Thimbles: A Geometric Solution to the Sign Problem

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Roadmap:

- The Sign Problem
- Motivational 1D example
- Thimbles in path integrals
- The Beltway Algorithm
- Application to Relativistic Bose Gas at Finite Density
The Sign Problem

Observables in QFT

\[ \langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{O}[\phi] e^{-S[\phi]} D[\phi] \]

\[ Z = \int e^{-S[\phi]} D[\phi] \]
The Sign Problem

In practice, generate fields \( \{ \phi_i \} \) distributed as \( \text{Pr}[\phi] = \frac{e^{-S[\phi]}}{Z} \)

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The Sign Problem

In practice, generate fields \( \{ \phi_i \} \) distributed as

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\text{Pr}[\phi] = \frac{e^{-S[\phi]}}{Z}
\]

Then, \( \langle O \rangle = \frac{1}{N} \sum_{i=1}^{N} O[\phi_i] \) with statistical errors.
The Sign Problem

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In practice, generate fields \( \{\phi_i\} \) distributed as \( \text{Pr}[\phi] = \frac{e^{-S[\phi]}}{Z} \)

Then, \( \langle \mathcal{O} \rangle = \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}[\phi_i] \) with statistical errors.

But if \( S = S_R + iS_I \) ....then what? You’ve got a “sign problem”.
The Sign Problem

A complex action occurs in a variety of situations
The Sign Problem

A complex action occurs in a variety of situations

1. QCD at finite chemical potential
The Sign Problem

A complex action occurs in a variety of situations

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2. Most theories with a chemical potential
The Sign Problem

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2. Most theories with a chemical potential
3. Hubbard Model away from half filling
The Sign Problem

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2. Most theories with a chemical potential
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4. Any real time dynamics, etc…
The Sign Problem

A complex action occurs in a variety of situations

1. QCD at finite chemical potential
2. Most theories with a chemical potential
3. Hubbard Model away from half filling
4. Any real time dynamics, etc…

So, is there a way around?
Reweighting

\[ \langle \mathcal{O} \rangle = \frac{\int e^{-S_R(\phi)} e^{-iS_I(\phi)} \mathcal{O}(\phi) d^n \phi}{\int e^{-S_R(\phi)} e^{-iS_I(\phi)} d^n \phi} \]

\[ = \frac{\int e^{-S_R(\phi)} e^{-iS_I(\phi)} \mathcal{O}(\phi) d^n \phi}{\int e^{-S_R(\phi)} d^n \phi} \cdot \frac{\int e^{-S_R(\phi)} d^n \phi}{\int e^{-S_R(\phi)} e^{-iS_I(\phi)} d^n \phi} \]

\[ = \frac{\langle e^{-iS_I} \mathcal{O} \rangle_{S_R}}{\langle e^{-iS_I} \rangle_{S_R}} \]

average phase \( \sim e^{-\# \beta V} \)
Geometric Solution

\[ \phi \in \mathbb{R}^N \rightarrow \phi \in \mathbb{C}^N \]
What’s a thimble?

Thimble = a surface of steepest descent/stationary phase

\[
\int_{-\infty}^{\infty} e^{-S(x)} f(x) dx = e^{-iS_I} \int_{C} e^{-S_R(z)} f(z) dz
\]

\[\frac{dS}{dz} = 0\]
What’s a thimble?

To find thimbles, solve flow equations

\[
\frac{dz}{d\tau} = -\left(\frac{\partial S}{\partial z}\right)
\]

\[z(\tau) \xrightarrow{\tau \to \infty} z_c\]
What’s a thimble?

