A Simple Approach Towards the Sign Problem in Lattice Field Theory

Michael Kroyter

Holon Institute of Technology

SFT 2018 – HRI
13-February-2018

Work in progress with *Francis Bursa*

Outline

1. Introduction
2. Lefschetz Thimbles
3. The Bose Gas at Finite Chemical Potential
4. Simulation Results
5. Summary and Future Directions

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Lattice Field Theory

A framework for a numerical study of field theories:
Evaluate path integrals numerically by discretizing space-time.

Challenges

- Lorenzian path integrals are highly oscillatory and divergent.
- A very large number of integration variables:
  d-dim. cubic lattice of size $L = aN$ (a is the lattice spacing).
  $N_{tot} \equiv \#(\text{integration variables}) = N^d \times \#(\text{component fields})$.
- Describing fermions.

Resolutions

- Wick rotate, $iS_L \to -S_E$: Oscillations are gone. Convergence.
  The action can be interpreted as a classical Boltzmann weight.
- Evaluate integrals using a statistical method:
  The Metropolis algorithm (Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, E. Teller 1953).
- In the quadratic case: Integrate fermions. Simulate only bosons.

The Metropolis Algorithm

The complexity of deterministic algorithms for evaluating integrals is multiplied by a constant for each added integration variable, $O(e^{\alpha N_{tot}})$.
Instead use a non-deterministic (Monte-Carlo) algorithm:

- Interpret the integrand as a probability density $P[x_n] = e^{-S[x_n]}$.
- Define a stochastic process in the space $[x_n]$, $x_n^{(1)}, x_n^{(2)}, ..., x_n^{(T)}$ by:
  - Given $x_k^{(i)}$ consider a random nearby point $\tilde{x}$.
  - If changing $x_k^{(i)} \to \tilde{x}$ increases the probability, apply this change.
  - If it lowers the probability, apply with probability $\tilde{P}/P[x_n^{(i)}]$ and keep $x_k^{(i+1)} = x_k^{(i)}$ otherwise. Repeat for all $k = 1...N_{tot}$.
- Detailed balance for a measure that equals the probability $P[x_n]$.
- The measure is obtained in the limit of a long simulation time T.
- Average any observables $\mathcal{O}$ along the process: $\langle \mathcal{O} \rangle \simeq \frac{1}{T} \sum_{i=1}^{T} \mathcal{O}[x_n^{(i)}]$.

Now, each x_k should be updated to get the new configuration $\Rightarrow O(N_{tot})$.
Evaluation of P might increase in cost and one might have to increase T.

The Sign Problem

A subtlety with fermions

- Expression after integrating fermions could become negative.
  It cannot be interpreted as a weight function $e^{-\tilde{S}[x_n]} = P[x_n]$.
- The Metropolis algorithm cannot work, since now we need a "negative probability" in configuration space.

The sign problem

- Define the expression obtained as $\pm e^{-\tilde{S}}$ (the *sign* problem).
  Work with the $e^{\tilde{S}}$ so defined.
- This has exponential computational cost (the sign *problem*).
  A significant challenge. It was claimed that, for a specific system, the sign problem is an **NP-complete** problem (Troyet, Wiese 2004).
- Seems quite unlikely that a general solution would ever be found.

Bosonic Sign Problem

Generalizing the sign problem

- Systems with a not necessarily real action have a "phase problem".
- Write $e^{-S} = \left|e^{-S}\right| e^{i\phi}$.
- For $\phi = \pi$ the phase is a negative sign, but problems occur whenever the phase $e^{i\phi}$ oscillates enough.
- This is still known as *the sign problem*.

Motivation for the bosonic sign problem

Why would one consider a complex action?

- PT-symmetric theories/String field theory.
- Theories, e.g. QCD, with a nonzero chemical potential $\mu \neq 0$.
  μ is coupled to terms of the form $\phi\partial_0\phi$.
  Such terms acquire i from Wick rotation and become imaginary.
- A toy model: Bose gas at finite chemical potential.

