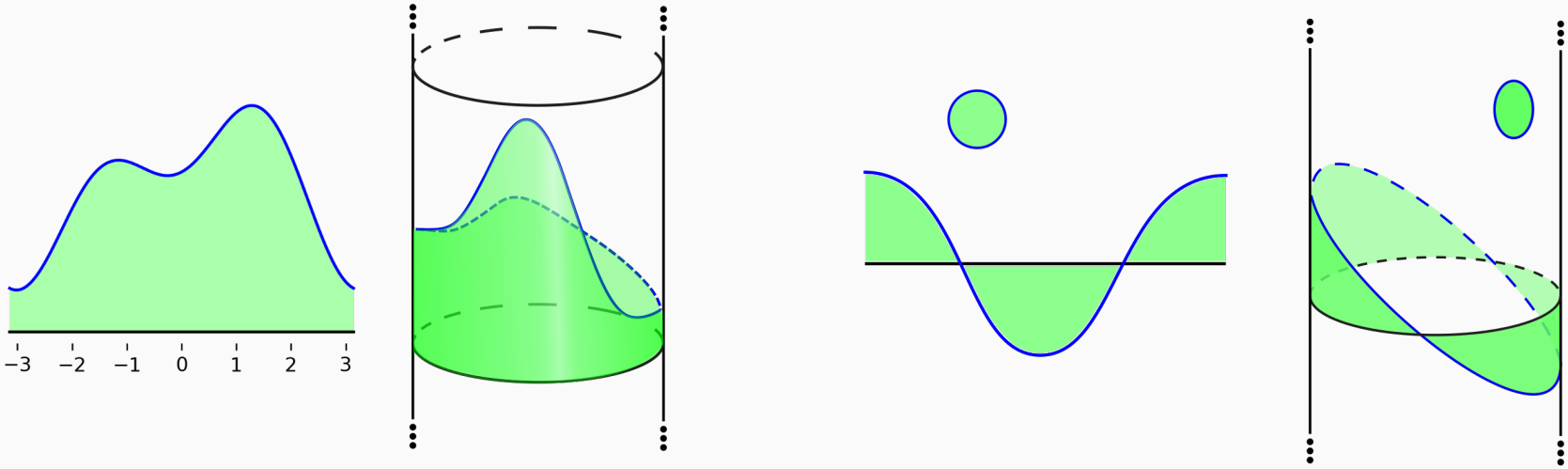

Theorem: Integrals of holomorphic functions are unchanged

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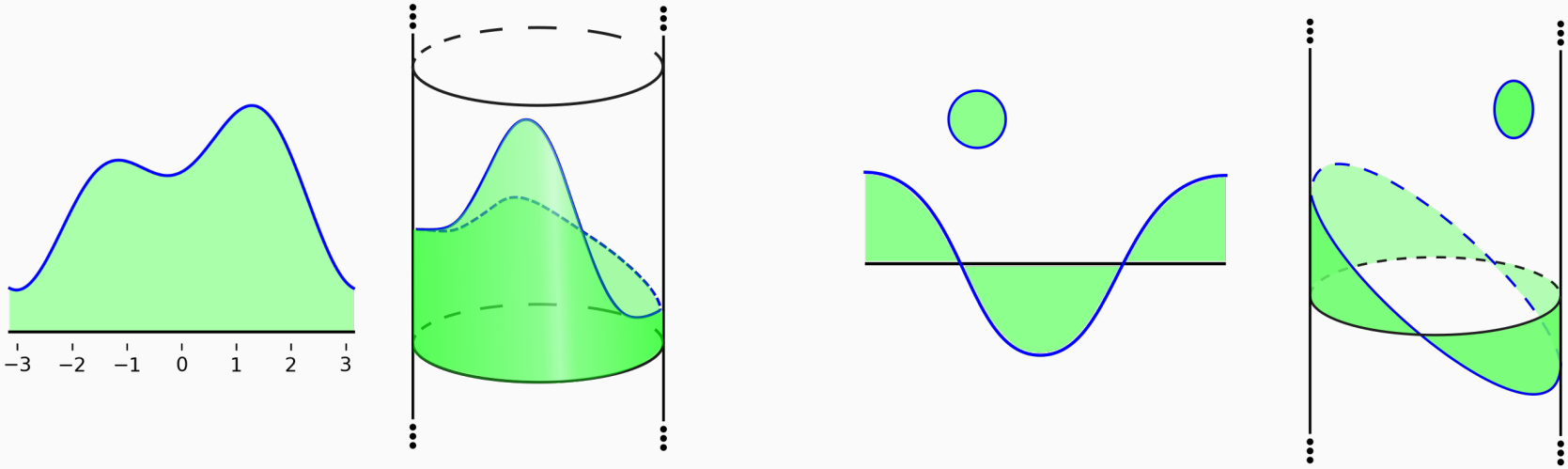
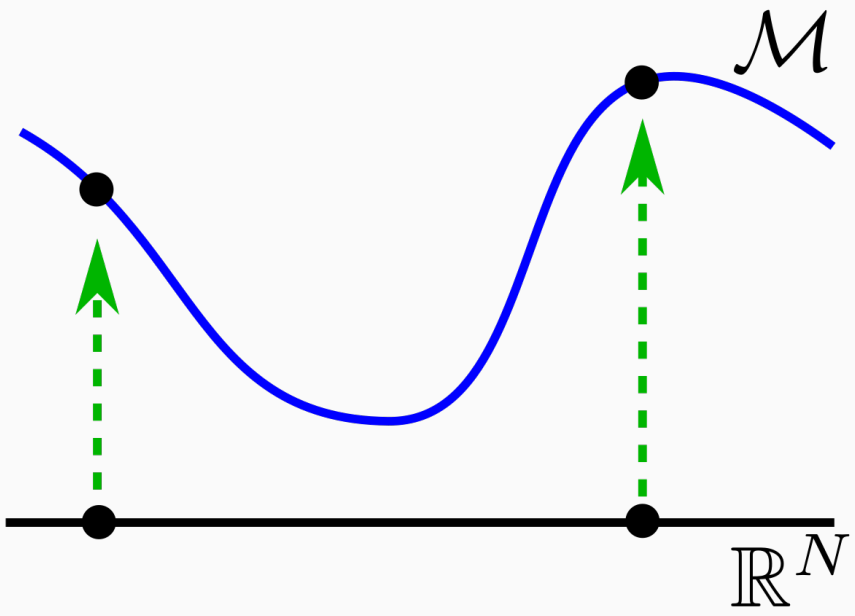


