A strong residual sign problem on the thimbles

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Phase density

- Consider complex action → weights $\exp(-S_R - iS_I) \equiv Re^{i\theta}$
- Density of states method for complex action: consider density $p(\theta)$ in phase quenched partition function (Gocksch, PRL 61 (1988) 2054)
- Thermodynamical observables accessible using derivatives of $\log Z$ with

$$Z = \langle e^{i\theta} \rangle Z_{\text{pq}}$$

and

average phase factor

$$\langle e^{i\theta} \rangle = \int d\theta \, p(\theta) \, e^{i\theta}$$

- $\langle e^{i\theta} \rangle$ is exponentially small in volume for $\mu \neq 0$ → computation plagued by strong sign problem
- Requires very precise knowledge of $p(\theta)$, e.g. from LLR method (Langfeld and Lucini, PRD90 (2014) 094502).

Using a fit Ansatz

- Improve accuracy and stability of integration using fit Ansatz for $p(\theta)$
- Simple example shows that $\langle e^{i\theta} \rangle$ obtained using fit:
  - not accurate when sign problem is strong
  - not stable under slight variations of fit parameters
- Thimble integration: hope to reduce sign problem as magnitude of integrand falls off in Gaussian like manner away from saddle point

Motivation

How can thimble integration yield exponentially small values for $\langle e^{i\theta} \rangle$?

Potential sign problem due to *residual phase* along the thimble, caused by:

- phase of complex measure along integration path
- the constant phase of the integrand on the thimble.

Phase: intensive vs extensive

- Intensive phase $\theta \in (-\pi, +\pi]$
  - strong sign problem: $p(\theta) \approx$ uniform distribution
  - tiny corrections to uniformity $\rightarrow$ exponentially small value for $\langle e^{i\theta} \rangle \rightarrow$ not measurable accurately
- Extensive phase *(Ejiri et al.)*: θ no longer bounded, avoid branch cut discontinuities
  - claim: as $V \nearrow \Rightarrow p(\theta) \sim$ Gaussian
    $\rightarrow$ use pure Gaussian Ansatz to compute $\langle e^{i\theta} \rangle$ and perform phenomenology at nonzero density
  - method questioned by *Greensite et al.*: higher order corrections in cumulant expansion, which involve delicate volume cancellations
    $\rightarrow$ invalidate Gaussian value of $\langle e^{i\theta} \rangle$
  - supported by our simple example of Gaussian-like distribution:
    - cumulant expansion converges slowly when sign problem becomes strong
      $\rightarrow$ higher order terms make $\langle e^{i\theta} \rangle$ several orders of magnitudes smaller than leading order Gaussian value

Ansatz for phase distribution

- Distribution $p(\theta)$ of extended phase: generically described by exponential of even polynomial in θ *(Greensite et al.)*

Ansatz: simplest extension of Gaussian distribution

$$p(\theta) = N \exp\left[-\frac{\theta^2}{2\sigma^2}\left(1 + a\frac{\theta^2}{\sigma^2}\right)\right]$$

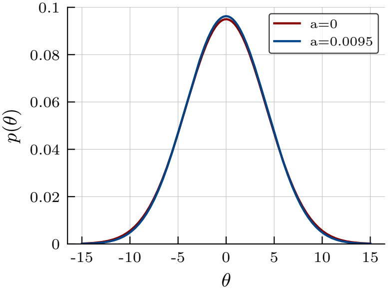
with normalization factor $N = 2\sqrt{a}/(\sigma e^\kappa K_{1/4}(\kappa))$, $\kappa = 1/(16a)$, $K_{1/4}$: modified Bessel function of fractional order, and $a \geq 0$.

- Ansatz also suggested by our MC simulations of random matrix theory: for $V \nearrow$: $p(\theta)$ *almost* Gaussian with small nonzero quartic contribution.
- Parameters σ and a: unambiguously extracted from $\langle\theta^2\rangle$ and $\langle\theta^4\rangle$ measured in phase quenched MC simulations.