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Lefschetz Thimbles

When $e^{-S} \notin \mathbb{R}$ it cannot be used as a measure for the Monte-Carlo.
Resolution: use *phase-quenching*: redefine $e^{-S} \to |e^{-S}|$ as the measure function: $\langle \mathcal{O} \rangle = \frac{\int D\phi \mathcal{O} |e^{-S}| e^{i\theta}}{\int D\phi |e^{-S}| e^{i\theta}} \equiv \frac{\langle \mathcal{O} e^{i\theta} \rangle_{\mathrm{PQ}}}{\langle e^{i\theta} \rangle_{\mathrm{PQ}}}$.

However, growing phase oscillations lead to exponential numerical cost.
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Methods towards a resolution: Stochastic quantizaion (complex Langevin); Analytical continuation; Taylor expansion...

Resolve using Lefschetz Thimbles (Witten 10; Cristoforetti, Di Renzo, Scorzato 12)

- Complexify all the d.o.f. The original integration contour is a cycle.
- A basis for cycles can be obtained by considering downward gradient flow of $Re(S)$ from stationary points.
- The union of these flows is a smooth manifold: Lefschetz Thimble.
- The gradient flow has $Im(S)$ as a *conserved quantity*.
- Efficient integration cycles. Useful for complex actions.

Implementation of Lefschetz Thimbles on the Lattice

Lefschetz Thimbles are manifolds, but no closed form expression.
Numerical algorithms over thimbles include *expensive checks* for verifying that the data is still on the thimble at each step (however (Alexandru et al. 16)).

For one integration variable the conservation of $Im(S)$ defines the thimble. With more variables the thimble is an N_{tot} dim real manifold in $2N_{tot}$ dim real space. The requirement $Im(S) = C$ leads to a $2N_{tot} - 1$ dim object.

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We don't care if the integration cycle is a thimble (also (Mori, Kashiwa, Ohnishi 17)).
Strategy: Pick *the simplest* integration cycle with proper asymptotic behaviour obeying the equation $Im(S) = C$ at least approximately.

Criteria for simplicity

- Explicit expression for the cycle: avoid expensive verifications.
- As local as possible: reduces numerical cost.
- Use variables that do not lead to expensive Jacobians.
- Trade accuracy of $Im(S) = C$ for simplicity if possible.

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The Bose Gas at Finite Chemical Potential

To illustrate the approach consider the Bose gas at finite μ:
A theory of a single complex scalar.
In the continuum the Euclidean action is given by

$$S = \int d^d x \Big(m^2 \phi^* \phi + \partial_\alpha \phi^* \partial_\alpha \phi + \lambda (\phi^* \phi)^2 + \mu \big(\partial_0 \phi^* \phi - \partial_0 \phi \phi^* \big) \Big) .$$

Discretize in lattice units ($a = c = \hbar = 1$). Impose periodic b. c.:

$$S = \sum_{\vec{x}} \Big(\big(2d + m^2 \big) \phi^*_{\vec{x}} \phi_{\vec{x}} + \lambda (\phi^*_{\vec{x}} \phi_{\vec{x}})^2 - \sum_{\nu=0}^{d-1} \big(\phi^*_{\vec{x}} e^{-\mu \delta_{\nu,0}} \phi_{\vec{x}+\hat{\nu}} + \phi^*_{\vec{x}+\hat{\nu}} e^{\mu \delta_{\nu,0}} \phi_{\vec{x}} \big) \Big) .$$

For simplicity and concreteness take $d = 1$:

$$S = \sum_{k=1}^{N} \Big(\big(2 + m^2 \big) \phi^*_k \phi_k + \lambda (\phi^*_k \phi_k)^2 - \big(\phi^*_k e^{-\mu} \phi_{k+1} + \phi^*_{k+1} e^{\mu} \phi_k \big) \Big) .$$

The Bose Gas in Components

For integrating define $\phi_k = \frac{u_k + i v_k}{\sqrt{2}}$. Now:

$$S = \sum_{k=1}^{N} \Big((1 + \frac{m^2}{2})(u_k^2 + v_k^2) + \frac{\lambda}{4}(u_k^2 + v_k^2)^2 - \cosh\mu\big(u_k u_{k+1} + v_k v_{k+1}\big) - i \sinh\mu\big(u_{k+1} v_k - u_{k+1} v_k\big) \Big).$$

