First steps in applying the density of states method to the Thirring model

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Motivation

Density of States

- Promising results usign the LLR method
- Sign problem from fermions at nonzero chemical potential
- Also in the Thirring Model
- Simple case: 1+1D

Fermion Bag or World Line

- Direct access to the determinant
- Numerically efficient

Plan

1. Quick review of LLR, DoS and The Thirring model
2. The Fermion Bag method
3. The world line
4. A discrete density of states

Introduction

Generalised density of states

$$Z(\beta) = \int [D\phi] e^{-\beta S[\phi] + i\mu Q[\phi]}$$

$$\rho(q) = \int [D\phi] e^{-\beta S[\phi]} \delta(Q[\phi] - q)$$

$$Z(\mu) = \int dq \rho(q) e^{i\mu q}$$

- Need great accuracy, LLR useful
- Compression through a polynomial fit

Introduction

A problem with fermions

- Pseudofermion actions

$$det(M) = N \int d\chi e^{\chi^\dagger \frac{1}{M} \chi}$$

- Normally we sample χ from a gaussian:

$$Z = e^{\psi^\dagger \psi}$$

$$\chi = \sqrt{M} \psi$$

- Restricting the imaginary part is not consistent

We need the determinant

The Thirring Model

$$S = \sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y - \sum_x m\bar{\chi}_x\chi_x - U\sum_{x,\nu} \bar{\chi}_x\chi_x\bar{\chi}_{x+\nu}\chi_{x+\nu}$$

$$D^{KS}_{x,y} = \frac{1}{2}\eta_{x,\nu}e^{\mu\delta_{\nu,0}}\delta_{y,x+\nu} - \frac{1}{2}\eta^{\dagger}_{x,\nu}e^{-\mu\delta_{\nu,0}}\delta_{y,x-\nu}$$

Similarities to QCD

- Asymptotically safe
- Dynamically generated fermion mass
- Massless boson but no chiral symmetry breaking [1]
- Sign problem at non-zero density

[1] (Witten 1978)

Auxiliary Field Representation

$$S = \sum_{x,\nu} \frac{N_F}{g^2} (1 - \cos A_{x,\nu}) + \sum_{x,y} \bar{\chi}_x D_{x,y} \chi_y$$

$$D_{x,y} = m' \delta_{x,y} + \frac{1}{2} \sum_{\nu=0,1} \eta_\nu e^{iA_{x,\nu} + \mu\delta_{\nu,0}} \delta_{x+\nu,y} - \eta_\nu^\dagger e^{-iA_{y,\nu} - \mu\delta_{\nu,0}} \delta_{x-\nu,y}$$

$$U = 0.25 \left(\frac{I_0\left(\frac{N_F}{g^2}\right)}{I_1\left(\frac{N_F}{g^2}\right)} \right)^2 - 0.25, \;\; m = \left(\frac{I_0\left(\frac{N_F}{g^2}\right)}{I_1\left(\frac{N_F}{g^2}\right)} \right) m'$$

$$g = 1 \;\; \rightarrow \;\; U \approx 0.26, \;\; m \approx 1.43 m'$$

Fermion Bag Representation

Starting with a free staggered fermion:

$$S = \sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y - \sum_x m\bar{\chi}_x\chi_x$$

$$D^{KS}_{x,y} = \frac{1}{2}\eta_{x,\nu} e^{\mu\delta_{\nu,0}}\delta_{y,x+\nu} - \frac{1}{2}\eta_{x,\nu} e^{-\mu\delta_{\nu,0}}\delta_{y,x-\nu}$$

Fermion Bag Representation

Expand the partition function

$$Z = \int d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y - m\bar{\chi}_x\chi_x}$$

Fermion Bag Representation

Expand the partition function

$$Z = \int d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y - m\bar{\chi}_x\chi_x}$$
$$= \int d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y} \prod_x (1 + m\bar{\chi}_x\chi_x)$$

Fermion Bag Representation

Expand the partition function

$$
\begin{aligned}
Z &= \int d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y - m\bar{\chi}_x\chi_x} \\
&= \int d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y} \prod_x (1 + m\bar{\chi}_x\chi_x) \\
&= \sum_{[m]} \int d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y} (m\bar{\chi}_x\chi_x)^{m_x}
\end{aligned}
$$

