

Beyond Thimbles: Sign-Optimized Manifolds for Finite Density

Scott Lawrence

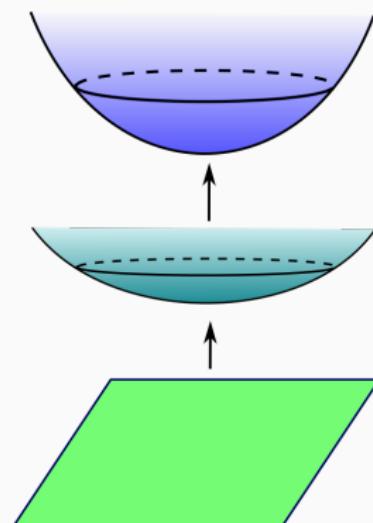
with Andrei Alexandru, Paulo Bedaque,

Henry Lamm, Neill Warrington

Based on 1804.00697 and 18xx.xxxxx

23 July 2018

Lattice 2018



The Fermion Sign Problem

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 $p(\phi) \propto e^{-S(\phi)}$.

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What if S isn't real?

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

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

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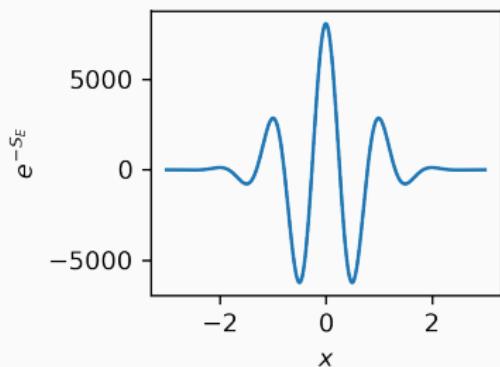
QCD (finite density), Hubbard model (away from half-filling)

Thirring model, **QED** (both at finite density)

The Sign Problem: A Gaussian Example

The simplest toy sign problem: $S_E = (x - i\mu)^2$.

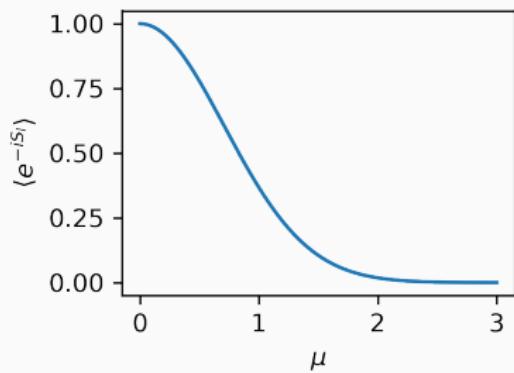
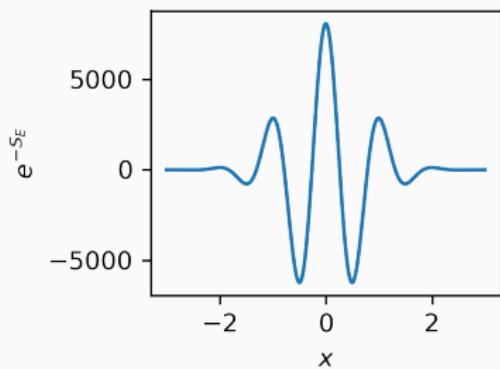
$$\langle x^2 \rangle = \frac{\int_{-\infty}^{\infty} dx \ x^2 \ e^{-(x-i\mu)^2}}{\int_{-\infty}^{\infty} dx \ e^{-(x-i\mu)^2}}$$



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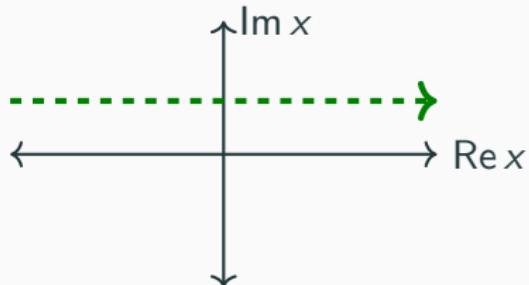
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Invoke Cauchy's theorem!