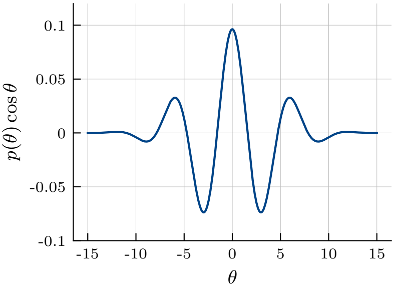
Distribution and integrand

- Investigate $\langle e^{i\theta} \rangle$ for small values of a where $p(\theta) \sim$ Gaussian
- All results given for $\sigma = 4.2$, without loss of generality. Typical parameter value from RMT simulations with strong sign problem and quasi-normal distribution distribution

$p(\theta)$ for $\sigma = 4.2$ and $a = 0.0095$

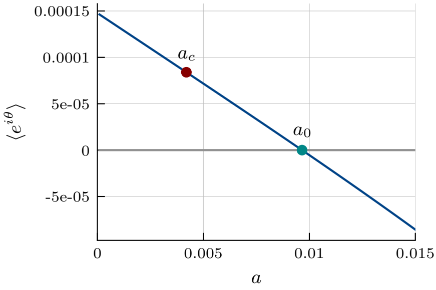


Real part $p(\theta)\cos\theta$ of oscillating integrand for $\sigma = 4.2$ and $a = 0.0095$.



$\langle e^{i\theta} \rangle$ versus a

$\langle e^{i\theta} \rangle$ as function of a for $\sigma = 4.2$ from standard quadrature formulas



- for $a = 0$: Gaussian result $\langle e^{i\theta} \rangle_{\text{Gauss}} = e^{-\sigma^2/2}$
- zero crossing $a_0 \approx 0.00965632$
- a_c: transition from single to double-thimble $\rightarrow$ residual sign problem sets in
- $a \in [0, a_0)$ releventant in physical simulations as $\langle e^{i\theta} \rangle > 0$ but $\propto e^{-V}$

Thimble analysis

Thimble formulation

$$\langle e^{i\theta} \rangle = \int d\theta \, p(\theta) \, e^{i\theta} = \sum_{\mathcal{T} \in \Omega} I_{\mathcal{T}}$$

- Ω: set of relevant thimbles contributing to integral
- thimbles: trajectories of constant phase ϕ through saddle points

Integral on a thimble $\mathcal{T}$

$$I_{\mathcal{T}} = \int_{\mathcal{T}} dz \, f(z) = \int_{\mathcal{T}} ds \, f(z(s)) \, \frac{dz}{ds}$$

- changed variable: real θ → complex z
- parametrized thimble by its arc length s.

Residual phase

- Complex measure along thimble: $dz = ds\, e^{i\eta(s)}$
  - Phase factor $e^{i\eta(s)}$: Jacobian of arc length parametrization
  - $\eta(s)$: angle of tangential to the thimble
- Thimbles: trajectories of constant phase $\phi \rightarrow f(z(s)) = r(s)\, e^{i\phi}$ with $r(s) = |f(z(s))|$ such that

$$I_{\mathcal{T}} = \int_{\mathcal{T}} ds\, r(s)\, e^{i(\phi+\eta(s))}$$

$\rightarrow$ useful form to investigate strong residual sign problem

Interlude: the Gaussian case

Gaussian distribution: thimble for $\langle e^{i\theta} \rangle$ trivially solves sign problem

- single saddle point at $z_0 = i\sigma^2$
- thimble $\parallel$ real axis
- constant phase $\phi = 0$
- oscillating integrand on real axis becomes Gaussian on thimble
- $\langle e^{i\theta} \rangle \propto e^{-V}$ as $f(z_0) \propto e^{-V}$ when path pushed up in $\mathbb{C}$ plane

No longer true when generalizing phase distribution $\longrightarrow$ different thimble mechanism at work close to a_0

Saddle point equation for $p(z) = N \exp\left[-\frac{z^2}{2\sigma^2}\left(1 + a\frac{z^2}{\sigma^2}\right)\right]$

- Rewrite integrand $f(z) = p(z)\,e^{iz}$ as $e^{-S(z)}$ with complex action:

$$S(z) = \frac{z^2}{2\sigma^2} + \frac{az^4}{2\sigma^4} - iz - \log N$$

- Complex saddle point equation:

$$\frac{\partial S}{\partial z} = \frac{z}{\sigma^2} + \frac{2az^3}{\sigma^4} - i = 0.$$