Fermion Bag Representation

Expand the partition function

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\begin{aligned}
Z &= \int d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y - m\bar{\chi}_x\chi_x} \\
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&= \sum_{[m]} \int d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y} (m\bar{\chi}_x\chi_x)^{m_x} \\
&= \sum_{[m]} m^{N_m} \int_{[f]} d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y}
\end{aligned}
$$

Fermion Bag Representation

Expand the partition function

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Z &= \int d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y - m\bar{\chi}_x\chi_x} \\
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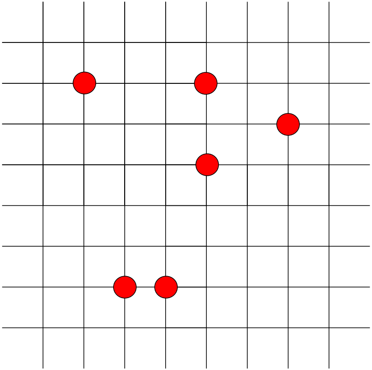
&= \sum_{[m]} \int d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y} (m\bar{\chi}_x\chi_x)^{m_x} \\
&= \sum_{[m]} m^{N_m} \int_{[f]} d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y} \\
&= \sum_{[m]} m^{N_m} \det\left(D([f],\mu)\right)
\end{aligned}
$$

Fermion Bag Representation

- Sites covered by (mass) monomers
- Determinant over free sites



Fermion Bag Representation

Adding a four fermion interaction

$$Z = \int e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu) \chi_y - m \sum_x \bar{\chi}_x \chi_x - U \sum_{x,\nu} \bar{\chi}_x \chi_x \bar{\chi}_{x+\nu} \chi_{x+\nu}}$$

Fermion Bag Representation

Adding a four fermion interaction

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$$= \int e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y} \prod_x (1 + m\bar{\chi}_x\chi_x) \prod_{x,\nu} (1 + U\bar{\chi}_x\chi_x\bar{\chi}_{x+\nu}\chi_{x+\nu})$$

Fermion Bag Representation

Adding a four fermion interaction

$$Z = \int e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y - m\sum_x \bar{\chi}_x\chi_x - U\sum_{x,\nu} \bar{\chi}_x\chi_x\bar{\chi}_{x+\nu}\chi_{x+\nu}}$$

$$= \int e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y} \prod_x (1 + m\bar{\chi}_x\chi_x) \prod_{x,\nu} (1 + U\bar{\chi}_x\chi_x\bar{\chi}_{x+\nu}\chi_{x+\nu})$$

$$= \sum_{[m],[d]} m^{N_m} U^{N_d} \int_{[f]} d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y}$$

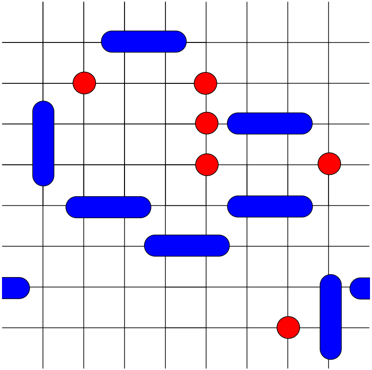
Fermion Bag Representation

Adding a four fermion interaction

$$
\begin{aligned}
Z &= \int e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y - m\sum_x \bar{\chi}_x\chi_x - U\sum_{x,\nu} \bar{\chi}_x\chi_x\bar{\chi}_{x+\nu}\chi_{x+\nu}} \\
&= \int e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y} \prod_x (1 + m\bar{\chi}_x\chi_x) \prod_{x,\nu} (1 + U\bar{\chi}_x\chi_x\bar{\chi}_{x+\nu}\chi_{x+\nu}) \\
&= \sum_{[m],[d]} m^{N_m} U^{N_d} \int_{[f]} d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu)\chi_y} \\
&= \sum_{[m],[d]} m^{N_m} U^{N_d} \det\left(D([f],\mu)\right)
\end{aligned}
$$