Complexify the components for finding improved integration contours:
$u_k = x_k + i y_k$, $v_k = \xi_k + i\zeta_k$.
Rescale the fields ($\alpha \equiv \frac{1}{2+m^2}$) and expand $y = \alpha \sinh\mu \tilde{y} + O(\alpha \sinh\mu)^2$:

$$Im(S) = \frac{\sinh\mu}{\lambda\alpha} \sum_k \Big(\Big(x_k(1 + x_k^2 + \xi_k^2) - \alpha(x_{k+1} + x_{k-1}) \Big) \tilde{y}_k + \Big(\xi_k(1 + x_k^2 + \xi_k^2) - \alpha(\xi_{k+1} + \xi_{k-1}) \Big) \tilde{\zeta}_k + (x_k \xi_{k+1} - x_{k+1} \xi_k) \Big).$$

Solve $Im(S) \simeq 0$ for $\tilde{y_k}$,$\tilde{\zeta_k}$: One linear equation in $2N$ variables.
Major difference between this expansion and the Taylor expansion method: Here we only approximate the integration contour. The action is exact.

Possible Local Contours

0. $\tilde{y_k} = \tilde{\zeta_k} = 0$.
   The original integration contour – sign problem.
1. $\tilde{y_k} = -\frac{\xi_{k+1}}{1+x_k^2+\xi_k^2}$, $\tilde{\zeta_k} = \frac{x_{k+1}}{1+x_k^2+\xi_k^2}$.
   Only first order in α. Asymptotic behaviour?
2. $\tilde{y_k} = -\frac{\xi_{k+1}}{1+x_k^2+\xi_k^2+\xi_{k+1}^2}$, $\tilde{\zeta_k} = \frac{x_{k+1}}{1+x_k^2+\xi_k^2+x_{k+1}^2}$.
   Only first order in α while $Im(S) \simeq 0$. Regular asymptotic behaviour.
3. $\tilde{y_k} = -\frac{\xi_{k+1}}{1+x_k^2+\xi_k^2+\kappa\xi_{k+1}^2}$, $\tilde{\zeta_k} = \frac{x_{k+1}}{1+x_k^2+\xi_k^2+\kappa x_{k+1}^2}$.
   Interpolate between the previous two contours in order to obtain the best from both. Find best value for κ (0.25).
5. Ansatz: $\tilde{y_k} = -\frac{\sum_{\mu\nu\rho\sigma\tau\phi} a_{\mu\nu\rho\sigma\tau\phi} x_k^\mu x_{k-1}^\nu x_{k+1}^\rho \xi_k^\sigma \xi_{k-1}^\tau \xi_{k+1}^\phi}{1+\sum_{\mu\nu\rho\sigma\tau\phi} b_{\mu\nu\rho\sigma\tau\phi} x_k^\mu x_{k-1}^\nu x_{k+1}^\rho \xi_k^\sigma \xi_{k-1}^\tau \xi_{k+1}^\phi}$, $\tilde{\zeta_k} = ...$
   Add free parameters for products of powers of all nearest neighbours.
   Fit *on a small lattice* for minimizing $Im(S)$ with 12 *parameters*:
   Linear in the numerator, quadratic in the denominator (9 non-zero).

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Simulation Results

Simulations were run with different lattice size (4,8,16,24,32,40) for a fixed value of the parameters: $m = \mu = \lambda = 1$.
The change of variables was implemented in the action ab initio.
Jacobians from the change of variables were included in the simulations.
10^5 configurations checked in each run.
Error estimation is achieved with the Jackknife method.

