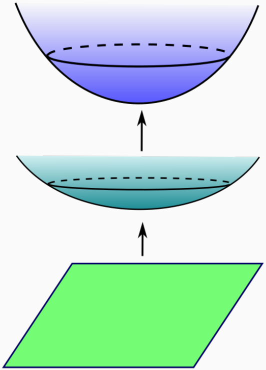
Beyond Thimbles:
Sign-Optimized Manifolds for Finite Density



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

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

What if S isn't real?

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

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

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

What if S isn't real?

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

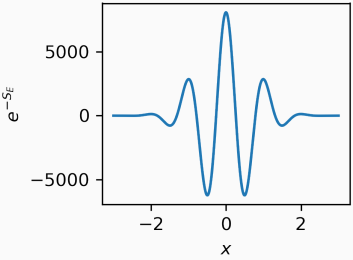
The **average phase** $\langle \sigma \rangle$ may be **small**.

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

The Sign Problem: A Gaussian Example

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

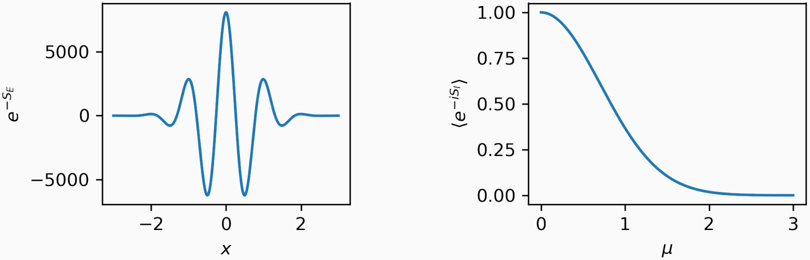
$$\left\langle x^2 \right\rangle = \frac{\int_{-\infty}^{\infty} \mathrm{d}x\ x^2\ e^{-(x-i\mu)^2}}{\int_{-\infty}^{\infty} \mathrm{d}x\ e^{-(x-i\mu)^2}}$$



The Sign Problem: A Gaussian Example

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

$$\left\langle x^2 \right\rangle = \frac{\int_{-\infty}^{\infty} \mathrm{d}x \; x^2 \; e^{-(x-i\mu)^2}}{\int_{-\infty}^{\infty} \mathrm{d}x \; e^{-(x-i\mu)^2}}$$



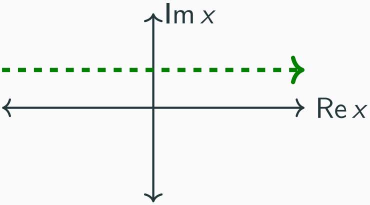
The Sign Problem: A Gaussian Solution

$$\left\langle x^2 \right\rangle = \frac{\int_{-\infty}^{\infty} \mathrm{d}x \; x^2 \; e^{-(x-i\mu)^2}}{\int_{-\infty}^{\infty} \mathrm{d}x \; e^{-(x-i\mu)^2}}$$

The Sign Problem: A Gaussian Solution

$$\left\langle x^2 \right\rangle = \frac{\int_{-\infty}^{\infty} \mathrm{d}x\ x^2\ e^{-(x-i\mu)^2}}{\int_{-\infty}^{\infty} \mathrm{d}x\ e^{-(x-i\mu)^2}}$$

Invoke Cauchy's theorem!

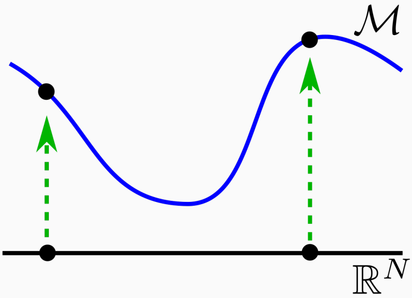


$$Z(\mu) = \int_{-\infty+i\mu}^{\infty+i\mu} \mathrm{d}x\ e^{-(x-i\mu)^2} = \int_{-\infty}^{\infty} \mathrm{d}x\ e^{-x^2}$$

No sign problem!