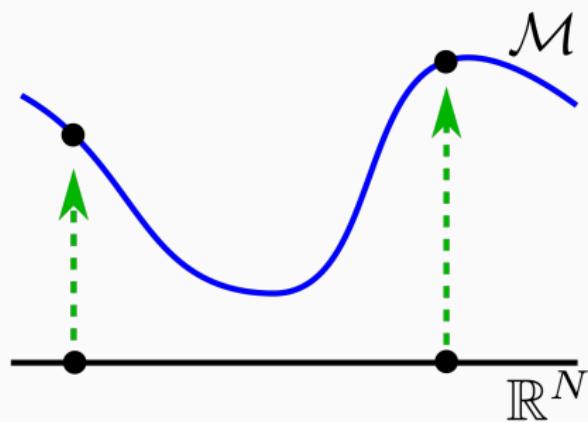


$$Z(\mu) = \int_{-\infty+i\mu}^{\infty+i\mu} dx \ e^{-(x-i\mu)^2} = \int_{-\infty}^{\infty} dx \ e^{-x^2}$$

No sign problem!

Integrating on Curved Manifolds

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



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

$$\begin{aligned} D_{xy}[A] = m\delta_{xy} + \frac{1}{2} \sum_\nu & \left[e^{iA_\nu(x) + \mu\delta_{\nu 0}} \delta_{x,(y+\hat{\mu})} (-1)^{x_0 + \dots + x_{\nu-1}} \right. \\ & \left. - e^{-iA_\nu(x) - \mu\delta_{\nu 0}} \delta_{(x+\hat{\mu}),y} (-1)^{x_0 + \dots + x_{\nu-1}} \right] \end{aligned}$$

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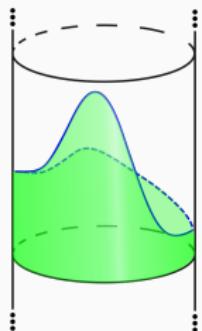
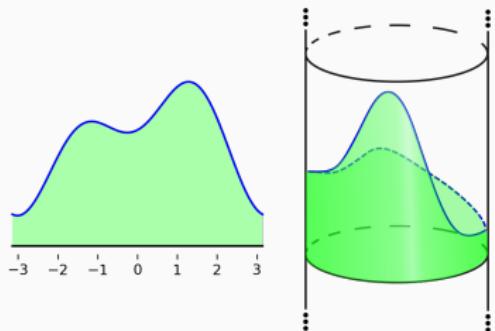
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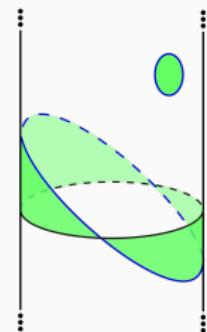
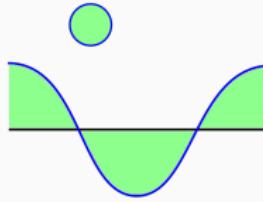
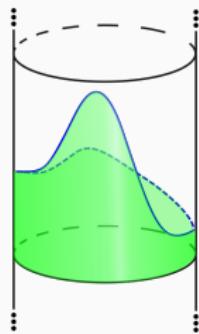
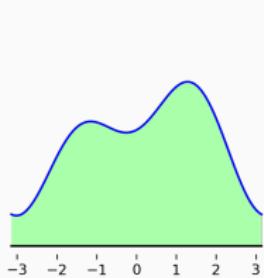
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Fields are periodic.

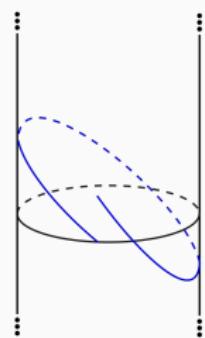
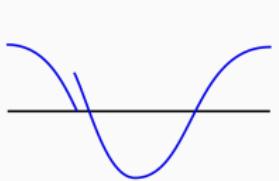
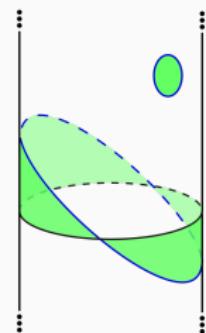
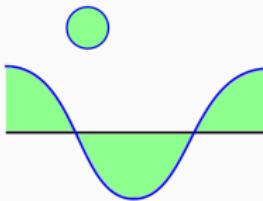
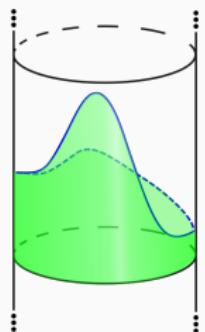
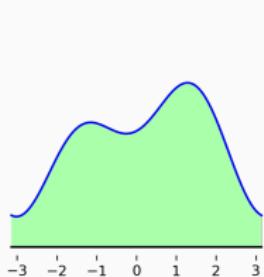
Contour Integration Rules!