To find thimbles, solve flow equations

Rewriting $z(\tau) = x(\tau) + iy(\tau)$:

\[
\frac{dx}{d\tau} = -\frac{\partial S_R}{\partial x} = -\frac{\partial S_I}{\partial y}
\]

\[
\frac{dy}{d\tau} = -\frac{\partial S_R}{\partial y} = \frac{\partial S_I}{\partial x}
\]

\[
\frac{dz}{d\tau} = -\left(\frac{\partial S}{\partial z}\right)
\]

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\[
\begin{align*}
\frac{dx}{d\tau} &= -\frac{\partial S_R}{\partial x} = -\frac{\partial S_I}{\partial y} \\
\frac{dy}{d\tau} &= -\frac{\partial S_R}{\partial y} = \frac{\partial S_I}{\partial x}
\end{align*}
\]

Gradient Flow of \( S_R \)

\( z(\tau) \xrightarrow{\tau \to \infty} z_c \)
What's a thimble?

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\end{align*}
\]

Gradient Flow of \( S_R \)  
Hamiltonian Flow of \( S_I \)
1D Example

1D Example: \( S(z) = -z^2 + z^4 + (h_R + i h_I)z \)
1D Example:

\[ S(z) = -z^2 + z^4 + (h_R + i h_I)z \]
1D Example: \( S(z) = -z^2 + z^4 + (h_R + i h_I)z \)

Notice: Not all thimbles contribute to integral
In general:

\[ \int_{-\infty}^{\infty} e^{-S(x)} f(x) dx = \sum_{\sigma = 0}^{N} n_{\sigma} e^{-iS_{I}(\sigma)} \int_{\mathcal{T}_{\sigma}} e^{-S_{R}(z)} f(z) dz \]
Many Variables

\[ S = S(z_1, \ldots, z_n) \]

\[ \frac{dz_i}{d\tau} = -\left( \frac{\partial S}{\partial z_i} \right) \]

\[ z(\tau) \xrightarrow{\tau \to \infty} z_c \]
Many Variables

\[ S = S(z_1, \ldots, z_n) \]

\[ \frac{dz_i}{d\tau} = -\left( \frac{\partial S}{\partial z_i} \right) \]

\[ z(\tau) \xrightarrow{\tau \to \infty} z_c \]

\[ \frac{dx_i}{dt} = -\left( \frac{\partial S_R}{\partial x_i} \right) = -\frac{\partial S_I}{\partial y_i} \]

\[ \frac{dy_i}{dt} = -\left( \frac{\partial S_R}{\partial y_i} \right) = \frac{\partial S_I}{\partial x_i} \]

Gradient Flow of \( S_R \)  Hamiltonian Flow of \( S_I \)
Many Variables

Harder to see (no pictures):

$$\int_{\mathbb{R}^n} e^{-S(x)} f(x) \, dx = \sum_{\sigma=0}^{N} n_{\sigma} e^{-i S_I(\sigma)} \int_{T_\sigma} e^{-S(z)} f(z) \, dz$$
Many Variables

Harder to see (no pictures):

$$\int_{\mathbb{R}^n} e^{-S(x)} f(x) \, dx = \sum_{\sigma=0}^{N} n_{\sigma} e^{-iS_{I}(\sigma)} \int_{\mathcal{T}_{\sigma}} e^{-S(z)} f(z) \, dz$$

Recall: $$\langle \mathcal{O} \rangle = \frac{\int e^{-S(\phi)} \mathcal{O}(\phi) d^n \phi}{\int e^{-S(\phi)} d^n \phi}$$
Many Variables

Harder to see (no pictures):

\[
\int_{\mathbb{R}^n} e^{-S(x)} f(x) \, dx = \sum_{\sigma=0}^{N} n_\sigma e^{-iS_I(\sigma)} \int_{T_\sigma} e^{-S(z)} f(z) \, dz
\]

Recall: 
\[
\langle O \rangle = \frac{\int e^{-S(\phi)} O(\phi) \, d^n \phi}{\int e^{-S(\phi)} \, d^n \phi}
\]

\[
\implies \langle O \rangle = \frac{\sum_{\sigma=0}^{N} n_\sigma e^{-iS_I(\sigma)} \int_{T_\sigma} e^{-S_R(\phi)} O(\phi) \, d^n \phi}{\sum_{\sigma=0}^{N} n_\sigma e^{-iS_I(\sigma)} \int_{T_\sigma} e^{-S_R(\phi)} \, d^n \phi}
\]
Beltway Algorithm

