One-thimble regularisation of lattice field theories:
is it only a dream?

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based on work mostly in collaboration with K. Zambello

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Agenda

- **THIMBLES**: a (minimal ...) primer ...
- ... including our preferred parametrisation of the thimble and ...
- ... importance sampling in the Steepest Ascents space.

- **HOW MANY THIMBLES?**
  - Single thimble dominance hypothesis ...
  - ... and a story of its failure: Thirring model

- **MULTIPLE THIMBLES SIMULATIONS** ...
  - ... a few examples.

- Still we would like **ONE THIMBLE SIMULATIONS**
  - A *simple* mechanism taking a step in that direction ...
  - ... mainly speculations (at the moment).

- Conclusions and outlook
Constructing thimbles

We want to compute

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

... but S is complex ...

One-thimble regularisation of lattice field theories?
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\[ S(x) = S_R(x) + iS_I(x) \rightarrow S(z) \]
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II. Look for **critical points**
\[ \partial_z S = 0 \]
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II Look for critical points \( \partial_z S = 0 \)

III Then for each critical point we then have to ...

\[ H(S; p_\sigma) v^{(i)} = \lambda_i \bar{v}^{(i)} \]

Solve the Takagi problem for the Hessian at the critical point

The Takagi vectors \( v^{(i)} \) provide a basis for the tangent space at the critical point (first piece of information on our manifold)

The Takagi values \( \lambda_i \) fixes the rate at which the real part of the action increases along the Steepest Ascents paths

The THIMBLE attached to the critical point is the union of all the STEEPEST ASCENT PATHS originating at the critical point, along which imaginary part of action stays constant while the real part of the action grows (ensuring convergence).

In order to construct the tangent space at a generic point on the thimble we have to PARALLEL TRANSPORT the Takagi vectors along the SA on which the given point sits.
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The main message is the THIMBLES DECOMPOSITION

\[
\langle O \rangle = \frac{\sum_\sigma n_\sigma e^{-i S_I(p_\sigma)} \int_{\mathcal{J}_\sigma} dz e^{-S_R} O e^{i\omega}}{\sum_\sigma n_\sigma e^{-i S_I(p_\sigma)} \int_{\mathcal{J}_\sigma} dz e^{-S_R} e^{i\omega}}
\]
Our preferred parametrisation of the thimbles

In the vicinity of a critical point we know the solution of the SA equations

\[
\frac{d}{dt} z_i = \frac{\partial S}{\partial z_i}
\]

\[
\begin{align*}
 z_j(t) &\approx z_{\sigma,j} + \sum_{i=1}^{n} n_i v_{\sigma j}^{(i)} e^{\lambda_i^{(\sigma)} t} \\
 V_{\sigma j}^{(i)}(t) &\approx v_{\sigma j}^{(i)} e^{\lambda_i^{(\sigma)} t}
\end{align*}
\]

(and the solution of parallel transportation of basis vectors as well…)

One-thimble regularisation of lattice field theories?
Our preferred parametrisation of the thimbles

In the vicinity of a critical point we know the solution of the SA equations

\[
\frac{d}{dt} z_i = \frac{\partial \tilde{S}}{\partial \tilde{z}^i} \]

\[
\begin{align*}
\tilde{z}_j(t) &\approx \tilde{z}_{\sigma,j} + \sum_{i=1}^{n} n_i \tilde{v}^{(i)}_{\sigma j} e^{\lambda_i(\sigma)t} \\
\tilde{V}^{(i)}_{\sigma j}(t) &\approx \tilde{v}^{(i)}_{\sigma j} e^{\lambda_i(\sigma)t}
\end{align*}
\]

(and the solution of parallel transportation of basis vectors as well…)

This in the end mean that a single SA is singled out by the direction along which it leaves the critical point, so that specifying this direction and the time of integration you can single out a given point on the thimble (like in Kikukawa et al 2013)

\[
\mathcal{J}_\sigma \ni z \leftrightarrow (\hat{n}, t) \in S_{\mathcal{R}}^{n-1} \times \mathbb{R}
\]
Our preferred parametrisation of the thimbles