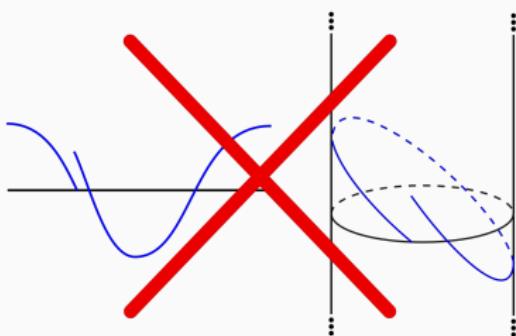
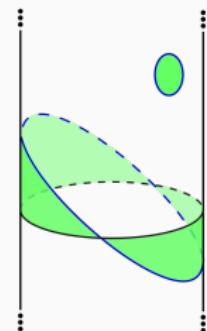
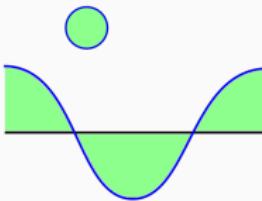
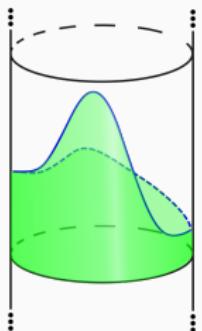
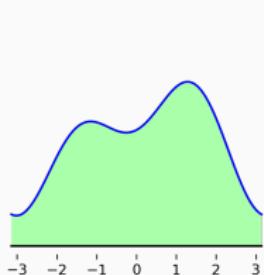
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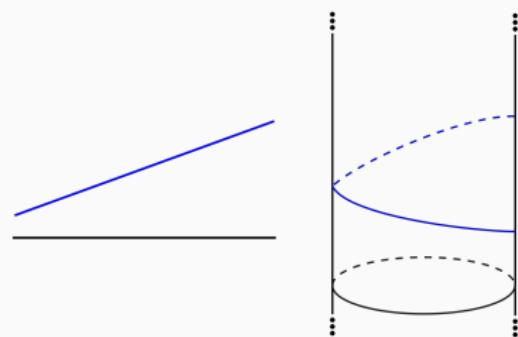
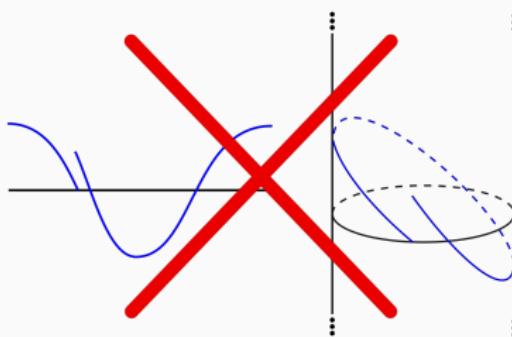
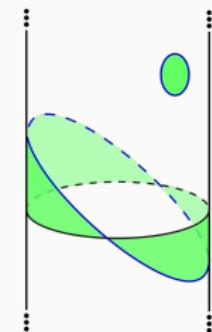
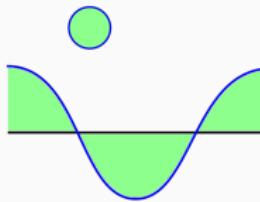
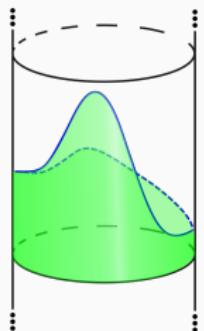
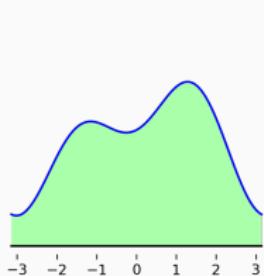
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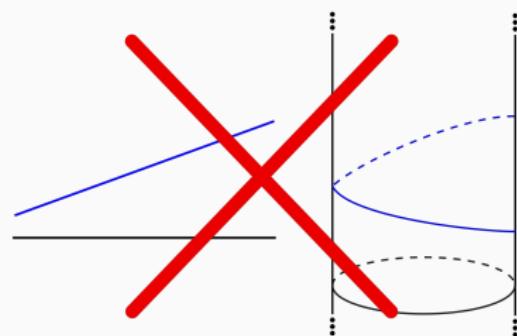
