Measuring Renyi entropies in finite-temperature QMC using Wang-Landau sampling

Stephen Christopher Inglis

University of Waterloo

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Outline

1. Motivation
2. Importance vs. Wang-Landau
3. Results
4. Discussion

The Renyi Entropy

Using Renyi Entropy we can detect qualities not possible using two-point correlation functions.

In one dimension, we can detect central charge.

In two dimensions we can test the area law and it's violations.

The Renyi Entropy

The Renyi Entropy is defined as

$$S_n(\rho_A) = \frac{1}{1-n} \ln[\mathrm{Tr}(\rho_A^n)]$$

$$\mathrm{Tr}(\rho_A^n) = \frac{Z(A, n, \beta)}{Z^n(\beta)}$$

where the second equation is the "replica trick" we can use to calculate the 2nd (or larger) Renyi Entropy with the normal, $Z(\beta)$, and modified, $Z(A, n, \beta)$, simulations.

Roger G. Melko, Ann B. Kallin, Matthew B. Hastings, Phys. Rev. B 82, 100409(R) (2010)

The classical Monte Carlo algorithm

Classical Monte Carlo with importance sampling is done by

- start with a random state of the system
- propose a test state, and accept the move to that state with some probability P
- whether accepted or rejected, measure observables in the current state

In this method the probability used is based on the Boltzmann distribution

$$P = \min \begin{cases} e^{\beta(E_i - E_f)} \\ 1 \end{cases} .$$

Observables in classical Monte Carlo

In statistical systems, the energy can be defined as

$$\langle E \rangle = \frac{\sum_i E_i e^{-\beta E_i}}{\sum_i e^{-\beta E_i}}.$$

In Monte Carlo simulations, we do large N sampling. If we let $W_i = e^{-\beta E_i} / \sum_i e^{-\beta E_i}$ and use importance sampling, we get

$$\langle E \rangle = \frac{\sum_i E_i \left(W_i N \right)}{N},$$

where $\left(W_i N \right)$ is the number of times state i is sampled.

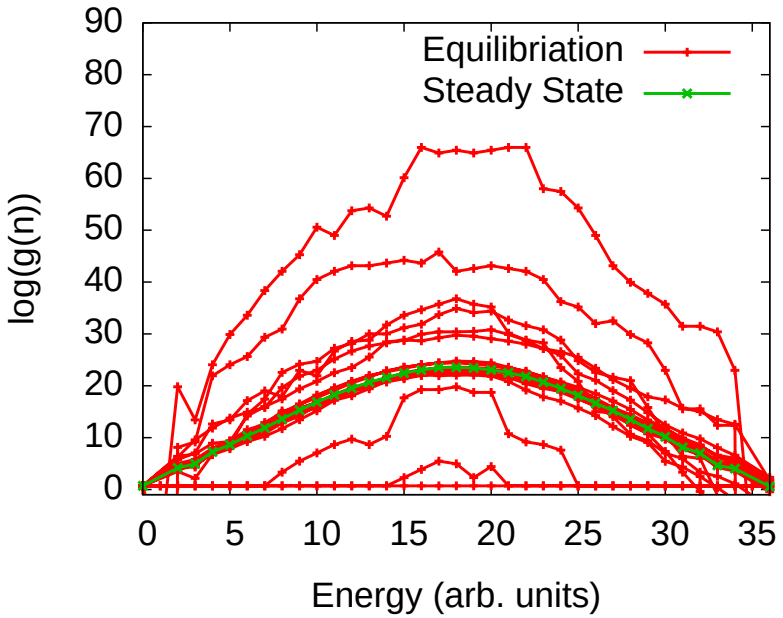
The Wang-Landau algorithm

The Wang-Landau algorithm calculates the density of states by

- assume an initial density of states $g_0(E)$
- generate a new state and visit it with a probability P
- update $g_{i+1}(E) = g_i(E) \times f$