Start with one thimble integration:

$$\langle \mathcal{O} \rangle_0 = \frac{\int_{\mathcal{T}_0} e^{-S_R(\phi)} \mathcal{O}(\phi) d^n \phi}{\int_{\mathcal{T}_0} e^{-S_R(\phi)} d^n \phi}$$

Generate points on the thimble according to:

$$\Pr[\phi] = \frac{e^{-S_R(\phi)}}{\int_{\mathcal{T}_0} e^{-S_R(\phi)} d^n \phi}$$

Non-trivial task!
Beltway Algorithm

\[ \tilde{\phi} = \text{Flow}(\phi, T) \]
Beltway Algorithm

Near critical point,

$$\frac{d\phi_i}{d\tau} = -\left(\frac{\partial S}{\partial \phi_i}\right) \approx -H_{ij}\phi_j$$

$$\implies$$ spanned by $\{\hat{\rho}_i\}$

such that $\overline{H\hat{\rho}_i} = \lambda_i\hat{\rho}_i$
\[ \langle \mathcal{O} \rangle = \frac{\int e^{-SR(\phi)} \mathcal{O}(\phi) d\phi}{\int e^{-SR(\phi)} d\phi} = \frac{\int e^{-SR(\tilde{\phi})} \mathcal{O}(\tilde{\phi}) \det \left( \frac{d\phi}{d\tilde{\phi}} \right) d\tilde{\phi}}{\int e^{-SR(\tilde{\phi})} \det \left( \frac{d\phi}{d\tilde{\phi}} \right) d\tilde{\phi}} \]

\[ \equiv J = e^{\text{Re}(\ln J) + i \text{Im}(\ln J)} \]
\[
\langle \mathcal{O} \rangle = \frac{\int e^{-S_R(\phi)} \mathcal{O}(\phi) d\phi}{\int e^{-S_R(\phi)} d\phi} = \frac{\int e^{-S_R(\tilde{\phi})} \mathcal{O}(\tilde{\phi}) \det\left(\frac{d\phi}{d\tilde{\phi}}\right) d\tilde{\phi}}{\int e^{-S_R(\tilde{\phi})} \det\left(\frac{d\phi}{d\tilde{\phi}}\right) d\tilde{\phi}}
\]

\[
\equiv S_{eff}
\]

\[
\equiv J = e^{\text{Re}(\ln J) + i \text{Im}(\ln J)}
\]

\[
= \frac{\int e^{-(S_R(\tilde{\phi}) - \text{Re}(\ln J))} e^{i \text{Im}(\ln J)} \mathcal{O}(\tilde{\phi}) d\tilde{\phi}}{\int e^{-(S_R(\tilde{\phi}) - \text{Re}(\ln J))} e^{i \text{Im}(\ln J)} d\tilde{\phi}} \equiv \text{“residual phase”}
\]
Beltway Algorithm

\[ \langle O \rangle = \frac{\int e^{-S_R(\phi)} O(\phi) d\phi}{\int e^{-S_R(\phi)} d\phi} = \frac{\int e^{-S_R(\tilde{\phi})} O(\tilde{\phi}) \det \left( \frac{d\phi}{d\tilde{\phi}} \right) d\tilde{\phi}}{\int e^{-S_R(\tilde{\phi})} \det \left( \frac{d\phi}{d\tilde{\phi}} \right) d\tilde{\phi}} \]

\[ \equiv S_{eff} \]

\[ = \frac{\int e^{-(S_R(\tilde{\phi}) - \text{Re}(\ln J))} e^{i\text{Im}(\ln J)} O(\tilde{\phi}) d\tilde{\phi}}{\int e^{-(S_R(\tilde{\phi}) - \text{Re}(\ln J))} e^{i\text{Im}(\ln J)} d\tilde{\phi}} \equiv \text{“residual phase”} \]