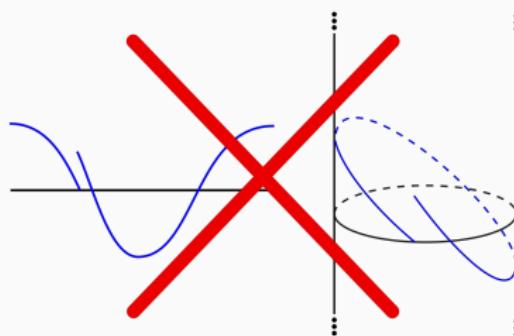
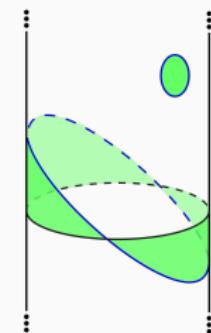
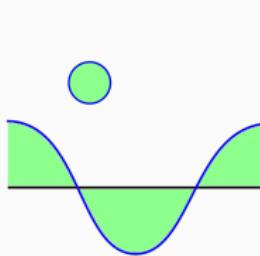
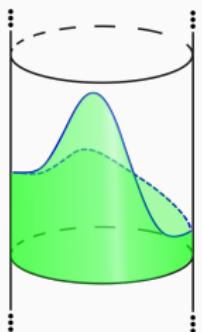
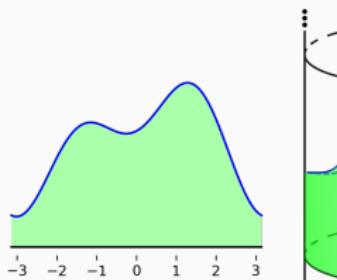
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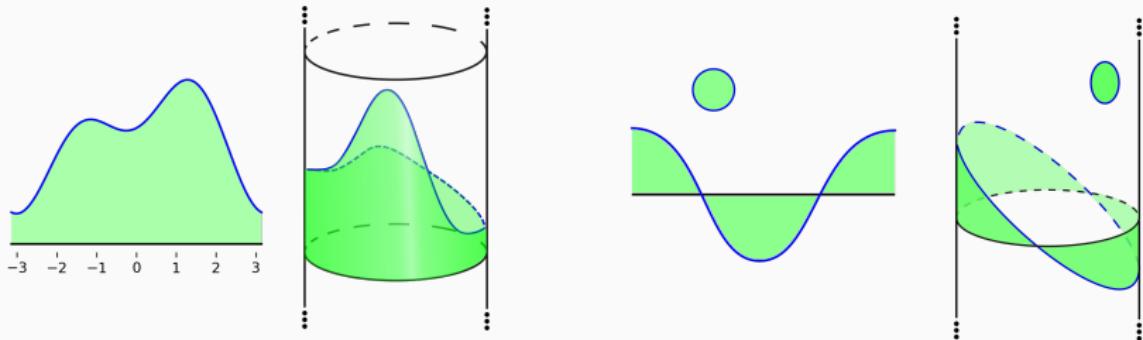
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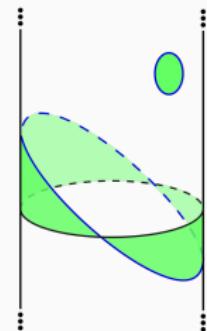
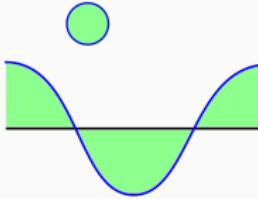
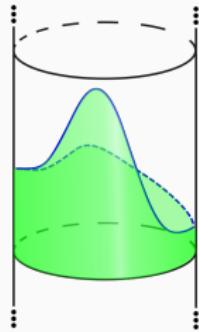
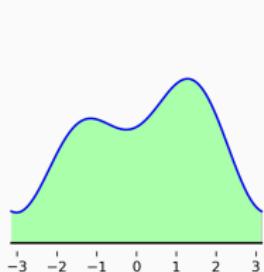