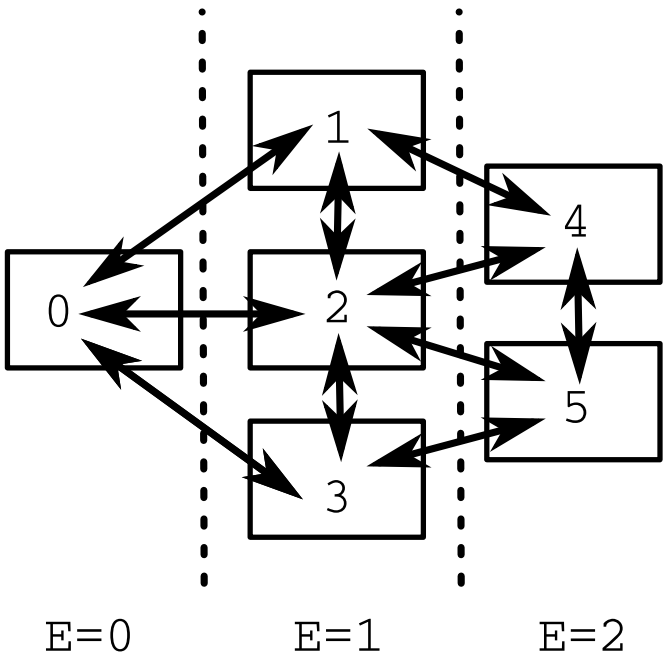
In Wang-Landau the probability is

$$P = \min \begin{cases} g(E_i)/g(E_f) \\ 1 \end{cases}$$



The evolution of the density of states, $g(E)$, as the simulation progresses

The Wang-Landau algorithm

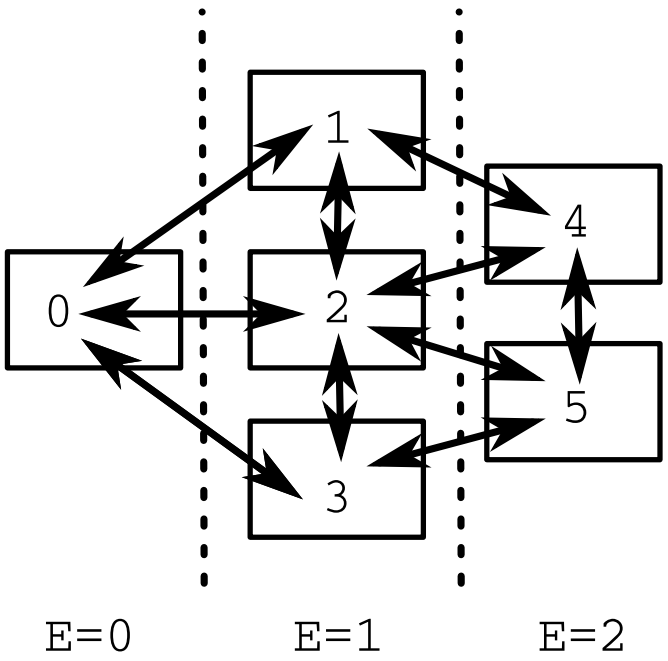


$g(0)$	$g(1)$	$g(2)$
1.0	1.0	1.0

Step	**0**	**1**	**2**	**3**	**4**	**5**
$i = 0$	100	0	0	0	0	0
$i = 1$	0	33	33	33	0	0
$i = 2$	29	7	22	7	17	17
$\cdots$						
$i = \infty$	15	15	25	15	15	15

$$W(E_0) = 15, W(E_1) = 55, W(E_2) = 30$$

The Wang-Landau algorithm

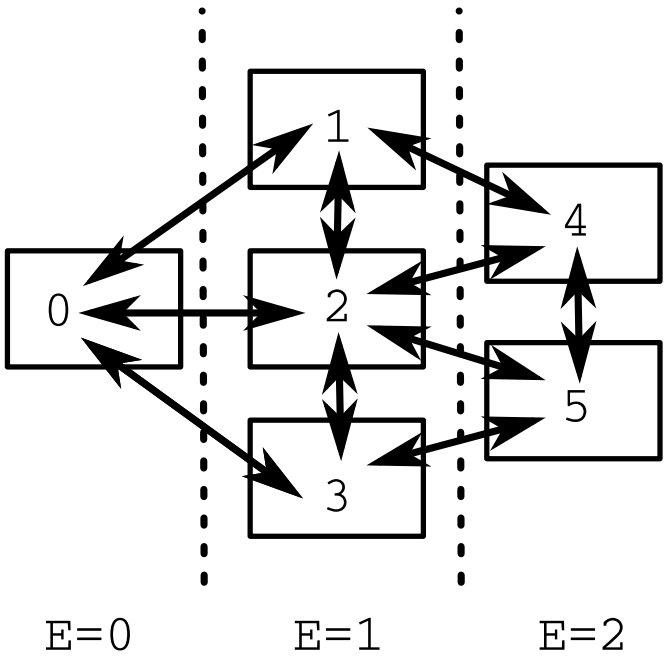


$g(0)$	$g(1)$	$g(2)$
1.0	3.0	2.0

Step	**0**	**1**	**2**	**3**	**4**	**5**
$i = 0$	100	0	0	0	0	0
$i = 1$	67	11	11	11	0	0
$i = 2$	54	9	15	9	6	6
$\cdots$						
$i = \infty$	31	10	17	10	15	15