Theorem: Integrals of holomorphic functions are unchanged

$$\langle \sigma \rangle = \frac{\int_{\mathcal{M}} e^{-S}}{\int_{\mathcal{M}} e^{-\operatorname{Re} S}}$$

Integrating on Curved Manifolds

$$\int_{\mathcal{M}} \mathrm{d}z\ e^{-S[z]} = \int_{\mathbb{R}^N} \mathrm{d}x\ e^{-S[z(x)]}\ \det J$$



Heavy-Dense Thirring

The sign problem is **worst** in the **large-μ limit**.

$$\det D \to e^{V\mu}\left[e^{i\sum A_0} + \mathcal{O}\left(e^{-\beta\mu}\right)\right]$$

$$Z \to \left[\int \mathrm{d}A_0\,\mathrm{d}A_1\ \exp\left(\frac{N_F}{g^2}\cos A_0 + iA_0\right)\exp\left(\frac{N_F}{g^2}\cos A_1\right)\right]^V$$

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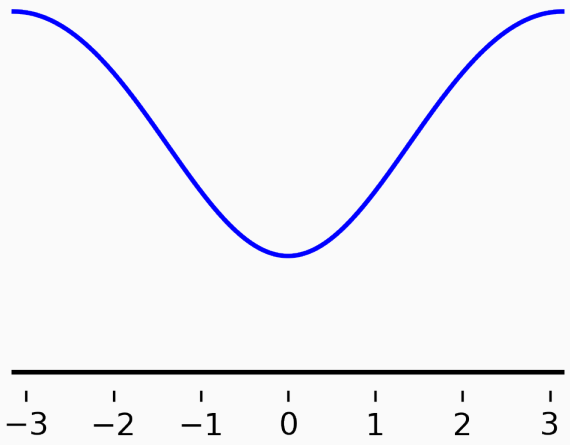

$$\mathrm{Im}\, A_0(x) = \lambda_0 + \lambda_1 \cos\left[\mathrm{Re}\, A_0(x)\right] + \cdots$$

$$J_{(\mu,x)(\nu,y)} = \delta_{\mu\nu}\delta_{xy}\left[1 - i\delta_{\mu 0}\lambda_1 \sin \mathrm{Re}\, A_0(x) + \cdots\right]$$

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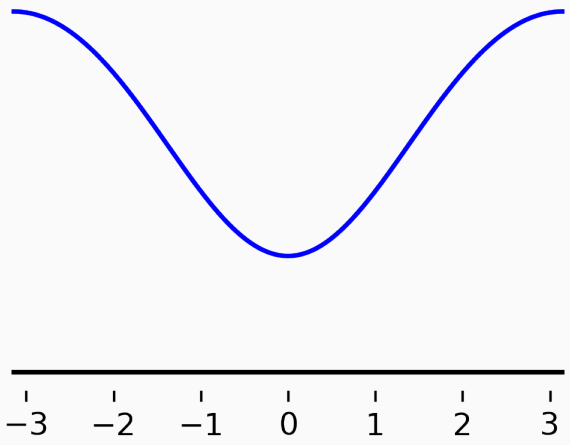