In the vicinity of a critical point we know the solution of the SA equations

\[ \frac{d}{dt} z_j(t) \approx z_{\sigma,j} + \sum_{i=1}^{n} n_i \, v_{\sigma j}^{(i)} \, e^{\lambda_j^{(\sigma)} t} \]

\[ V_{\sigma j}^{(i)}(t) \approx v_{\sigma j}^{(i)} \, e^{\lambda_j^{(\sigma)} t} \]

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\[ \mathcal{J}_\sigma \ni z \leftrightarrow (\hat{n}, t) \in S_{\mathcal{R}}^{n-1} \times \mathbb{R} \]

… in terms of which the thimble decomposition of the functional integral reads

\[
\langle O \rangle = \frac{\sum_{\sigma} n_\sigma \, e^{-i S_I(z_\sigma)} \int_{\sigma} D\hat{n} \, 2 \sum_{i=1}^{n} \lambda_i^{(\sigma)} \, n_i^2 \, \int_{-\infty}^{+\infty} dt \, e^{-S^{(\sigma)}_{\text{eff}}(\hat{n}, t)} \, O(\hat{n}, t) \, e^{i \omega(\hat{n}, t)} \, e^{i \omega(\hat{n}, t)}}{\sum_{\sigma} n_\sigma \, e^{-i S_I(z_\sigma)} \int_{\sigma} D\hat{n} \, 2 \sum_{i=1}^{n} \lambda_i^{(\sigma)} \, n_i^2 \, \int_{-\infty}^{+\infty} dt \, e^{-S^{(\sigma)}_{\text{eff}}(\hat{n}, t)} \, e^{i \omega(\hat{n}, t)}}
\]

Notice normalization \( D\hat{n} \equiv \prod_{k=1}^{n} d n_k \delta (|\hat{n}|^2 - \mathcal{R}) \)

… and the appearance of \( S^{(\sigma)}_{\text{eff}}(\hat{n}, t) = S_{\mathcal{R}}(\hat{n}, t) - \log |\det V_\sigma(\hat{n}, t)| \)

One-thimble regularisation of lattice field theories?
Our preferred parametrisation of the thimbles

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\[
\begin{align*}
z_j(t) &\approx z_{\sigma,j} + \sum_{i=1}^{n} n_i v^{(i)}_{\sigma_j} e^{\lambda^{(\sigma)}_i t} \\
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(and the solution of parallel transport of basis vectors as well...)

This in the end mean that a single SA is singled out by the direction along which it leaves the critical point, so that specifying this direction and the time of integration you can single out a given point on the thimble (like in Kikukawa et al 2013)

\[
J_{\sigma} \ni z \leftrightarrow (\hat{n}, t) \in S^{n-1}_R \times \mathbb{R}
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Notice normalization \( D\hat{n} \equiv \prod_{k=1}^{n} dn_k \delta (|\hat{n}|^2 - R) \)

... and the appearance of \( S_{\text{eff}}^{(\sigma)}(\hat{n}, t) = S_R(\hat{n}, t) - \log |\det V(\hat{n}, t)| \)

All in all, this can be implemented in a Monte Carlo ...
Importance sampling

If only one thimble is in place, it is easy to see that one can rephrase

\[ \langle O \rangle = \frac{\langle O e^{i\omega} \rangle}{\langle e^{i\omega} \rangle} \]

where

\[ \langle f \rangle_{\sigma} = \frac{1}{Z_{\sigma}} \int d^n y f e^{-S_R} = \frac{1}{Z_{\sigma}} \int \mathcal{D}\hat{n} \left( 2 \sum_{i=1}^{n} \lambda_i \hat{n}_i^2 \right) \int dt f(\hat{n}, t) e^{-S_{\text{eff}}(\hat{n}, t)} = \int \mathcal{D}\hat{n} \frac{Z_{\sigma}^{(\sigma)}}{Z_{\sigma}} f(\hat{n}) \]

with

\[ Z_{\sigma} = \int \mathcal{D}\hat{n} Z_{\hat{n}}^{(\sigma)} \quad Z_{\hat{n}}^{(\sigma)} = 2 \sum_{i=1}^{n} \lambda_i^{(\sigma)} \hat{n}_i^2 \int dt e^{-S_{\text{eff}}^{(\sigma)}(\hat{n}, t)} \]
If only one thimble is in place, it is easy to see that one can rephrase