Integrating on Curved Manifolds

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



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

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

Testbed: Thirring Model

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

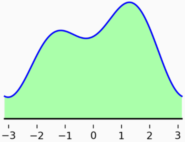
$$S_{\text{eff}}[A] = -\frac{N_F}{g^2}\sum_{x,\mu}\cos A_\mu(x) - N_F \log\det D[A]$$

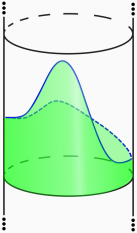
with Kogut-Susskind staggered fermions

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

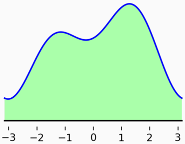
Fields are periodic.

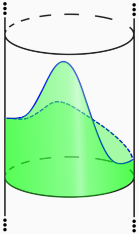
Contour Integration Rules!

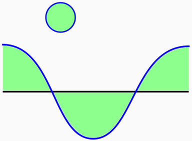


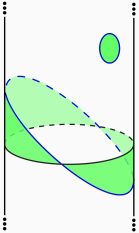


Contour Integration Rules!

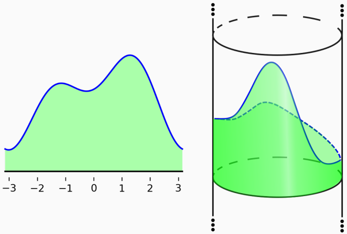


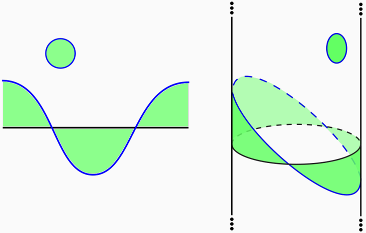


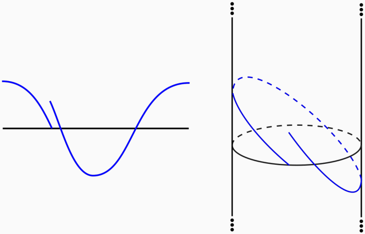




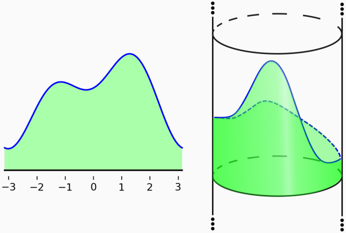
Contour Integration Rules!

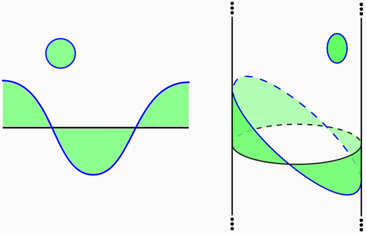


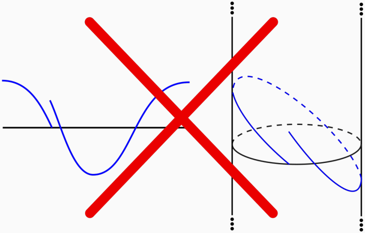




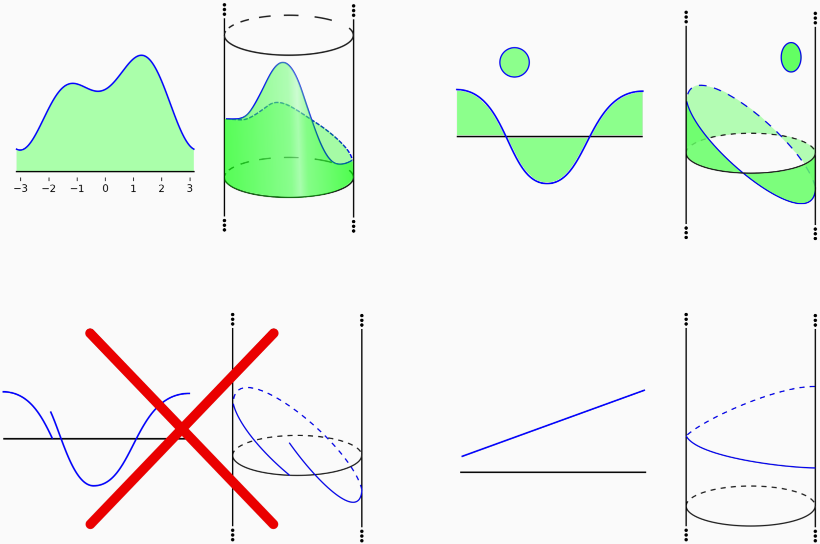
Contour Integration Rules!