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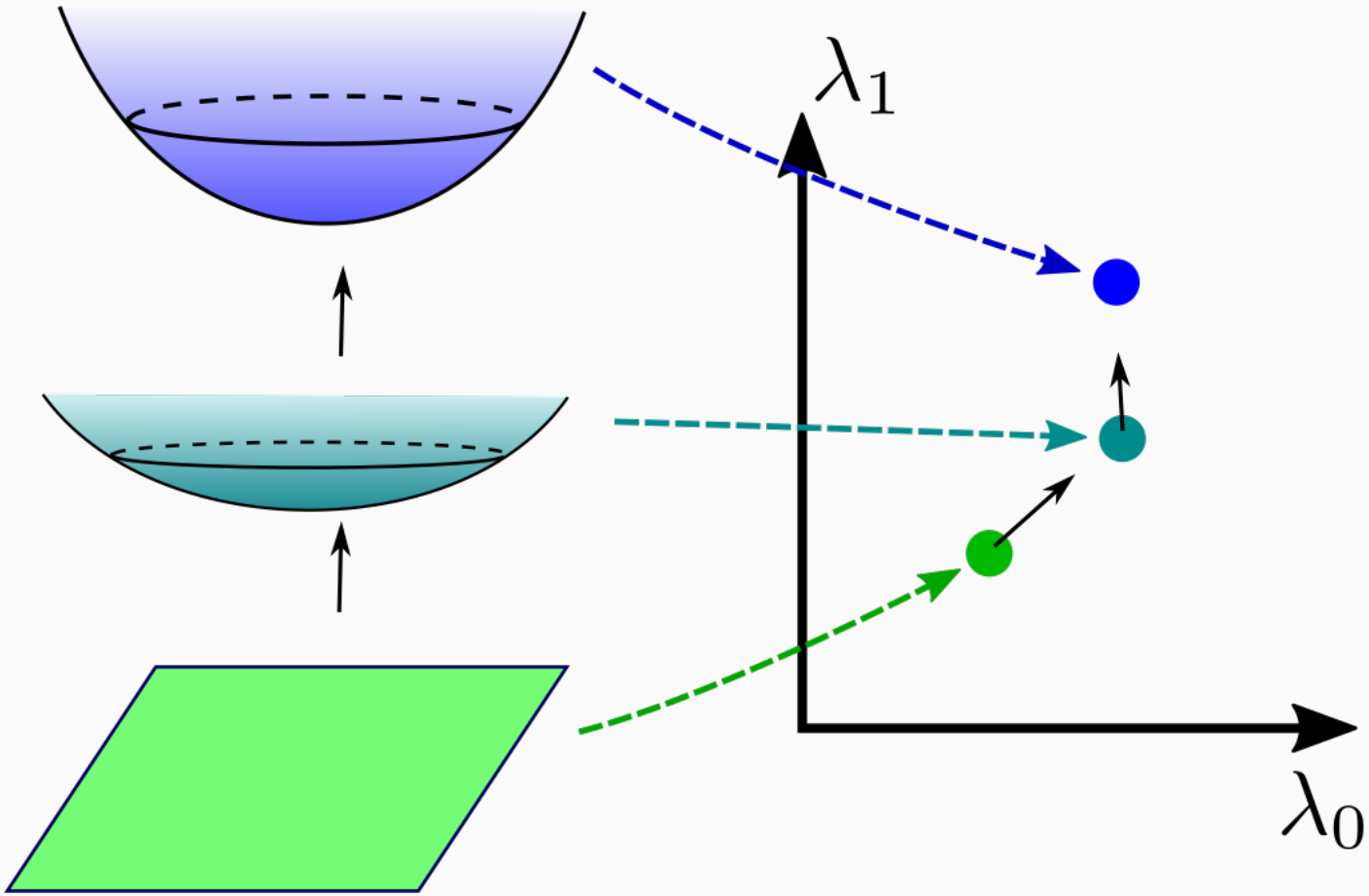
What should λ_0 and λ_1 be?

Optimizing Manifolds



Sign-Optimized Manifold Method

$$\langle \sigma \rangle \equiv \frac{\int \mathcal{D}A \; e^{-S(\phi(A)) + \log\det J}}{\int \mathcal{D}A \; e^{-S_R(\phi(A)) + \mathrm{Re}\log\det J}} = \frac{Z}{Z_{\mathrm{PQ}}}$$

Gradient descent: calculate $\nabla_\lambda \langle \sigma \rangle$. **This is hard!**

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Gradient descent: calculate $\nabla_\lambda \langle\sigma\rangle$. **This is not hard!**

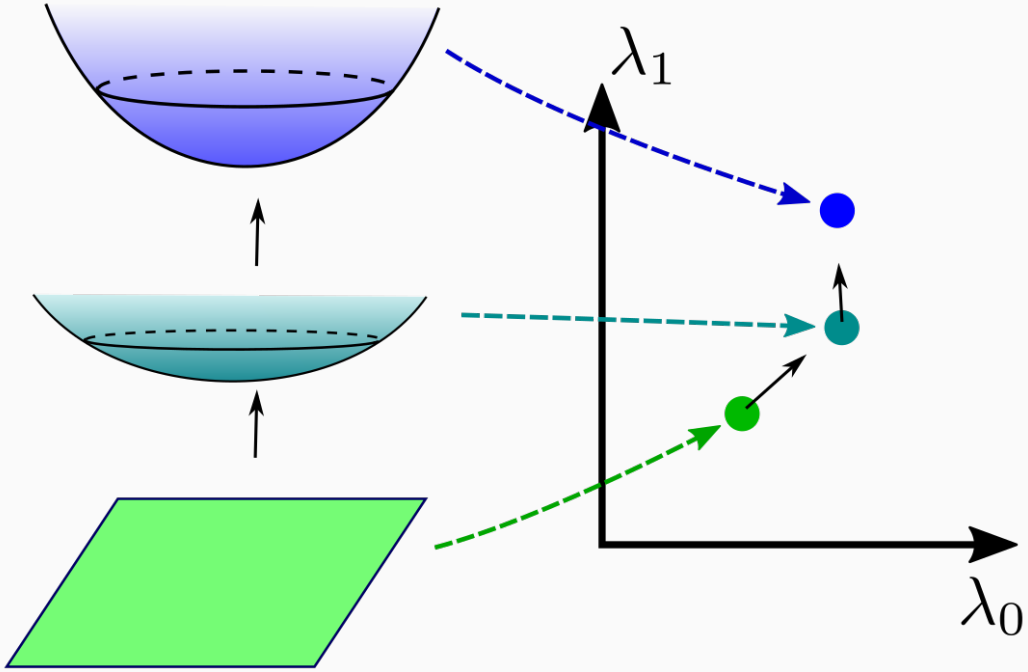
$$\nabla_\lambda Z = 0$$

That leaves $\nabla_\lambda Z_{\mathrm{PQ}}$, which is a phase-quenched observable. No sign problem!