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\langle O \rangle = \frac{\langle O e^{i\omega} \rangle_\sigma}{\langle e^{i\omega} \rangle_\sigma}
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with

\[
Z_\sigma = \int D\hat{n} \, Z_\sigma^{(\sigma)} \quad Z_\sigma^{(\sigma)} = 2 \sum_{i=1}^{n} \lambda_i^{(\sigma)} \hat{n}_i^2 \int_{-\infty}^{+\infty} dt \, e^{-S_{\text{eff}}^{(\sigma)}(\hat{n}, t)}
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and

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f_{\hat{n}} \equiv \frac{1}{Z_\sigma^{(\sigma)}} \left(2 \sum_{i=1}^{n} \lambda_i \hat{n}_i^2 \right) \int_{-\infty}^{+\infty} dt \, f(\hat{n}, t) \, e^{-S_{\text{eff}}(\hat{n}, t)}
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... which almost looks like a functional integral along a single flow line ...

One-thimble regularisation of lattice field theories?
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... which almost looks like a functional integral along a single flow line ...

... so that in the end you can think of generating contributions along single flow lines, and importance sampling is with respect to their overall relative weight ... à la Metropolis

\[ P_{\text{acc}} (\hat{n}' | \hat{n}) = \min \left\{ 1, \frac{Z^{(\sigma)}_{\hat{n}'}}{Z^{(\sigma)}_{\hat{n}}} \right\} \]

... and we can compute on multiple thimbles and then put results together (see later)
SINGLE THIMBLE DOMINANCE?
Prolegomena

We have already mentioned that not all the thimbles do contribute!

In order that a critical point contributes the associated unstable thimble must intersect the original domain of integration

A trivial example; the usual toy model: 0-dim *quartic oscillator*…

*blue* lines are thimbles, *red* ones are unstable thimbles

---

**PS** Unstable thimbles are those along which the real part of the action decreases.
SINGLE THIMBLE DOMINANCE?
The original conjecture

On the dominant thimble (lowest value of the real part of the action)

- you collect a contribution that dominates more and more in the thermodynamic limit
- you have a theory with the right (i.e. original) symmetries
- you recover the standard Perturbation Theory

so that in the end you can conjecture that it can capture the result you are interested in (at least in given regimes)
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SINGLE THIMBLE DOMINANCE?
A famous counterexample

Monte Carlo study of Lefschetz thimble structure in one-dimensional Thirring model at finite density

Hirotsgu Fujii, Syo Kamata and Yoshio Kikukawa

Figure 4. 
(a) Number density. 
(b) Scalar condensate.

One-thimble regularisation of lattice field theories?
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See also

Sign problem and Monte Carlo calculations beyond Lefschetz thimbles

Andrei Alexandru, Gökçe Başar, Paulo F. Bedaque, Gregory W. Ridgway, and Neill C. Warrington
SINGLE THIMBLE DOMINANCE?
… so, what?

Never give up! but there are two ways not to give up …

- either you sit down and try to do the very right thing, i.e. when you understand the thimble structure, you take everything into account (multi thimble simulations)
- or you insist and try to take single thimble simulations at least a few steps further
SINGLE THIMBLE DOMINANCE?