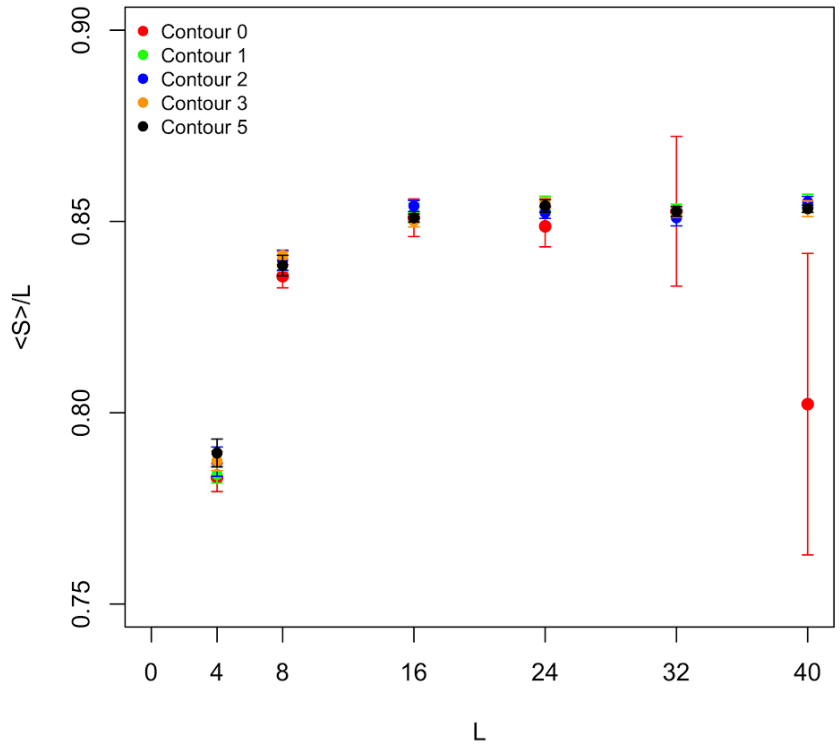
The observables evaluated are the action $\langle S \rangle$ and $\left\langle u_k^2 + v_k^2 \right\rangle$.
In the thermodynamical limit $\frac{\langle S \rangle}{N}$ should approach a constant.

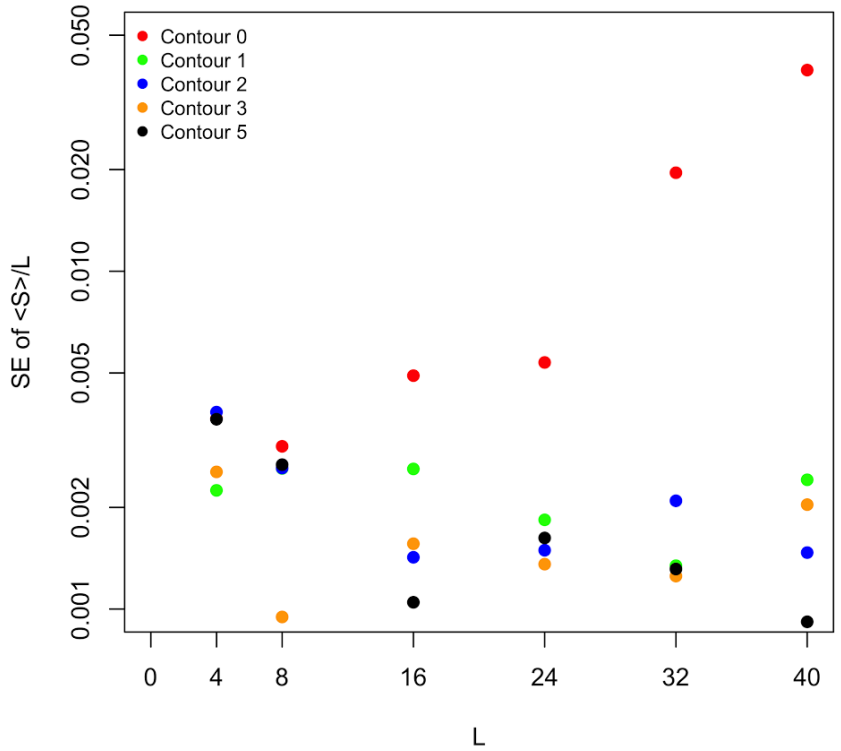
All expressions are complex. Observables could have been complex.
They turns out to be real to a high accuracy, as they should.