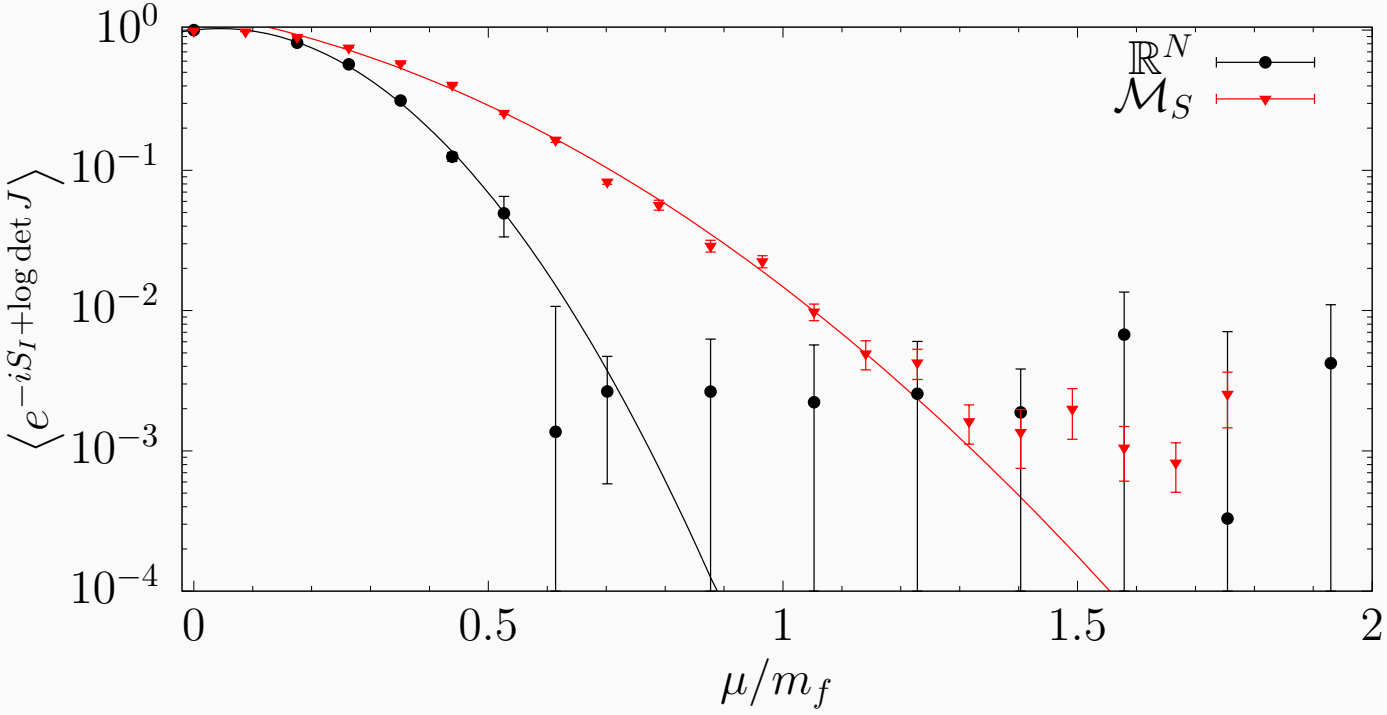
$$\nabla_\lambda \log\langle\sigma\rangle = \left\langle \nabla_\lambda S - \mathrm{Tr}\log J^{-1}\nabla_\lambda J \right\rangle_{\mathrm{Re}\, S_{\mathrm{eff}}}$$

Sign-Optimized Manifold Method

1. Start with $\mathcal{M}(\lambda^{(0)}) = \mathbb{R}^N$.
2. Evaluate $\nabla_\lambda \log \langle \sigma \rangle = \langle \nabla_\lambda S - \mathrm{Tr} \log J^{-1} \nabla_\lambda J \rangle_{\mathrm{Re}\, S_{\mathrm{eff}}}$
3. Step (with SGD) $\lambda^{(i+1)} = \lambda^{(i)} + \eta \nabla_\lambda \log \langle \sigma \rangle$
4. Repeat 2 and 3 until bored