Contour Integration Rules!



Theorem: Integrals of holomorphic functions are unchanged

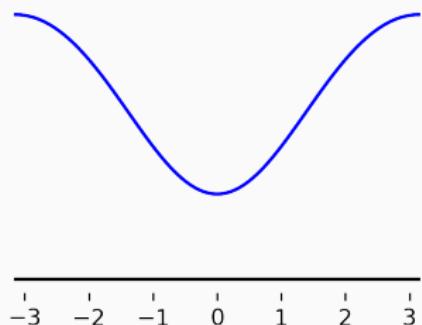
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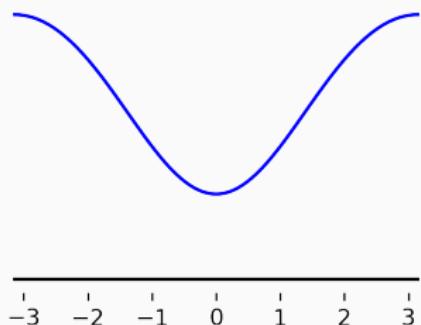
$$\langle \sigma \rangle = \frac{\int_{\mathcal{M}} e^{-S}}{\int_{\mathcal{M}} e^{-\text{Re } S}}$$

An Ansatz for Thirring



$$\operatorname{Im} A_0(x) = \lambda_0 + \lambda_1 \cos [\operatorname{Re} A_0(x)] + \dots$$

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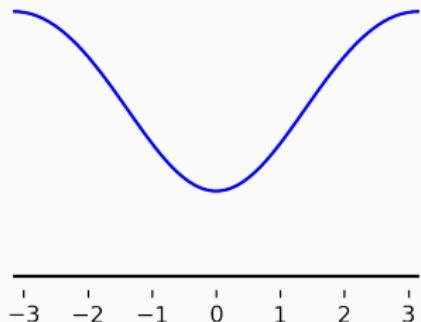


$$\operatorname{Im} A_0(x) = \lambda_0 + \lambda_1 \cos [\operatorname{Re} A_0(x)] + \dots$$

A very special property: J is diagonal!

$$J_{(x,\mu)(y,\nu)} \equiv \delta_{ij} + \frac{\partial \operatorname{Im} A_\mu(x)}{\partial \operatorname{Re} A_\nu(y)} = \delta_{ij} (1 - i \delta_{0\mu} \sin [\operatorname{Re} A_0(x)])$$

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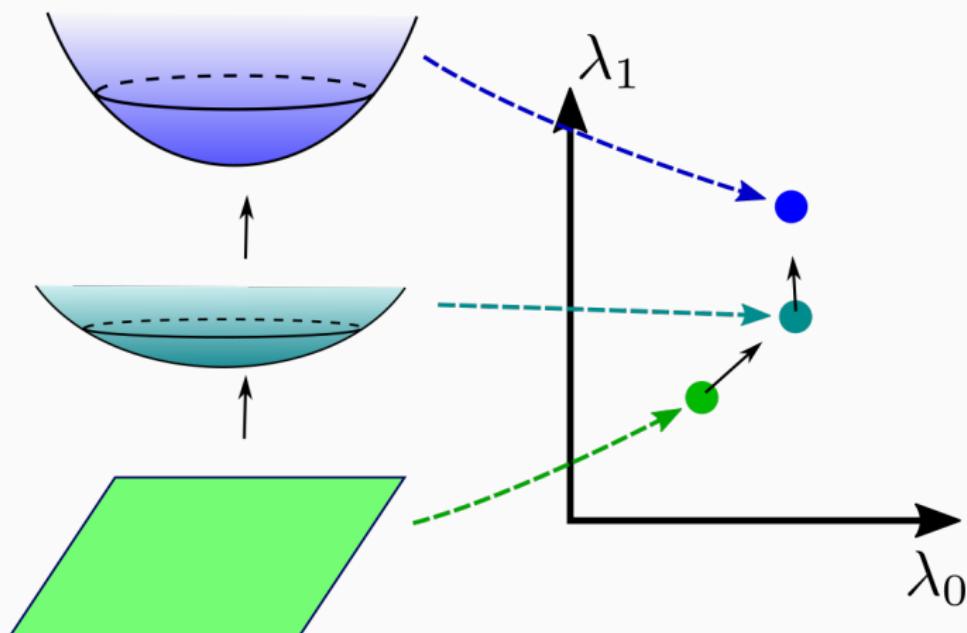
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What should λ_0 and λ_1 be?