Fermion Bag Representation

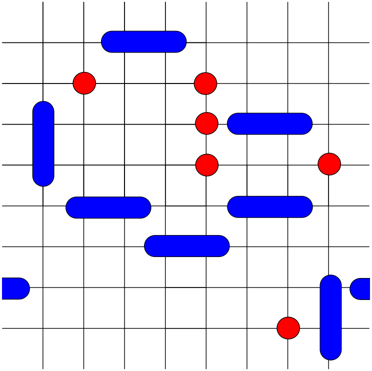
- Two new fields, d and m
- Each interaction term represented by dual field
- Partition function given by the determinant



Fermion Bag Algorithm

Local Updates:

1. Add / remove monomer
2. Add / remove dimer
3. Replace dimer with monomers
4. Replace two monomers with dimer
5. Swap monomer and dimer



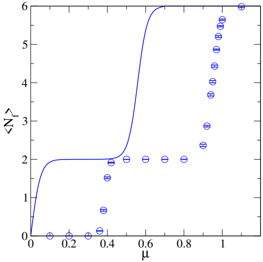
(github.com/rantahar/Thirring2D/tree/v1.0)

Fermion Bag Algorithm

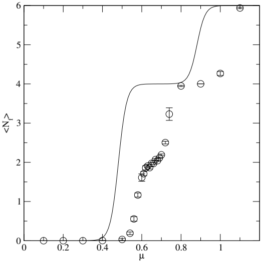
The point is to calculate (thermal) expectation values

$$< O > = \int d\bar{\chi} d\chi O e^{-S}$$
$$= \sum_{[d],[m]} O m^{N_m} \det (D([f], \mu))$$

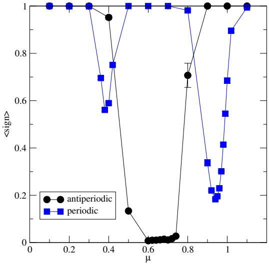
Sign Problem



Periodic



Anti-periodic



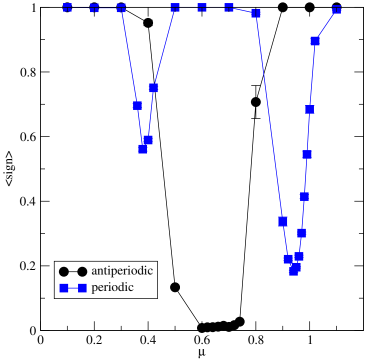
Average sign

- Small lattice, $L_X = 6$ and $L_T = 48$
- Intermediate coupling $U = 0.3$
- Levels determined by symmetry

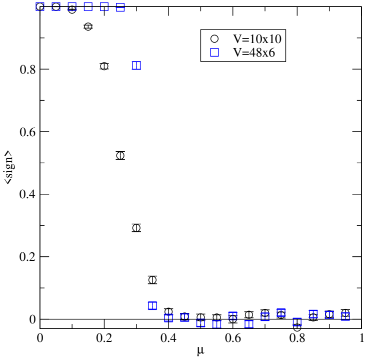
(Ayyar, Chandrasekharan, Rantaharju 2018)

Sign Problem

A quick test with the auxiliary field



Fermion Bag



Auxiliary field

Determinant

Problem: the determinant is real

- Cannot apply extended DoS directly
- Measure DoS as afunction of the determinant?
- Failure at $E = 0$: LLR requires finite $\log(\rho)$

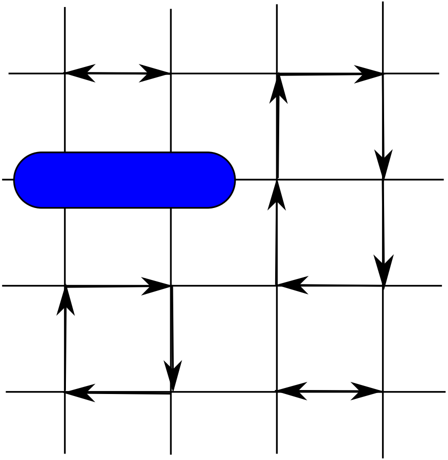
World Line Representation

$$
\begin{aligned}
&\det\left(W([f],\mu)\right) \\
&= \prod_{x\in[f]} \left(\int d\bar{\chi}_x d\chi_x \right) e^{-\sum_{x\in[f]}\left(\frac{1}{2}\eta_{x,\nu} e^{\mu\delta_{\nu,0}}\bar{\chi}_x\chi_{x+\nu} - \frac{1}{2}\eta^{\dagger}_{x,\nu} e^{-\mu\delta_{\nu,0}}\bar{\chi}_{x+\nu}\chi_x\right)} \\
&= \sum_{[l]} \prod_{loop\in l} \left(- \prod_{x,\alpha\in loop} e^{\pm\mu\delta_{\pm\alpha,\hat{t}}} \frac{s_\alpha \eta_{x,\alpha}}{2} \right)
\end{aligned}
$$