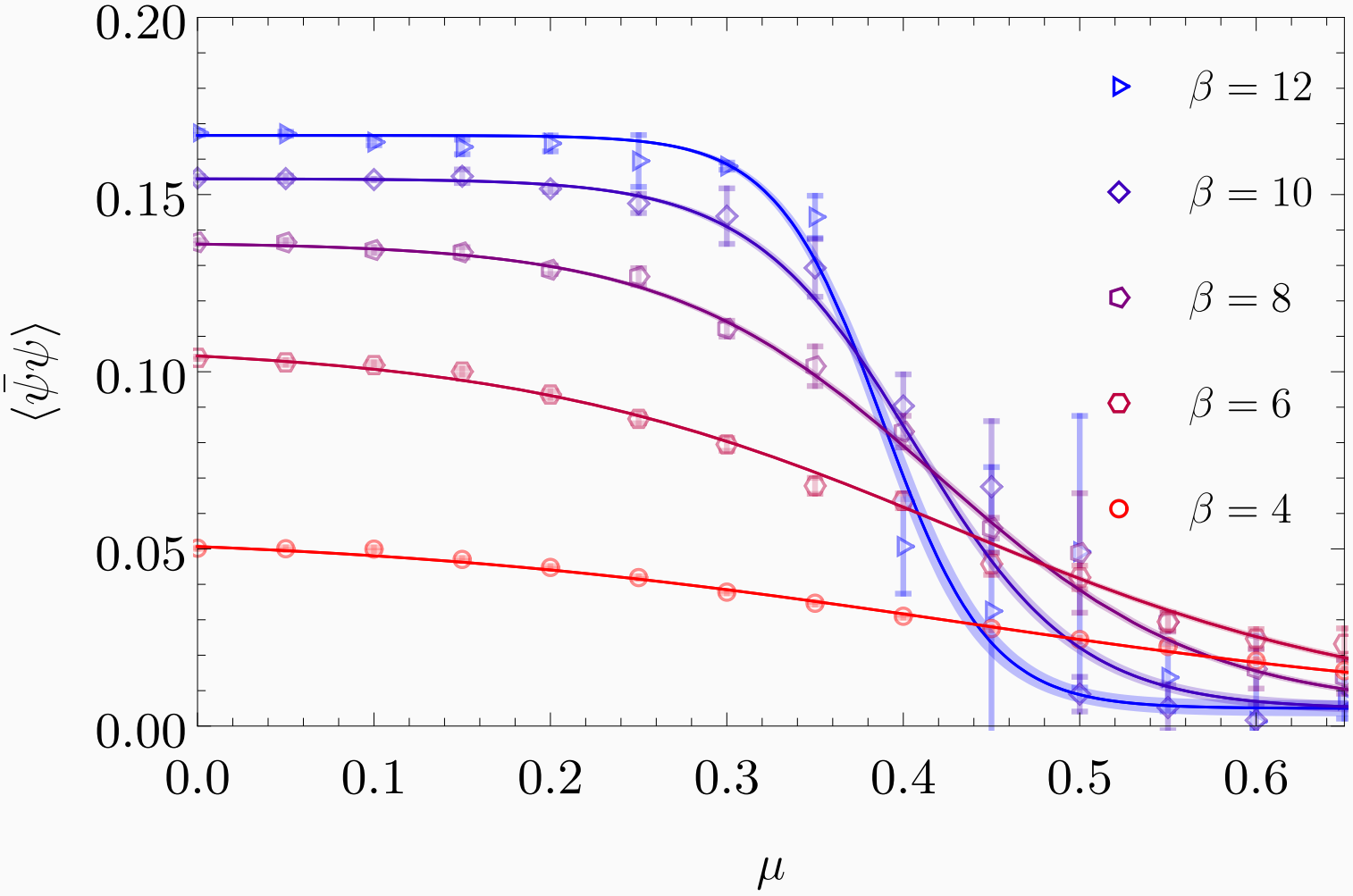


Thirring $2+1$: Sign Problem



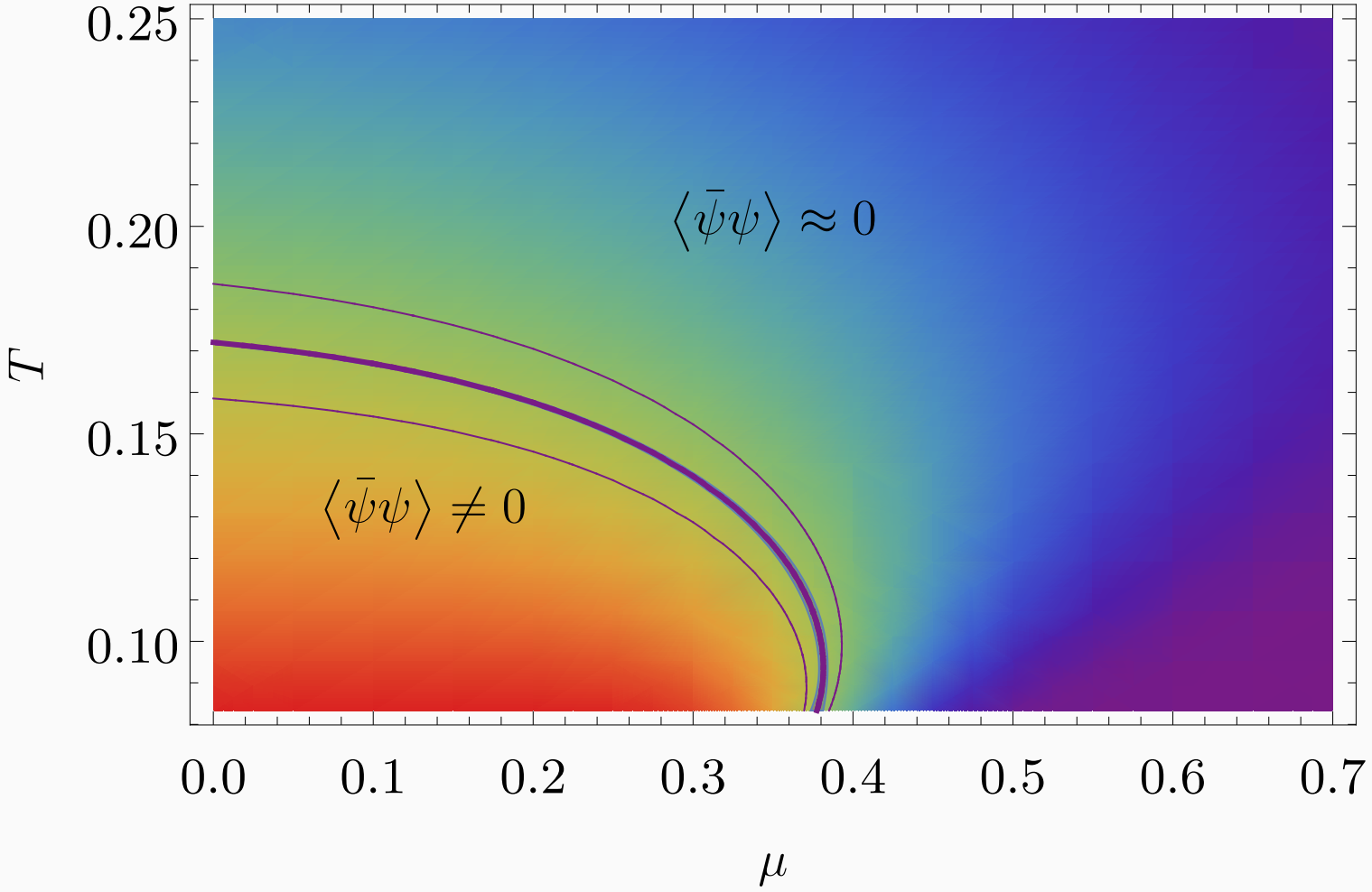
6^3 lattice with $am = 0.01$, $aM_f = 0.56 \pm 0.02$, $g = 1.08$