We also check explicitly the mean phase in the simulation, since the sign problem is characterized by a vanishing mean phase.

The Action

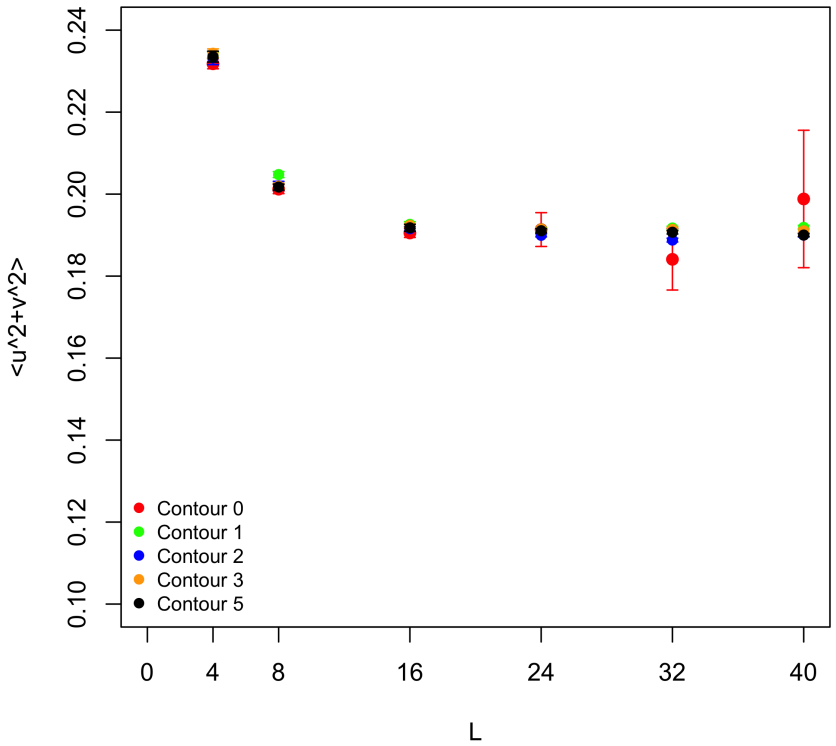
Left: The action density as a function of lattice size.
Right: The standard error in the evaluation of the action.
Contours 0,1,2,3,5 are color marked.