Rewrite $z = it$ → cubic equation in t

$$t^3 + p\,t + q = 0$$

with real coefficients:

$$p = -\frac{\sigma^2}{2a}, \quad q = \frac{\sigma^4}{2a}$$

Saddle points: $\Delta \geq 0$

Discriminant

$$\Delta = -4p^3 - 27q^2$$

$\Delta = 0$ when $a = a_c$ with

$$a_c = \frac{2}{27\sigma^2}$$

$a \leq a_c$: three real roots

$$t_k = 2\sqrt{-\frac{p}{3}}\cos\left[\frac{1}{3}\arccos\left(\frac{3}{2}\frac{q}{p}\sqrt{-\frac{3}{p}}\right) - \frac{2\pi k}{3}\right], \quad k = 0, 1, 2$$

$\rightarrow$ three saddle points $z_k = it_k$ on imaginary axis

Relevant thimble

Similar to Gaussian case $\rightarrow$ one relevant thimble through saddle point $z_1 = it_1$, constant phase $\phi = 0$

Saddle points: $\Delta < 0$

When $a > a_c$: one real and two complex conjugate solutions

- Real solution:

$$t_0 = -2\sqrt{-\frac{p}{3}}\cosh\left(\frac{1}{3}\operatorname{arcosh}\left(-\frac{3}{2}\frac{q}{p}\sqrt{-\frac{3}{p}}\right)\right)$$

- Complex conjugate solutions $t_\pm$:

$$t_\pm = -\frac{t_0}{2} \pm \frac{i}{2}\sqrt{4p + 3t_0^2}.$$

- Saddle points:
  - $z_0 = it_0$ on imaginary axis
  - complex pair $(z, -z^*) = (it_+, it_-)$ left and right of imaginary axis.

Relevant thimbles

- Thimble through imaginary saddle point does *not* contribute
- Thimble integration given by sum of two thimbles $\mathcal{T}_-$ and $\mathcal{T}_+$ mirrored about imaginary axis, going through $(z, -z^*)$ pair of saddle points.
- Contributions of $\mathcal{T}_-$ and $\mathcal{T}_+$ are complex conjugate $\rightarrow$ real sum
- $\phi \neq 0 \rightarrow$ possible residual sign problem in integration on each thimble

Table of thimble properties

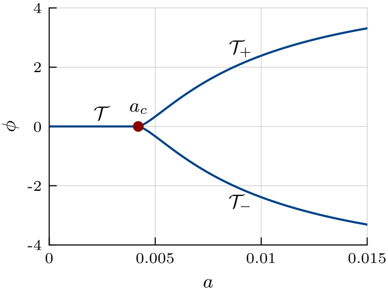
Summary of thimble properties for $\sigma = 4.2$

	a	z_0	ϕ	$\langle e^{i\theta} \rangle$
Gauss	0	$i\,17.64$	0	1.477×10^{-4}
single-thimble	0.001	$i\,18.3393$	0	1.326×10^{-4}
	0.004	$i\,23.6046$	0	8.698×10^{-5}
double-thimble	0.00425	$\pm 1.66704 + i\,26.319$	0.0066	8.318×10^{-5}
	0.009	$\pm 9.85516 + i\,18.9484$	2.098	1.022×10^{-5}
	0.0095	$\pm 9.98268 + i\,18.5119$	2.249	2.439×10^{-6}
	0.00965	$\pm 10.0157 + i\,18.3875$	2.292	9.869×10^{-8}
	0.009656	$\pm 10.0170 + i\,18.3826$	2.293	5.022×10^{-9}
	0.0096563	$\pm 10.0171 + i\,18.3824$	2.293	3.383×10^{-10}
	0.00965632	$\pm 10.0171 + i\,18.3824$	2.293	2.610×10^{-11}

How can exponentially small integral values arise in thimble framework?

Constant phase

- Constant phase along relevant thimbles: $\phi = -S_I(z_0)$, with iS_I imaginary part of action and saddle point z_0.