Thirring $2+1$: Chiral Condensate



$6^2 \times \beta$ lattice with $am = 0.01$, $aM_f = 0.56 \pm 0.02$, $g = 1.08$

Thirring $2+1$: Chiral Phase Transition



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Residual Phase on Lefschetz Thimbles (Heavy-Dense)

$$Z = \int_{\mathbb{R}^N} \mathcal{D}\phi \; e^{-S[\tilde{\phi}(\phi)] + \log\det J}$$

The **residual phase** is $\mathrm{Im}\log\det J$.

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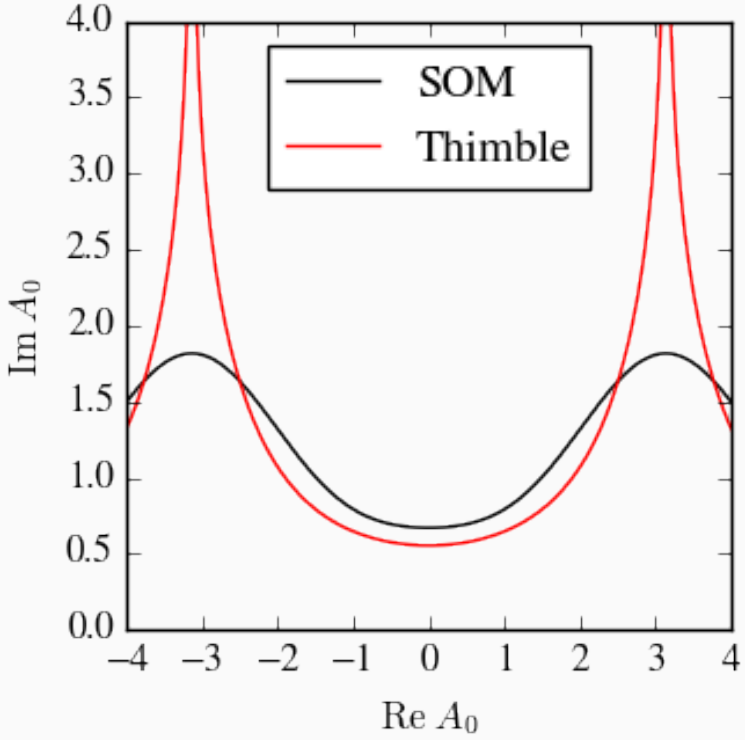

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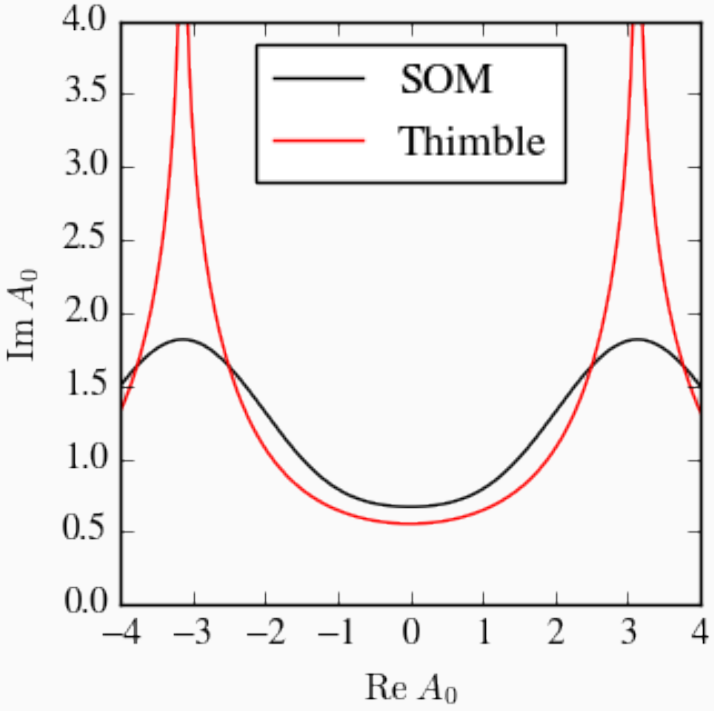