$s_\alpha = +1$ (-1) for positive (negative) directions α

World Line Representation

- Fermion world line variable $l_{x,\nu}$
- Closed loops of fermion world lines



World Line Representation

No sign problem with

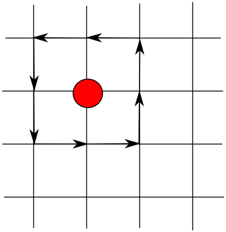
- Open boundary conditions

$$\bar{\chi}_x = \chi_x = 0 \text{ when } x_1 = 0, L_X$$

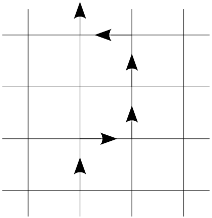
- $m = 0$ (no monomers)

World Line Representation

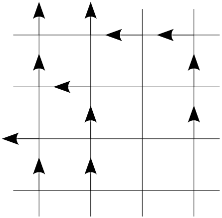
Examples of negative loops:



$m \neq 0$



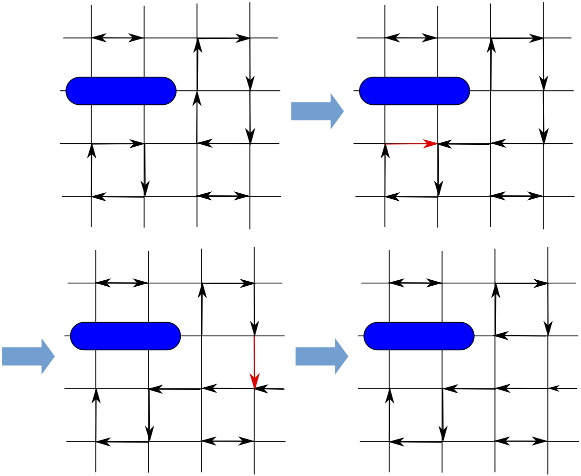
(Anti-)periodic



Anti-periodic

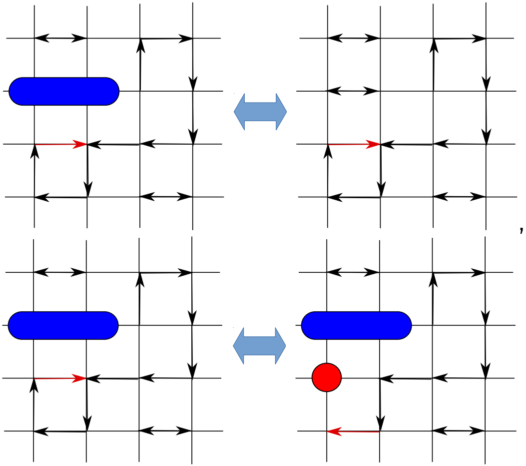
World Line Algorithm

- Avoids trapping in regions of N_f



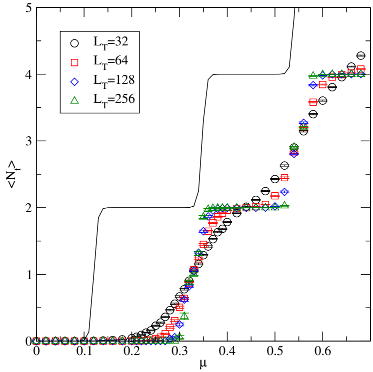
World Line Algorithm

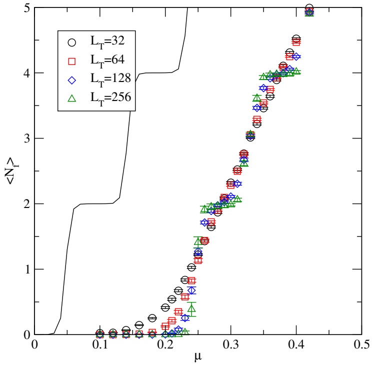
- Updating links and monomers



(github.com/rantahar/worldline)