Optimizing Manifolds



Sign-Optimized Manifold Method

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

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

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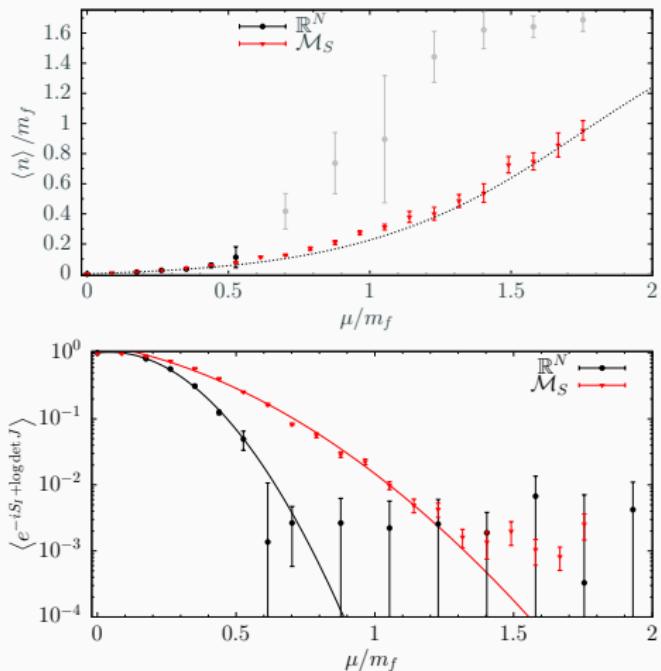
Gradient descent: calculate $\nabla_\lambda \langle \sigma \rangle$. **This is not hard!**

$$\nabla_\lambda Z = 0$$

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

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

Finite Density Thirring Model in $2+1$ Dimensions



6^3 lattice

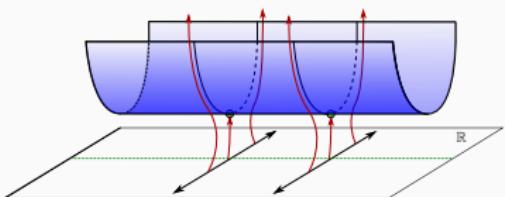
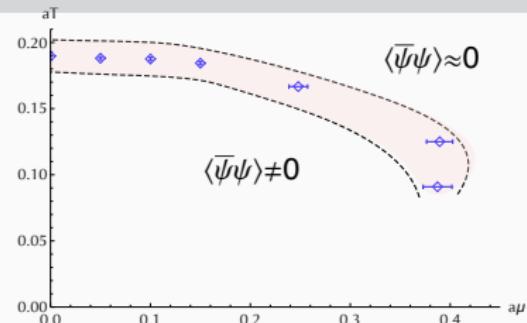
$am = 0.01$

$aM_f \approx 0.56 \pm 0.02$

$g = 1.08$

Outlook, Near And Far

Get a phase diagram!
(Neill Warrington)

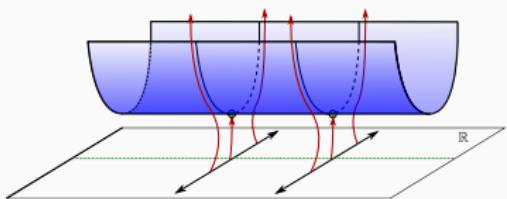
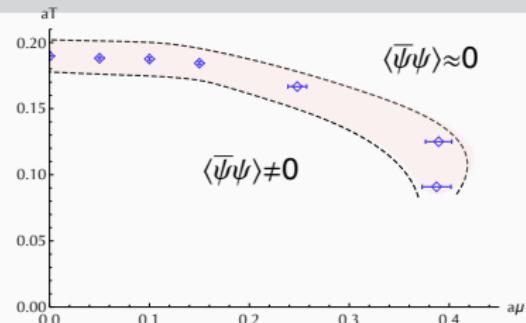