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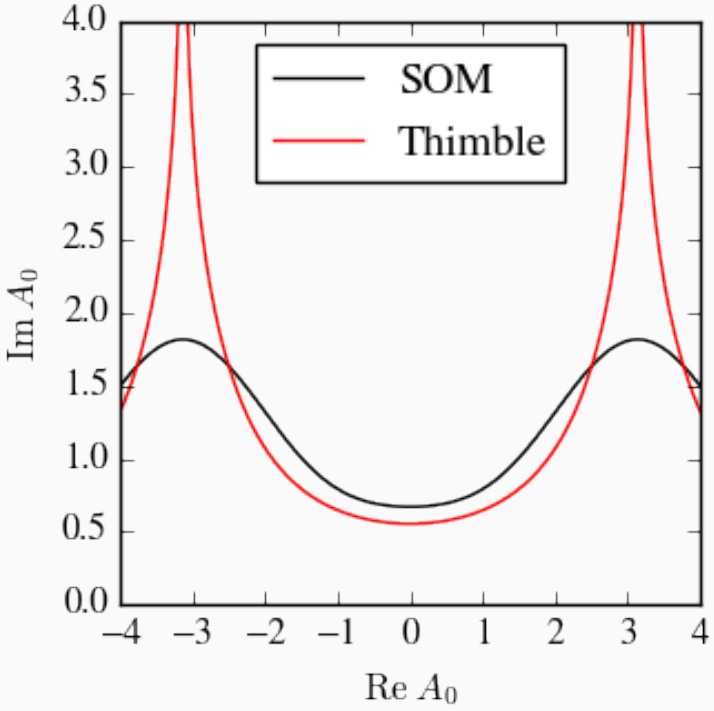

	Single site	10^3 lattice
$\mathbb{R}^N$	0.645	10^{-190}
$\mathcal{M}_T$	0.985	3×10^{-7}
$\mathcal{M}_{\mathrm{SOM}}$	0.9996	0.67

Holomorphic Integrands for Physical Observables

$$Z = \int \mathcal{D}A \, e^{-S_B} \det D = \int \mathcal{D}A \, e^{-\overbrace{S_B - \log \det D}^{S_{\text{eff}}}}$$

Effective action isn't holomorphic, but the integrand is!

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$$\int \mathrm{d}\bar{\psi}\mathrm{d}\psi \int \mathcal{D}A\, e^{-S_B} \underbrace{e^{-\bar{\psi}_a D_{ab}(A)\psi_b}}_{=1-\bar{\psi}_a D_{ab}(A)\psi_b+\cdots} \bar{\psi}_i \psi_j \bar{\psi}_j \psi_i$$

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$$\int \mathrm{d}\bar{\psi}\mathrm{d}\psi \int \mathcal{D}A \left[f_0(A) + f_{ab}(A)\bar{\psi}_a\psi_b + \cdots \right] \bar{\psi}_i \psi_j \bar{\psi}_j \psi_i$$

Obstacles and Outlook

- What manifolds are good for gauge theories?
- Are there always manifolds with $\langle \sigma \rangle \sim 1$?

- New families of manifolds (Bursa, Kroyter, arXiv:1805.04941)
- Apply to gauge theories (following arXiv:1807.02027)
- Real-time calculations: transport coefficients, etc.

Outline

Fermion Sign Problem

Cauchy Generalized

Thirring Model

Contour Integration

Curved Manifolds

SOMME

Results

Beating the Thimbles

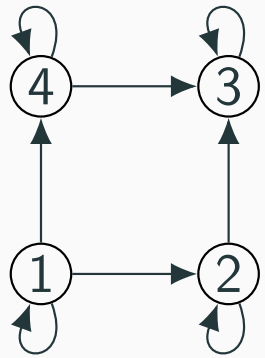
Holomorphic Integrands

Future Work

Origin of the Smile

Subgraph Expansion of the Fermion Determinant

$$D = \begin{pmatrix} m & e^{iA_1(x_1)} & 0 & e^{\mu+iA_0(x_1)} \\ e^{-iA_1(x_1)} & m & e^{\mu+iA_0(x_2)} & 0 \\ 0 & e^{-\mu-iA_0(x_2)} & m & e^{-iA_1(x_3)} \\ e^{-\mu-iA_0(x_1)} & 0 & e^{iA_1(x_3)} & m \end{pmatrix} \sim$$



$\longrightarrow = e^{iA_1(x)}$ $\uparrow = e^{iA_0(x)+\mu}$ $\downarrow = e^{-iA_0(x)-\mu}$  $= m$