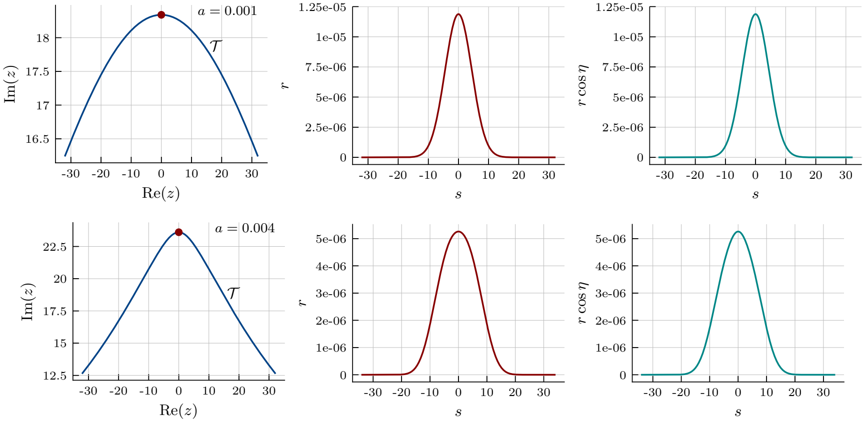
- At $a = a_c$: transition from single-thimble mode with $\phi = 0$
  $\longrightarrow$ double-thimble mode with $\phi \neq 0$

$a \leq a_c$ – single-thimble

complex path of thimble

magnitude $r(s) \sim$ fall off of Re(f) and Im(f) away from saddle point as ϕ constant

Real part of integrand $r(s)\, e^{i(\phi+\eta(s))}$



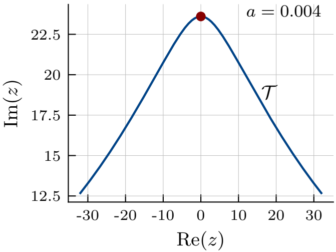
- Constant phase $\phi = 0$
- Small variation of phase $\eta(s) \rightarrow \cos\eta(s) \approx 1$

$\Big\} \rightarrow$ no sign problem

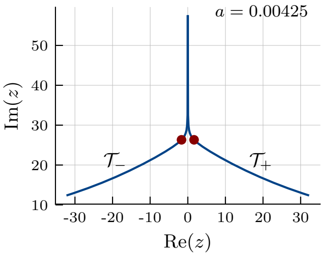
$a \approx a_c$ – Transition single to double-thimble

- Transition between single and double-thimble regions at $a_c \approx 0.0042$
- $a \to a_c$ from below: two purely imaginary saddle points move toward each other and merge when $a = a_c$
- $a > a_c$: saddle points move apart as $(z, -z^*)$ pair left and right of imaginary axis
- two mirrored thimbles $\mathscr{T}_-$ and $\mathscr{T}_+$ with complex conjugate contributions
- Constant phase $\phi = 0.0066$

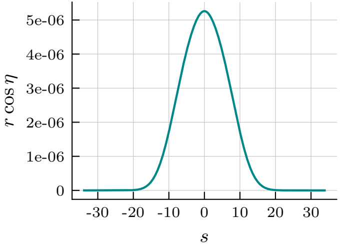
complex path of thimble $\mathscr{T}$



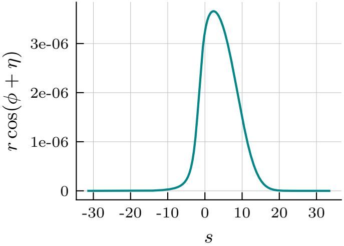
complex path of thimbles $\mathscr{T}_-$ and $\mathscr{T}_+$