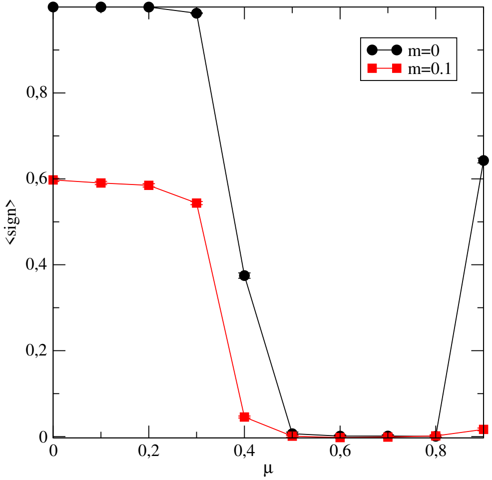
Fermion Number





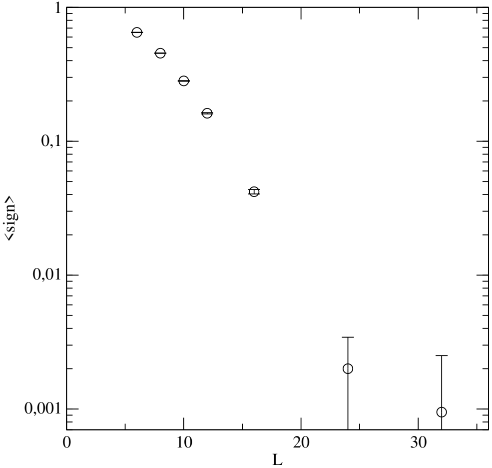
Fermion number at $U = 0.3$ and $L_X = 12$ (left) and 32 (right)

Sign Problem



The overlap as a function of μ with antiperiodic boundaries and $T = 48$, $L = 6$ and $U = 0.3$.

Sign Problem



The overlap as a function of L on a square lattice with $U = 0.3$, $m = 0.1$ and $\mu = 0$.

The Sector Number

Attempt to get a handle on the sign

- Count the number of negative loops

$$s = \sum_{loop \in l} \delta_{\mathrm{sign}\,(l),-1}$$

- The sign of a configuration is

$$-1^{s}$$

The Sector Number

Sector number

- A density of negative loops
- Approaches a continuous function
- Polynomial fit?
- Discrete, no LLR

Wang Landau

$$W_s = e^{-F_s} = \sum_{[d],[n],[l]} m^{N_m} U^{N_d} \delta(s(l), s).$$

1. Initialize $F_s = 0$
2. After worm update, accept new sector s' with propability

$$P = \max\left(1, e^{F_s - F_{s'}}\right).$$

3. Update F_s by

$$F_s(n) = F_s(n-1) + \frac{\delta}{n + n_{initial}}$$

Wang Landau

- Converges to correct free energy (up to a constant)
- But no proof gaussian distributition (Robbins Monro)