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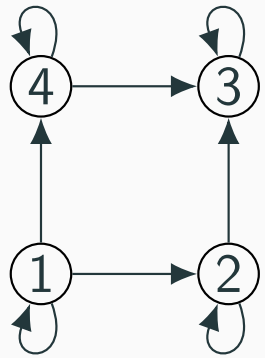
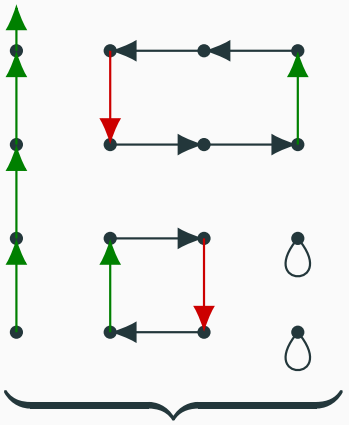


$\longrightarrow = e^{iA_1(x)}$ $\quad \uparrow = e^{iA_0(x)+\mu}$ $\quad \downarrow = e^{-iA_0(x)-\mu}$ $\quad$  $= m$

$\det D =$

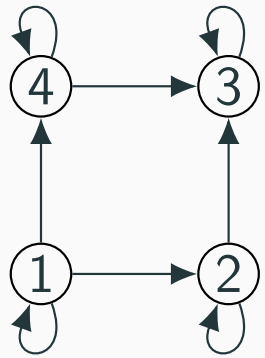


$+ \cdots$

$\propto e^{\beta\mu}$

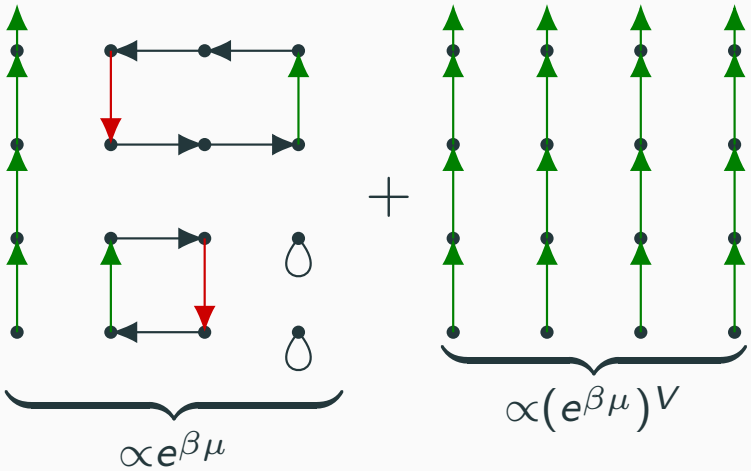
Subgraph Expansion of the Fermion Determinant

$$D = \begin{pmatrix} m & e^{iA_1(x_1)} & 0 & e^{\mu+iA_0(x_1)} \\ e^{-iA_1(x_1)} & m & e^{\mu+iA_0(x_2)} & 0 \\ 0 & e^{-\mu-iA_0(x_2)} & m & e^{-iA_1(x_3)} \\ e^{-\mu-iA_0(x_1)} & 0 & e^{iA_1(x_3)} & m \end{pmatrix} \sim$$



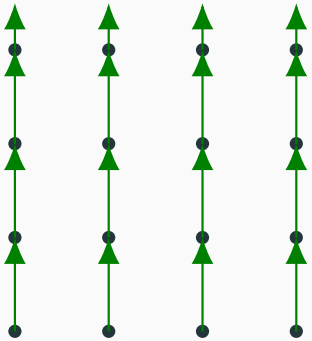
$\longrightarrow = e^{iA_1(x)}$ $\uparrow = e^{iA_0(x)+\mu}$ $\downarrow = e^{-iA_0(x)-\mu}$  $= m$

$\det D =$

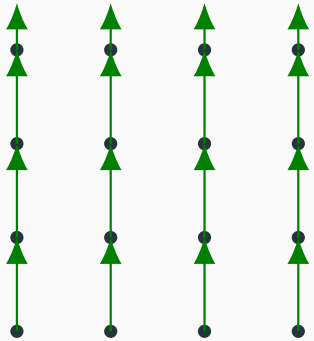


$+ \cdots$

Origin of the Smile: Large-μ Limit

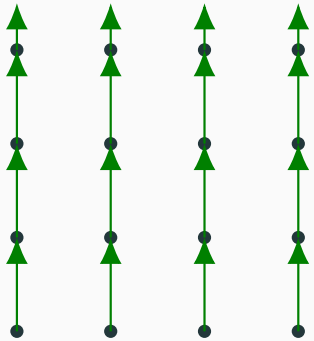
$\det D =$  $= e^{V\beta\mu}\left[e^{i\sum_x A_0(x)} + O\left(e^{-\beta\mu}\right)\right]$

Origin of the Smile: Large-μ Limit

$\det D =$  $= e^{V\beta\mu}\left[e^{i\sum_x A_0(x)} + O\left(e^{-\beta\mu}\right)\right]$

$$Z \approx e^{V\beta\mu}\int\left[\prod_x \mathrm{d}A_0(x)\mathrm{d}A_1(x)\right]\prod_x e^{\cos A_0(x)+iA_0(x)}e^{\cos A_1(x)}$$

Origin of the Smile: Large-μ Limit

$\det D =$  $= e^{V\beta\mu}\left[e^{i\sum_x A_0(x)} + O\left(e^{-\beta\mu}\right)\right]$

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$$Z \approx e^{V\beta\mu}\left[\int \mathrm{d}A_1(x)\; e^{\cos A_1(x)}\right]^V\left[\int \mathrm{d}A_0(x)\; e^{\cos A_0(x)+ix}\right]^V$$