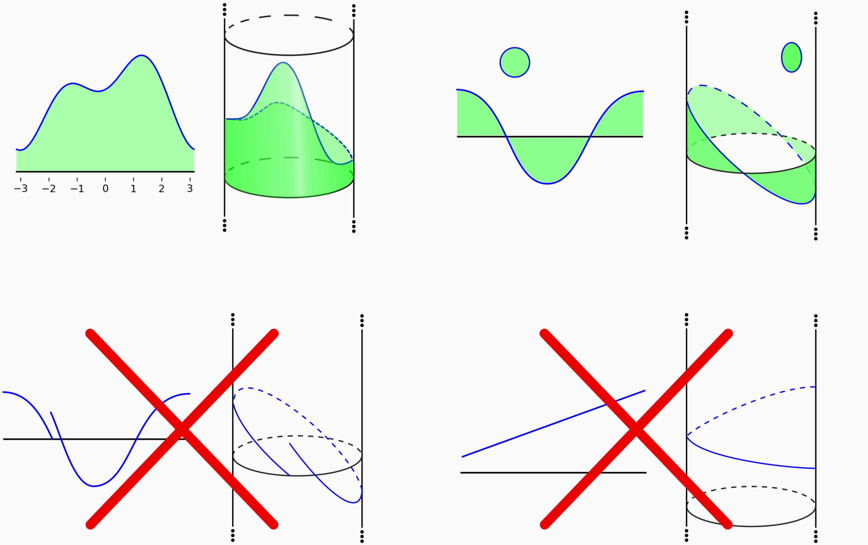




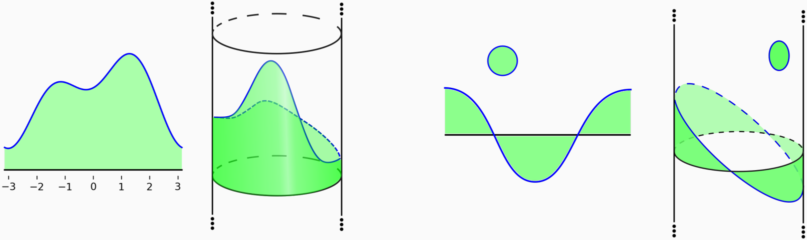
Contour Integration Rules!



Contour Integration Rules!

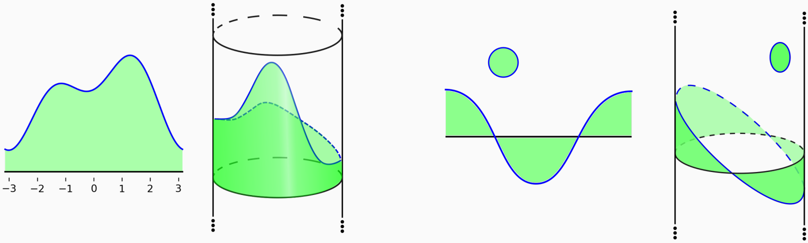


Contour Integration Rules!



Theorem: Integrals of holomorphic functions are unchanged

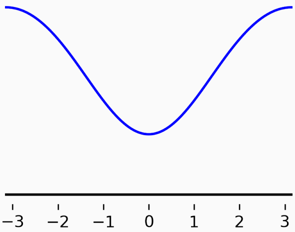
Contour Integration Rules!