\[ = \frac{\langle O e^{i\text{Im}(\ln J)} \rangle_{S_{eff}}}{\langle e^{i\text{Im}(\ln J)} \rangle_{S_{eff}}} \]

\[ \equiv J = e^{\text{Re}(\ln J) + i\text{Im}(\ln J)} \]
Beltway Algorithm

\[(\phi, S_R) = (\tilde{\phi}, S_{eff})\]
Relativistic Bose Gas

\[ S[\phi] = \int \left( |\partial \phi|^2 + (m^2 - \mu^2)|\phi|^2 + \mu j_0 + \lambda|\phi|^4 + h(\phi_1 + \phi_2) \right) d^4x \]

Where: \( \phi = \phi_1 + i\phi_2 \)

\[ j_0 = 2i\text{Im}(\phi \partial_0 \phi^* - \phi^* \partial_0 \phi) \]
Relativistic Bose Gas

\[ S[\phi] = \int \left( |\partial \phi|^2 + (m^2 - \mu^2)|\phi|^2 + \mu j_0 + \lambda |\phi|^4 + h(\phi_1 + \phi_2) \right) d^4 x \]

Where: \( \phi = \phi_1 + i\phi_2 \)

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Here's the sign problem!
Relativistic Bose Gas

\[ S[\phi] = \int \left( |\partial \phi|^2 + (m^2 - \mu^2)|\phi|^2 + \mu j_0 + \lambda |\phi|^4 + h(\phi_1 + \phi_2) \right) d^4 x \]

Where: \( \phi = \phi_1 + i\phi_2 \)

\[ j_0 = 2i \text{Im}(\phi \partial_0 \phi^* - \phi^* \partial_0 \phi) \]

\[ S = \left( 4 + \frac{m^2}{2} \right) \sum_{x,a} \phi_{a,x}^2 - \sum_{x,a} \sum_{\nu=1}^3 \left( \phi_{a,x} \phi_{a,x+\nu} \right) \]

\[ + \sum_{x,a,b} \left( \cosh \mu \ \phi_{a,x} \phi_{b,x+\hat{0}} \delta_{a,b} - i \sinh \mu \ \epsilon_{ab} \phi_{a,x} \phi_{b,x+\hat{0}} \right) \]

\[ + \frac{\lambda}{4} \sum_x \left( \phi_{1,x}^2 + \phi_{2,x}^2 \right)^2 + h \sum_x \phi_1,x + \phi_2,x \]

Here’s the sign problem!
Relativistic Bose Gas

Global min of $S[\phi] \implies$ constant field solution
Relativistic Bose Gas

Global min of $S[\phi] \implies$ constant field solution

$$V(\phi) = (m^2 - \mu^2)|\phi|^2 + \lambda|\phi|^4 + h(\phi_1 + \phi_2)$$
Relativistic Bose Gas

Global min of $S[\phi] \implies$ constant field solution

$$V(\phi) = (m^2 - \mu^2)|\phi|^2 + \lambda|\phi|^4 + h(\phi_1 + \phi_2)$$

$\mu < \mu_{\text{crit}}$

$\mu > \mu_{\text{crit}}$
\( \mu < \mu_{\text{crit}} \)
Is there a sign problem?

$\text{Re}\langle e^{-i S_I} \rangle$

$m = 1.0$

$\lambda = 1.0$
Is there a sign problem?

\[ \text{Re}\langle e^{-i S I} \rangle \]

- \( m = 1.0 \)
- \( \lambda = 1.0 \)
- \( T_{\text{flow}} = 0.2 \)
Phase due to curvature?

\[ \text{Re}(e^{i \text{Im}(J)}) \]

- \( m = 1.0 \)
- \( \lambda = 1.0 \)
- \( T_{\text{flow}} = 0.2 \)
The Jacobian

\[ S_{\text{eff}}(\tilde{\phi}) = S_R(\phi(\tilde{\phi})) - \text{Re}(\ln J(\tilde{\phi})) \]