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In order to (also) go through the second path, let’s anticipate a question:

- QUESTION: how can I learn of multiple thimbles structure?
- ANSWER: look for and into Stokes phenomena!
Multi thimbles computations: QCD 0+1

In this case we have 2 contributions (remember the symmetry!) and we rephrase like

\[
\langle O \rangle = \frac{n_0 e^{-i S_I(p_0)} Z_0 \langle O e^{i\omega} \rangle_0 + n_{12} e^{-i S_I(p_{12})} Z_{12} \langle O e^{i\omega} \rangle_{12}}{n_0 e^{-i S_I(p_0)} Z_0 \langle e^{i\omega} \rangle_0 + n_{12} e^{-i S_I(p_{12})} Z_{12} \langle e^{i\omega} \rangle_{12}}
\]

Putting all our ignorance into one single parameter...

\[
\langle O \rangle = \frac{\langle O e^{i\omega} \rangle_0 + \alpha \langle O e^{i\omega} \rangle_{12}}{\langle e^{i\omega} \rangle_0 + \alpha \langle e^{i\omega} \rangle_{12}} \quad \alpha \equiv \frac{n_{12} e^{-i S_I(p_{12})} Z_{12}}{n_0 e^{-i S_I(p_0)} Z_0}
\]

... which can be computed taking one known result as a normalization point! This can be done quite well, e.g. for

\[N_f = 1 \quad m = 0.1 \quad \mu/T = 2\]

we get, depending on the quantity we use to fix the normalization

\[\alpha = 0.2686(13) \quad 0.2682(8)\]
Multi thimbles computations: towards HDQCD

Here we have much the same as in QCD01

\[
\langle O \rangle = \frac{n_0 e^{-iS_1(p_0)} Z_0 \langle O e^{i\omega} \rangle_0 + n_{12} e^{-iS_1(p_{12})} Z_{12} \langle O e^{i\omega} \rangle_{12}}{n_0 e^{-iS_1(p_0)} Z_0 \langle e^{i\omega} \rangle_0 + n_{12} e^{-iS_1(p_{12})} Z_{12} \langle e^{i\omega} \rangle_{12}}
\]

… but this time the relevant parameter \( Z_{12} \)…

- is first computed in semiclassical approximation
- and then corrected as the simulation proceeds
Multi thimbles computations: Thirring

Well ... stay and listen to next talk ...
SINGLE THIMBLE DOMINANCE?

… do you remember?

QUESTION: how can I learn of multiple thimbles structure?
ANSWER: look for and into Stokes phenomena!

Stokes phenomena occur when two thimbles go on top of each other; thimble decomposition fails in that point of the parameter space and there is a discontinuity in the number of thimbles contributing.
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Stokes phenomena occur when two thimbles go on top of each other; thimble decomposition fails in that point of the parameter space and there is a discontinuity in the number of thimbles contributing.
But imaginary part of the action is constant on thimbles...
... and that’s why you look for CROSSINGS!

Figure 6. (a) \(\text{Im}S(\sigma_i)\) on the right half plane as a function of \(\hat{\mu}\). (b) Enlarged plot of (a).
(c) \(\text{Re}S(\sigma_i)\). The dashed line indicates \(\min_{x \in \mathbb{R}} \text{Re}S(x)\). Parameters are set to \(L = 4, \beta = 3\) and \(ma = 1\).

One-thimble regularisation of lattice field theories?
ONE THIMBLE REVISITED
... a more modest attitude ...

If, in the parameter space, you are interested in a point that lies in the region where more than one thimble contribute, you can reach that point by taking a few steps forward from the region where only one thimble contributes...

We mean that you can compute a Taylor expansion of your observable in a one thimble simulation ... 

... and notice: you can expand in either $\beta$ or $\mu$ or both ... (the two rows below are at different $\beta$ values)
Does it work? Here we go!

(expansion in $\mu$)
Conclusions and outlook

- One-thimble regularisation of lattice field theories: is it only a dream? … probably YES …

- BUT
  - you can take advantage from the rich structure of Stokes phenomena …
  - … and at least take a few steps further from the region where only one thimble counts …
  - … and this can be done in a way that we (already) know: simply Taylor expand.

- We are collecting the very first results, using as a lab 1-D Thirring model. Here you know a priori what to expect and up to where you can go, but we want to see whether the funny composite operators are computable within a reasonable precision. Notice that this is not such an extra work in our setting…

- As a byproduct, we can gain some more insight into Taylor expansions methods per se.