Theorem: Integrals of holomorphic functions are unchanged

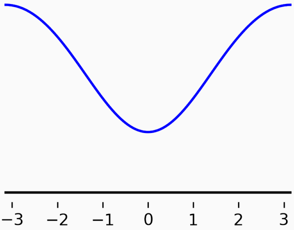
$$\langle \sigma \rangle = \frac{\int_{\mathcal{M}} e^{-S}}{\int_{\mathcal{M}} e^{-\operatorname{Re} S}}$$

An Ansatz for Thirring



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

An Ansatz for Thirring

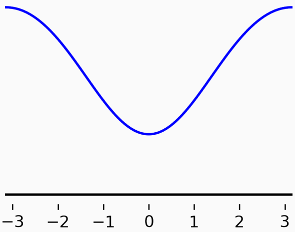


$$\operatorname{Im} A_0(x) = \lambda_0 + \lambda_1 \cos\left[\operatorname{Re} A_0(x)\right] + \cdots$$

A very special property: J is diagonal!

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

An Ansatz for Thirring



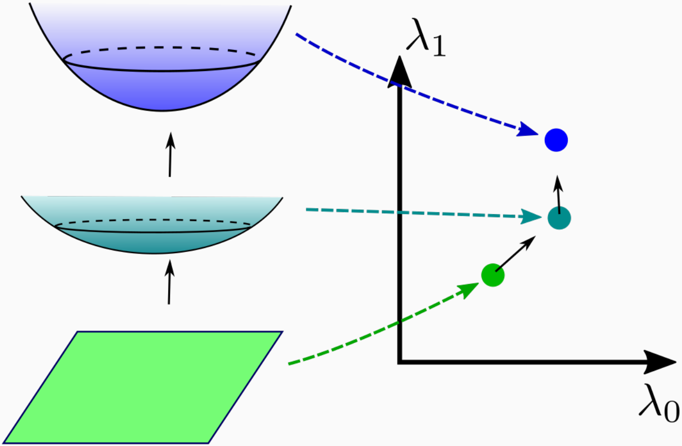
$$\mathrm{Im}\, A_0(x) = \lambda_0 + \lambda_1 \cos\left[\mathrm{Re}\, A_0(x)\right] + \cdots$$

A very special property: J is diagonal!

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

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!**

Sign-Optimized Manifold Method

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

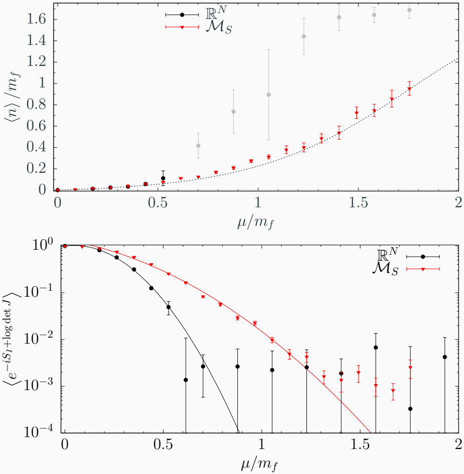
Gradient descent: calculate $\nabla_\lambda \langle\sigma\rangle$. **This is not hard!**

$$\nabla_\lambda Z = 0$$

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

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

Finite Density Thirring Model in $2+1$ Dimensions



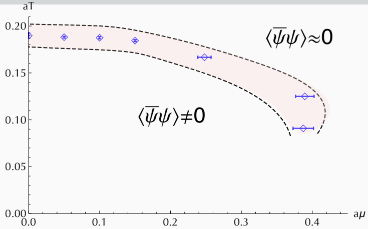
6^3 lattice

$am = 0.01$

$aM_f \approx 0.56 \pm 0.02$

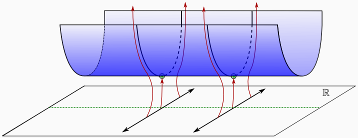
$g = 1.08$

Outlook, Near And Far



Get a phase diagram!