Finegrain with Monte Carlo

$$Z'(d,n,l) = Z(d,n,l)e^{-F_s}$$

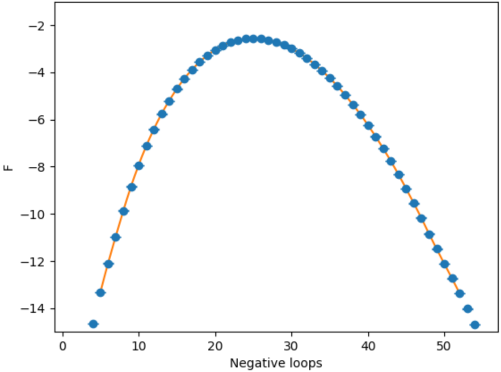
- Measure W_s directly

$$W_{s'} = \left\langle \delta_{s,s'} \right\rangle e^{F_s}$$

- Error roughly

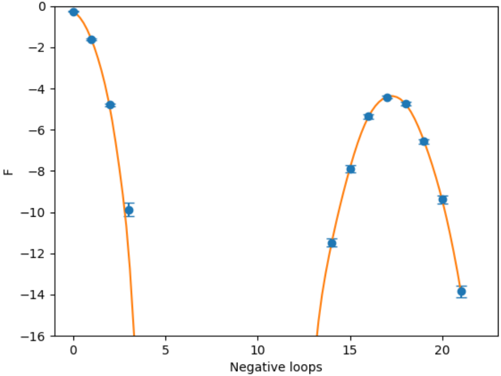
$$\frac{e^{-F_s}}{\sqrt{N}}$$

Density of States



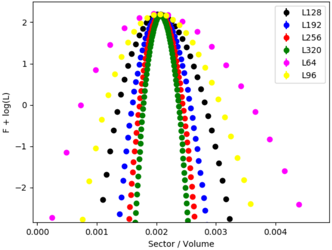
Density of states as a function of the sector s at $U = 0$, $m = 0.1$, $\mu = 0.1$ and $L_X = L_T = 128$

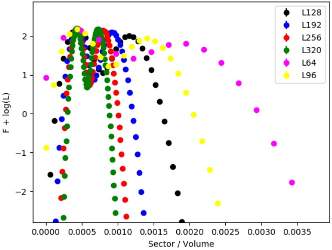
Density of States



Density of states as a function of the sector s at $U = 0$, $m = 0$, $\mu = 0.4$ and $L_X = L_T = 64$

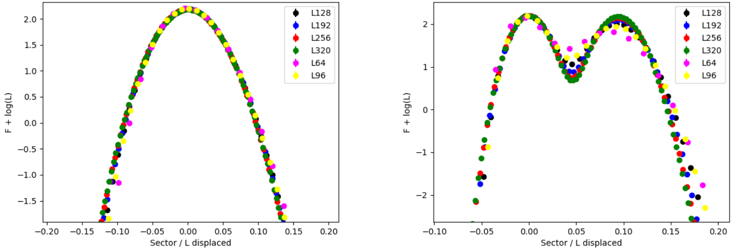
Density of States





Volume scaling of the sector density at $U = 0$, $m = 0.1$ and $\mu = 0$ (left) and 0.3 (right). The x axis shows the negative loop density, or the sector scaled by the volume. The y axis is shifted by $\log(L)$ for each volume to increase legibility.

Density of States



Same figure with the negative loop count scaled by L instead the volume and with the x-axis shifted so that the maximum free energy is at 0.

Wang Landau

A moving polynomial fit $p(x) = \sum_{i=0}^{2} p_i x^i$

$$\chi_s = \sum_{s'} \frac{(p(x) - F_x)^2}{\sigma_x e^{\frac{|x-s'|^2}{2w^2}}}$$

- Calculate the overlap

$$\langle sign(Z) \rangle = \frac{\sum_s (-1)^s e^{p(s)}}{\sum_s e^{p(s)}}.$$

Wang Landau

Volume	Updates	w	$\max\left(\frac{p(s)-F_s}{\sigma_s}\right)$	$\langle \mathrm{sign}\,(Z)\rangle$
64x64	3.1M + 6.62M	0	0	-0.001s(2)
64x64	3.1M + 6.62M	1	0.9	-0.0003(8)
64x64	3.1M + 6.62M	2	4.0	-9.0(9)e-5
128x128	5M + 3M	0	0	0.002(3)
128x128	5M + 3M	2	1.1	1(2)e-5
128x128	5M + 3M	4	1.6	6(8)e-9
128x128	5M + 3M	6	3.2	-0(3)e-10
256x256	6.1M + 12M	0	0	-0.00(1)
256x256	6.1M + 12M	2	1.2	0(2)e-5
256x256	6.1M + 12M	8	2.0	-0(7)e-11
256x256	6.1M + 12M	16	3.2	-0(1)e-10

$U = 0,\ \mu = 0,\ m = 0.1$

Conclusions

World line formalism with mass $\rightarrow$ bad sign problem

- Number of negative loops as an interpolator for the sign
- Simple scaling with volume
- Exponential scaling of accuracy
- Stress testing the method

Is there a better measurable correlated with the sign?