$$W(E_0) = 31, W(E_1) = 37, W(E_2) = 30$$

The Wang-Landau algorithm



$g(0)$	$g(1)$	$g(2)$
1.0	3.666	2.0

Step	**0**	**1**	**2**	**3**	**4**	**5**
$i = 0$	100	0	0	0	0	0
$i = 1$	72	9	9	9	0	0
$i = 2$	60	8	13	8	5	5
$\cdots$						
$i = \infty$	33	9	15	9	16	16

$$W(E_0) = 33, W(E_1) = 33, W(E_2) = 32$$

Wang-Landau and SSE

Wang-Landau works by calculating the density of states as a function of energy. In SSE QMC, the energy of the system is equal to

$$E = \frac{-\langle N \rangle}{\beta} + C,$$

where $\langle N \rangle$ is the average number of operators sampled, β is the inverse temperature and C is the sum of the constants added to the Hamiltonian.

A. W. Sandvik, Phys. Rev. B 59, R14157R14160 (1999)

Wang-Landau and SSE

Instead of sampling $g(E)$, we sample $g(n)$ in SSE QMC such that

$$E(\beta) = \sum_n \frac{-n}{\beta} \left[\beta^n g(n)\right] + C.$$

We modify the diagonal update such that (i.e. for adding an operator)

$$P_I = \frac{W\beta}{(M-n)}$$

$$P_{W-L} = \frac{W\beta g(n)}{(M-n)g(n+1)}$$

Matthias Troyer, Stefan Wessel, Fabien Alet, Phys. Rev. Lett. 90, 120201 (2003)

Calculating Renyi Entropy

Using importance sampling we calculate the Renyi Entropy as

$$\begin{aligned} S_2(A,\beta) &= -\ln(Z[A,2,\beta]) + 2\ln(Z[\beta]) \\ &= -S_2(A,\beta=0) + 2S_1(\beta=0) + \\ &\int_0^\beta < E >_{A,\beta'} d\beta' - 2\int_0^\beta < E >_{1,\beta'} d\beta' \end{aligned}$$

Calculating Renyi Entropy

In Wang-Landau we can directly evaluate the entropy as

$$S_2(A,\beta) = -\ln(Z[A,2,\beta]) + 2\ln(Z[\beta])$$

directly, as we have access to $Z[\beta]$ and $Z[A,2,\beta]$ through

$$Z(\beta) = \sum_n \left[\beta^n g(n)\right],$$

Mutual Information

At finite temperature we must use the Mutual Information instead of just the Renyi Entropy to account for the thermal contributions to the entropy.

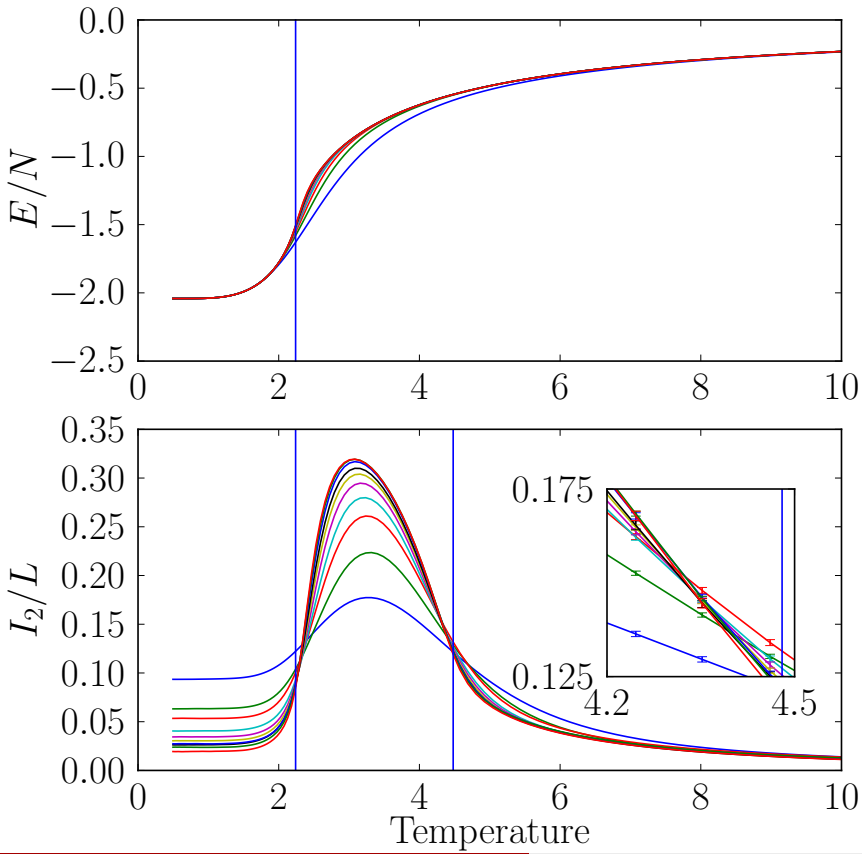
$$I_2(A:B,\beta) = S_2(A,\beta) + S_2(B,\beta) - S_2(A\cup B,\beta),$$