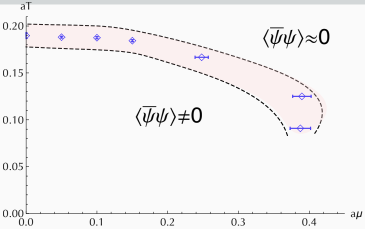
(Neill Warrington)



Extend to gauge theories!

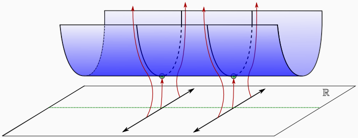
(Henry Lamm)

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



Get a phase diagram!

(Neill Warrington)



Extend to gauge theories!

(Henry Lamm)

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

Holomorphic Integrands for Physical Observables

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

Integrand doesn't look holomorphic!

Holomorphic Integrands for Physical Observables

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

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

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

Holomorphic Integrands for Physical Observables

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

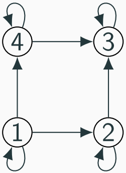
Integrand doesn't look holomorphic! Look at the pre-fermion-integration expression.

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

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

Subgraph Expansion of the Fermion Determinant

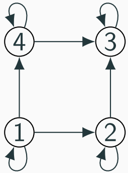
$$D = \begin{pmatrix} m & e^{iA_1(x_1)} & 0 & e^{\mu + iA_0(x_1)} \\ e^{-iA_1(x_1)} & m & e^{\mu+iA_0(x_2)} & 0 \\ 0 & e^{-\mu-iA_0(x_2)} & m & e^{-iA_1(x_3)} \\ e^{-\mu-iA_0(x_1)} & 0 & e^{iA_1(x_3)} & m \end{pmatrix} \sim$$



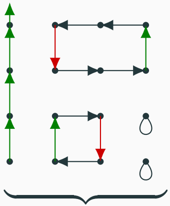
$\longrightarrow = e^{iA_1(x)}$ $\quad \uparrow = e^{iA_0(x)+\mu}$ $\quad \downarrow = e^{-iA_0(x)-\mu}$  $= m$

Subgraph Expansion of the Fermion Determinant

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



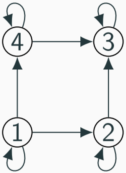
$\longrightarrow = e^{iA_1(x)}$ $\quad$ $\uparrow = e^{iA_0(x)+\mu}$ $\quad$ $\downarrow = e^{-iA_0(x)-\mu}$ $\quad$  $= m$

$\det D =$  $+ \cdots$

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

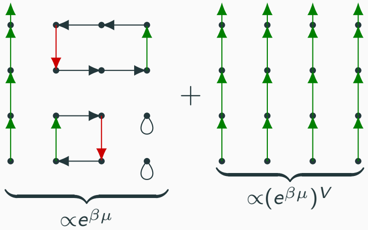
Subgraph Expansion of the Fermion Determinant

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



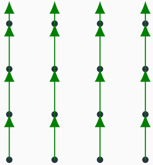
$\longrightarrow = e^{iA_1(x)}$ $\quad \uparrow = e^{iA_0(x)+\mu}$ $\quad \downarrow = e^{-iA_0(x)-\mu}$  $= m$

$\det D =$



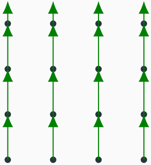
$+ \cdots$

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

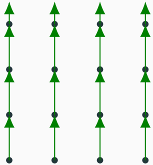
$$\det D =$$



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

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

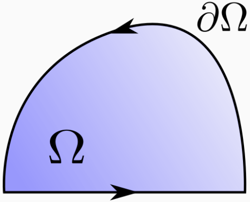
Origin of the Smile: Large-μ Limit

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

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

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

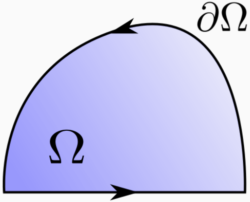
Cauchy's Integral Theorem



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.