Transition single to double-thimble



$\rightarrow$

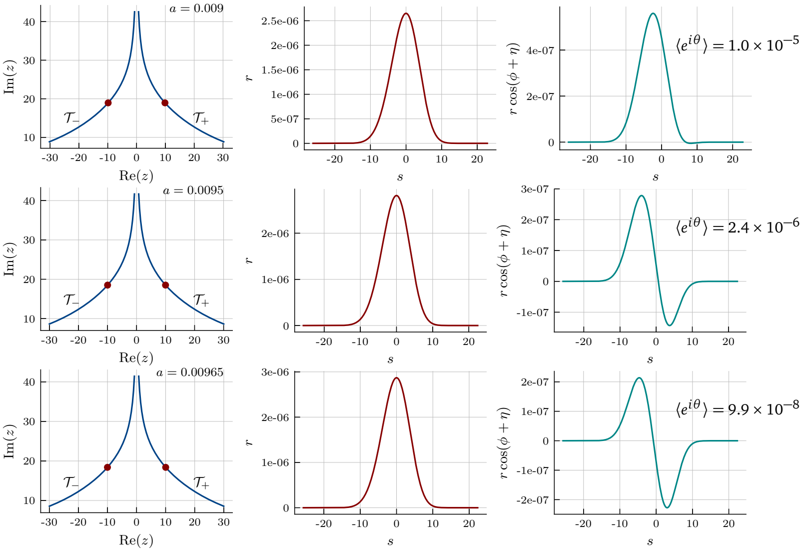


- $a \le a_c$ region smoothly connects to $a > a_c$ region:
  - single thimble splits in two mirrored thimbles
  - almost vertical for $s < 0 \rightarrow \eta(s < 0) \approx \mp\pi/2$
  - $\phi = \pm 0.0066$.

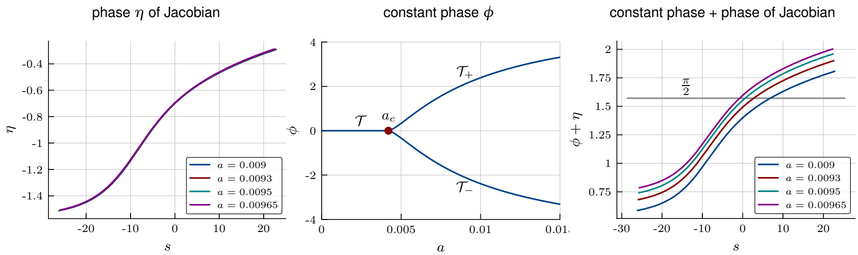
  $\rightarrow \cos(\phi + \eta(s)) \approx 0$ for $s < 0$
- Gaussian-like curve on $\mathscr{T}$ for $a \lessapprox a_c \rightarrow$ sum of two half-Gaussians, on $\mathscr{T}_-$ and $\mathscr{T}_+$ for $a \gtrapprox a_c$

$a_c < a < a_0$ – double-thimble

- Zoom in on $a \in [0.009, a_0]$, with $a_0 \approx 0.00965632$.



Residual sign problem



Integrand: $r(s)\cos(\phi + \eta(s))$

- η varies with s along thimble; but insensitive to small changes of a
- Increasing a from $a_c \to a_0$: constant phase ϕ on $\mathscr{T}_+$ increases from $\phi = 0 \to \phi \approx 2.3$
- Total phase $\phi + \eta(s)$: intersection with $\pi/2$ shifts towards saddle point $\to$ integrand oscillates $\to$ strong residual sign problem

$\to \langle e^{i\theta} \rangle$ many orders of magnitude smaller than Gaussian value

Summary

- Result:

a	0	0.009	0.0095	0.00965	0.00965632
$\langle e^{i\theta} \rangle$	1.5×10^{-4}	1.0×10^{-5}	2.4×10^{-6}	9.9×10^{-8}	2.6×10^{-11}

- Exponentially small $\langle e^{i\theta} \rangle$ obtained at cost of strong residual sign problem in thimble integration
- Problem related with existence of a zero crossing in $\langle e^{i\theta} \rangle$ versus a
- No cancellations between thimbles with different phases ϕ
- Strong sign problem occurs inside one thimble when $\phi \neq 0$ conspires with phase of Jacobian
- Situation is physically relevant as
    - $\langle e^{i\theta} \rangle > 0$ and $\propto e^{-V}$ for physical systems with complex action
    - distribution and parameter values σ and a obtained from MC simulations of RMT at nonzero chemical potential
- Binder cumulant very close to 3 $\rightarrow$ no indication that $\langle e^{i\theta} \rangle$ takes its Gaussian value