Flow \( \frac{\text{Flow}(V(\tilde{\phi}), T_{\text{flow}})}{V(\tilde{\phi})} \)
The Jacobian

\[ S_{\text{eff}}(\tilde{\phi}) = S_R(\phi(\tilde{\phi})) - \text{Re}(\ln J(\tilde{\phi})) \]

Flow \( \frac{\text{Flow}(V(\tilde{\phi}), T_{\text{flow}})}{V(\tilde{\phi})} \)

Evolves as:

\[ J = \det(M) \]
\[ \frac{dM}{d\tau} = HM \]
\[ M(0) = (\hat{\rho}_1, \hat{\rho}_2, \ldots, \hat{\rho}_V) \]

This is really hard to do!
Compromise: Reweighting

\[ \langle \mathcal{O} \rangle = \int \frac{e^{- \left[ S_R(\tilde{\phi}) - \text{Re}[\log(J)] \right]} e^{\text{Im}(\log(J))} \mathcal{O}(\tilde{\phi}) d\tilde{\phi}}{\int e^{- \left[ S_R(\tilde{\phi}) - \text{Re}[\log(J)] \right]} e^{\text{Im}(\log(J))} d\tilde{\phi}} \]
Compromise: Reweighting

\[
\langle \mathcal{O} \rangle = \frac{\int e^{-\left[ S_R(\tilde{\phi}) - \text{Re}[\log(J)] \right]} e^{\text{Im}(\log(J))} \mathcal{O}(\tilde{\phi}) d\tilde{\phi}}{\int e^{-\left[ S_R(\tilde{\phi}) - \text{Re}[\log(J)] \right]} e^{\text{Im}(\log(J))} d\tilde{\phi}}
\]

Modified distribution

“reweighting factor”
Compromise: Reweighting

\[ \langle \mathcal{O} \rangle = \frac{\int e^{-\left[ S_R(\tilde{\phi}) - \text{Re}[\log(J)] \right]} e^{\text{Im}(\log(J))} \mathcal{O}(\tilde{\phi}) d\tilde{\phi}}{\int e^{-\left[ S_R(\tilde{\phi}) - \text{Re}[\log(J)] \right]} e^{\text{Im}(\log(J))} d\tilde{\phi}} \]

Modified distribution

\[ = \frac{\int e^{-\left[ S_R(\tilde{\phi}) - \text{Re}[\log(W_1)] \right]} e^{\text{Re} \left[ \log(J) - \log(W_1) \right]} e^{\text{Im}(\log(J))} \mathcal{O}(\tilde{\phi}) d\tilde{\phi}}{\int e^{-\left[ S_R(\tilde{\phi}) - \text{Re}[\log(J)] \right]} e^{\text{Re} \left[ \log(J) - \log(W_1) \right]} e^{\text{Im}(\log(J))} d\tilde{\phi}} \]

"reweighting factor"

\[ = \frac{\langle e^{\text{Re} \left[ \log(J) - \log(W_1) \right]} e^{\text{Im}(\log(J))} \mathcal{O} \rangle e^{\text{Re} \left[ \log(J) - \log(W_1) \right]} e^{\text{Im}(\log(J))} S_R(\tilde{\phi}) - \text{Re}[\log(W_1)]}{\langle e^{\text{Re} \left[ \log(J) - \log(W_1) \right]} e^{\text{Im}(\log(J))} \rangle e^{\text{Re} \left[ \log(J) - \log(W_1) \right]} e^{\text{Im}(\log(J))} S_R(\tilde{\phi}) - \text{Re}[\log(W_1)]} \]
The Estimators

The problem: \( \log(J) = \log(\det(M)) \sim \mathcal{O}(N^3) \)

Solution 1: \( \log(W_1) = \int_0^{T_{flow}} dt' \sum_a \rho_a^\dagger H(t') \rho_a \sim \mathcal{O}(N) \)