Extend to gauge theories!
(Henry Lamm)

Ohnishi et al., Saturday 11:15 (1805.08940, 1712.01088)

Outlook, Near And Far

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Extend to gauge theories!
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Ohnishi et al., Saturday 11:15 (1805.08940, 1712.01088)

- Identify more general families of manifolds
- Apply to the Hubbard model
- Real-time calculations: transport coefficients, etc.

Outline

Fermion Sign Problem

Curved Manifolds

Thirring Model

Contour Integration

SOMME

Results

Future Work

Holomorphic Integrands

Origin of the Smile

Cauchy Generalized

Holomorphic Integrands for Physical Observables

$$\left\langle \bar{\psi}_i \psi_j \bar{\psi}_j \psi_i \right\rangle = \frac{1}{Z} \int \mathcal{D}A e^{-S_B} \left(D_{ij}^{-1} D_{ji}^{-1} - D_{ii}^{-1} D_{jj}^{-1} \right) \det D$$

Integrand doesn't look holomorphic!

Holomorphic Integrands for Physical Observables

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Integrand doesn't look holomorphic! Look at the pre-fermion-integration expression.

$$\int d\bar{\psi} d\psi \int \mathcal{D}A e^{-S_B} \underbrace{e^{-\bar{\psi}_i D_{ij}(A) \psi_j}}_{=1-\bar{\psi}_i D_{ij}(A) \psi_j + \dots} \bar{\psi}_i \psi_j \bar{\psi}_j \psi_i;$$

Holomorphic Integrands for Physical Observables

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$$\int d\bar{\psi} d\psi \int \mathcal{D}A \left[f_0(A) + f_{ij}(A) \bar{\psi}_i \psi_j + \dots \right] \bar{\psi}_i \psi_j \bar{\psi}_j \psi_i$$

Subgraph Expansion of the Fermion Determinant

$$D = \begin{pmatrix} m & e^{iA_1(x_1)} & 0 & e^{\mu+iA_0(x_1)} \\ e^{-iA_1(x_1)} & m & e^{\mu+iA_0(x_2)} & 0 \\ 0 & e^{-\mu-iA_0(x_2)} & m & e^{-iA_1(x_3)} \\ e^{-\mu-iA_0(x_1)} & 0 & e^{iA_1(x_3)} & m \end{pmatrix} \sim \begin{array}{c} \text{Diagram of a directed graph with 4 nodes (1, 2, 3, 4) and edges (1,2), (2,3), (3,4), (4,1). Each node has a self-loop arrow pointing upwards.} \\ \longrightarrow = e^{iA_1(x)} \quad \uparrow = e^{iA_0(x)+\mu} \quad \downarrow = e^{-iA_0(x)-\mu} \quad \text{---} = m \end{array}$$

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

$$\det D = \underbrace{\dots}_{\propto e^{\beta \mu}} + \dots$$

The diagram shows a subgraph expansion of the determinant. It consists of two parts: a summand proportional to $e^{\beta \mu}$ (indicated by a brace under the first term) and higher-order terms. The first term is represented by a directed graph with four nodes (1, 2, 3, 4) and edges (1,2), (2,3), (3,4), (4,1). Each node has a self-loop. Arrows indicate directionality: nodes 1, 2, and 3 have green arrows pointing upwards, while node 4 has a red arrow pointing downwards. The second part is indicated by a plus sign followed by three dots.