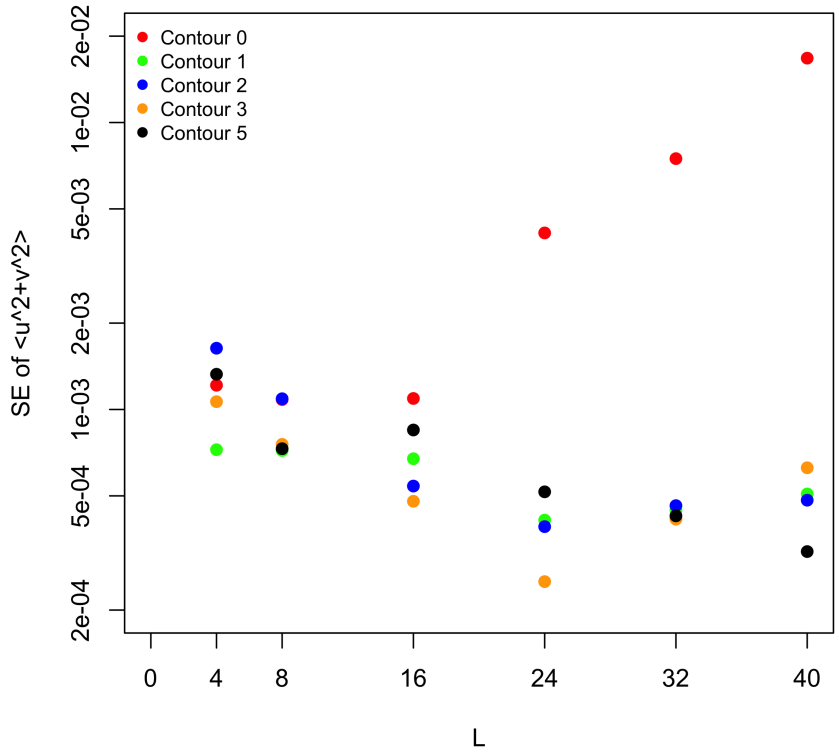




$\langle u_k^2 + v_k^2 \rangle$

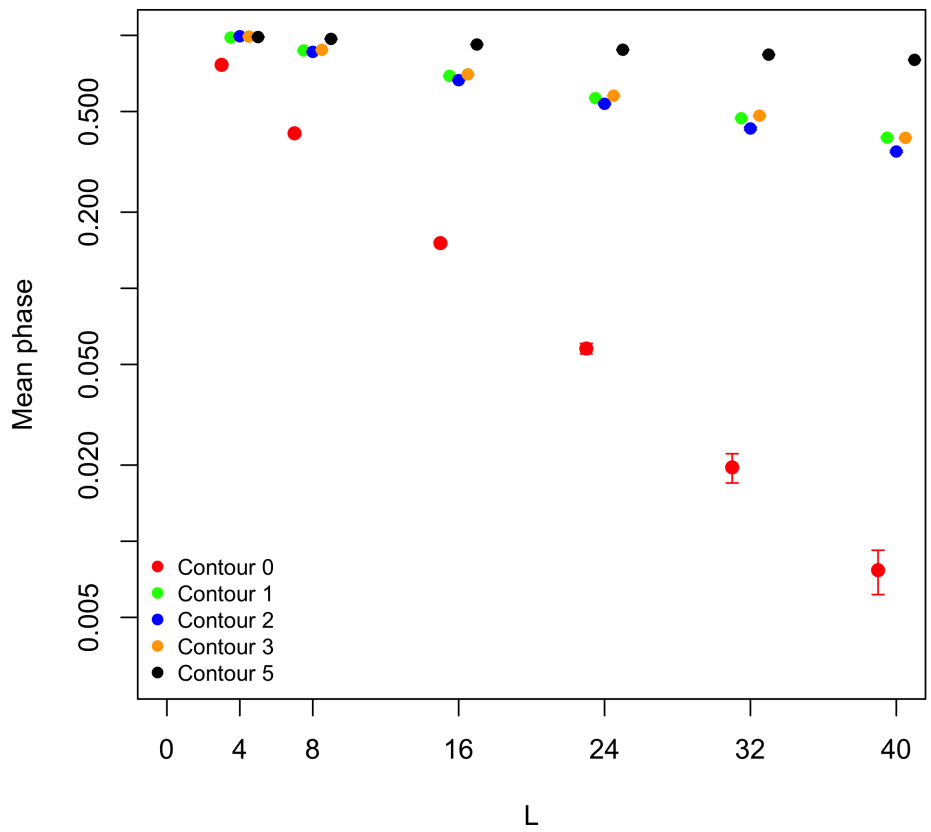
Left: $\langle u_k^2 + v_k^2 \rangle$ as a function of lattice size.
Right: The standard error in the evaluation of $\langle u_k^2 + v_k^2 \rangle$.
Contours 0,1,2,3,5 are color marked.





The Mean Phase

The mean phase as a function of lattice size.
Contours 0,1,2,3,5 are color marked. Points were separated for clarity.
(Note logarithmic scale)



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Summary and Future Directions

Results

- A very simple method can address a complicated question.
- More results:
  - Variants of the contours shown can be used for small $\alpha\lambda$.
  - Non-local contour: The non-locality is hidden in a single variable. An efficient computational method with a determinant that can be evaluated with $O(N)$ instead of $O(N^4)$ per swipe.

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- More results:
  - Variants of the contours shown can be used for small $\alpha\lambda$.
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What's next

- Examine the approach in higher dimensions.
- Apply to other systems, including to systems with fermions.
- Evaluate the continuum limit.
- Apply to PT-symmetric theories and to string field theory.

THANK YOU