Solution 2: \( \log(W_2) = \int_0^{T_{flow}} dt' \text{Tr}(H(t')) \sim \mathcal{O}(N) \)

Just reweigh after the fact!
Do they work?

\[ \mu = \frac{\lambda}{\lambda + \rho} \]

\[ \lambda = \frac{\beta}{1 + \beta} \]

\[ m = \frac{\rho}{\lambda + \rho} \]

\[ \Sigma = \frac{1}{N} \frac{\langle r \rangle^2}{\langle r^2 \rangle} \]

\[ \{ r_i \} = \{ \frac{1}{N}, \ldots, \frac{1}{N} \} \]

\[ \{ r_i \} = \{ 1, 0, \ldots, 0 \} \]

\[ = \frac{1}{N} \]
Charge

\[ \lambda = 1.0 \]
\[ T_{\text{flow}} = 0.2 \]

\[ m = 1.0 \]

Re\langle n \rangle

Conclusions

• One thimble computations below $\mu_c$
• Fast jacobian estimator makes algorithm possible
• Analysis of Bose gas above $\mu_c$ possible with alternate surfaces

Marching on

• Perfect simultaneous multi-thimble calculations
• Application to real time dynamics
• Thimbles in gauge theories
Backup Slides
\[ \mu > \mu_{\text{crit}} \]
In continuum \[ \mu_c = m \]

On lattice \[ \cosh(\mu_c) - 1 = \frac{m^2}{2} \]
Thimbles of…

Project to…
Charge: Tangent Plane

$m=1.0$

$\lambda=1.0$

Blue = Contraction Algorithm

Orange = Hybrid Monte Carlo

Equivalent Surfaces

\[
\int_{\mathbb{R}^n} e^{-S(\phi)} \mathcal{O}(\phi) d^n\phi
\]
\[ \langle \mathcal{O} \rangle = \frac{n_1 e^{-iS_I(\phi_1)} \int_{T_1} e^{-S_R(\phi)} \mathcal{O}(\phi) d\phi + n_2 e^{-iS_I(\phi_2)} \int_{T_2} e^{-S_R(\phi)} \mathcal{O}(\phi) d\phi}{n_1 e^{-iS_I(\phi_1)} \int_{T_1} e^{-S_R(\phi)} d\phi + n_2 e^{-iS_I(\phi_2)} \int_{T_2} e^{-S_R(\phi)} d\phi} \]

\[ = \frac{\langle \tilde{\mathcal{O}} \rangle}{\langle \tilde{\mathcal{I}} \rangle} \]

\[ \text{Pr}[\phi] = \frac{e^{-S_R(\phi)}}{Z} \quad Z = \int_{T_1 \cup T_2} e^{-S_R(\phi)} \]

\[ \tilde{\mathcal{O}}(\phi) = \begin{cases} 
  n_1 e^{-iS_I(\phi_1)} \mathcal{O}(\phi) & \phi \in T_1 \\
  n_2 e^{-iS_I(\phi_2)} \mathcal{O}(\phi) & \phi \in T_2 
\end{cases} \]

\[ \tilde{\mathcal{I}}(\phi) = \begin{cases} 
  n_1 e^{-iS_I(\phi_1)} & \phi \in T_1 \\
  n_2 e^{-iS_I(\phi_2)} & \phi \in T_2 
\end{cases} \]
\[ \langle \tilde{O} \rangle = \frac{\int_{\mathcal{T}_1 \cup \mathcal{T}_2} \tilde{O}(\phi) e^{-S_R(\phi)} d\phi}{\int_{\mathcal{T}_1 \cup \mathcal{T}_2} e^{-S_R(\phi)} d\phi} = \frac{\int \tilde{O}(\phi, i) e^{-S_{\text{eff}}(\phi, i)} e^{i \text{Im}(\ln J)} d\phi}{\int e^{-S_{\text{eff}}(\phi, i)} e^{i \text{Im}(\ln J)} d\phi} \]

Common set of coordinates + integer