Subgraph Expansion of the Fermion Determinant

$$D = \begin{pmatrix} m & e^{iA_1(x_1)} & 0 & e^{\mu+iA_0(x_1)} \\ e^{-iA_1(x_1)} & m & e^{\mu+iA_0(x_2)} & 0 \\ 0 & e^{-\mu-iA_0(x_2)} & m & e^{-iA_1(x_3)} \\ e^{-\mu-iA_0(x_1)} & 0 & e^{iA_1(x_3)} & m \end{pmatrix} \sim \begin{array}{c} \text{Diagram of a directed graph with nodes } 1, 2, 3, 4 \text{ and edges } (1,2), (2,3), (3,4), (4,1). \text{ Nodes } 1, 2, 3 \text{ have self-loops.} \\ \text{Legend: } \rightarrow = e^{iA_1(x)}, \uparrow = e^{iA_0(x)+\mu}, \downarrow = e^{-iA_0(x)-\mu}, \text{ loop } = m \end{array}$$

$$\det D = \underbrace{\text{Diagram with vertical lines and a loop}}_{\propto e^{\beta\mu}} + \underbrace{\text{Diagram with vertical lines and multiple loops}}_{\propto (e^{\beta\mu})^V} + \dots$$

Origin of the Smile: Large- μ Limit

$$\det D = \begin{array}{c} \text{Diagram showing four vertical paths from bottom to top, each with arrows pointing up. The paths consist of vertical segments with dots at the intersections.} \\ \text{The paths are:} \\ \text{Path 1: } \cdot \rightarrow \cdot \rightarrow \cdot \rightarrow \cdot \rightarrow \uparrow \\ \text{Path 2: } \cdot \rightarrow \cdot \rightarrow \cdot \rightarrow \cdot \rightarrow \uparrow \\ \text{Path 3: } \cdot \rightarrow \cdot \rightarrow \cdot \rightarrow \cdot \rightarrow \uparrow \\ \text{Path 4: } \cdot \rightarrow \cdot \rightarrow \cdot \rightarrow \cdot \rightarrow \uparrow \end{array} = e^{V\beta\mu} \left[e^{i \sum_x A_0(x)} + O(e^{-\beta\mu}) \right]$$

Origin of the Smile: Large- μ Limit

$$\det D = \begin{array}{c} \text{Diagram showing four vertical paths from bottom to top, each with four dots and green arrows pointing up.} \\ \text{The paths are separated by small gaps.} \end{array} = e^{V\beta\mu} \left[e^{i \sum_x A_0(x)} + O(e^{-\beta\mu}) \right]$$

$$Z \approx e^{V\beta\mu} \int \left[\prod_x dA_0(x) dA_1(x) \right] \prod_x e^{\cos A_0(x) + i A_0(x)} e^{\cos A_1(x)}$$

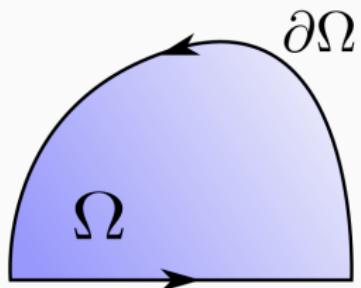
Origin of the Smile: Large- μ Limit

$$\det D = \begin{array}{c} \text{Diagram showing four vertical columns of dots with arrows pointing up.} \\ \text{The first column has 4 dots, the second 3, the third 2, and the fourth 1.} \end{array} = e^{V\beta\mu} \left[e^{i \sum_x A_0(x)} + O(e^{-\beta\mu}) \right]$$

$$Z \approx e^{V\beta\mu} \int \left[\prod_x dA_0(x) dA_1(x) \right] \prod_x e^{\cos A_0(x) + iA_0(x)} e^{\cos A_1(x)}$$

$$Z \approx e^{V\beta\mu} \left[\int dA_1(x) e^{\cos A_1(x)} \right]^V \left[\int dA_0(x) e^{\cos A_0(x) + ix} \right]^V$$

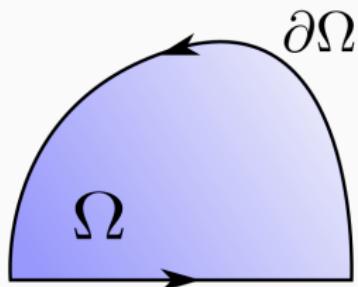
Cauchy's Integral Theorem



For any holomorphic function $f(z)$:

$$0 = \int_{\partial\Omega} f \, dz$$

Cauchy's Integral Theorem



For any holomorphic function $f(z)$:

$$0 = \int_{\partial\Omega} f \, dz$$

$$\int_{\gamma_1} f \, dz = \int_{\gamma_2} f \, dz$$

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