By measuring this quantity we can extend the idea of an area law to finite temperature quantum systems

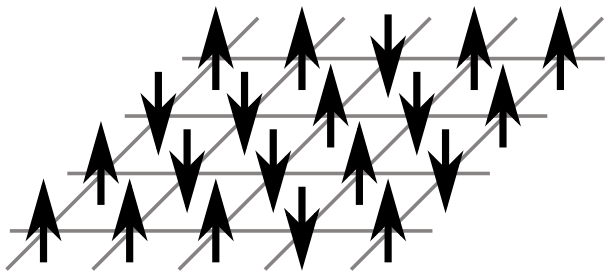
Preliminary Results

We are currently testing this method on 2D-XXZ Models and the 3D Heisenberg model.

2D Anisotropic Ising (Delta=4)



$$H = -\sum_{<ij>}\left(\Delta S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y\right)$$



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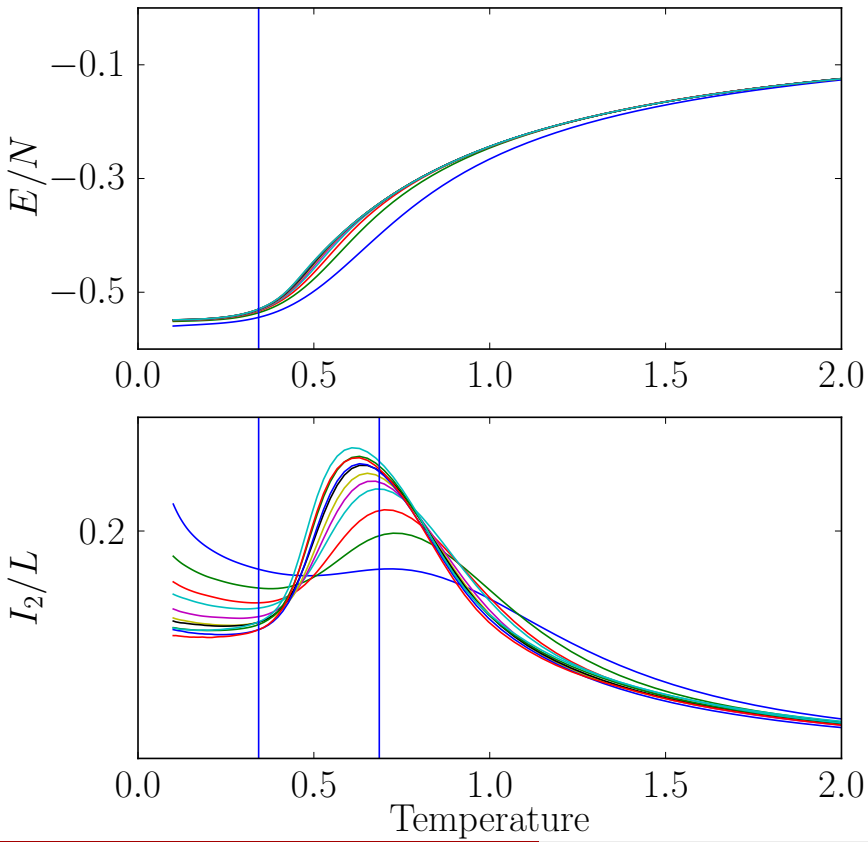
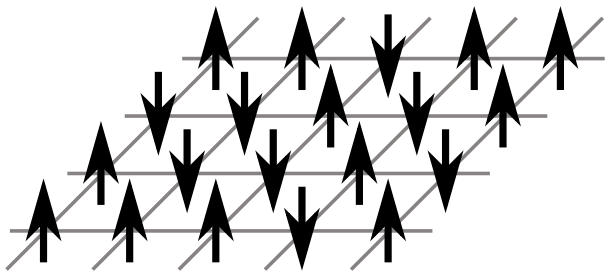
2D XY (Delta = 0)



$$H = -\sum_{<ij>} \left(\Delta S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y \right)$$



Preliminary Results

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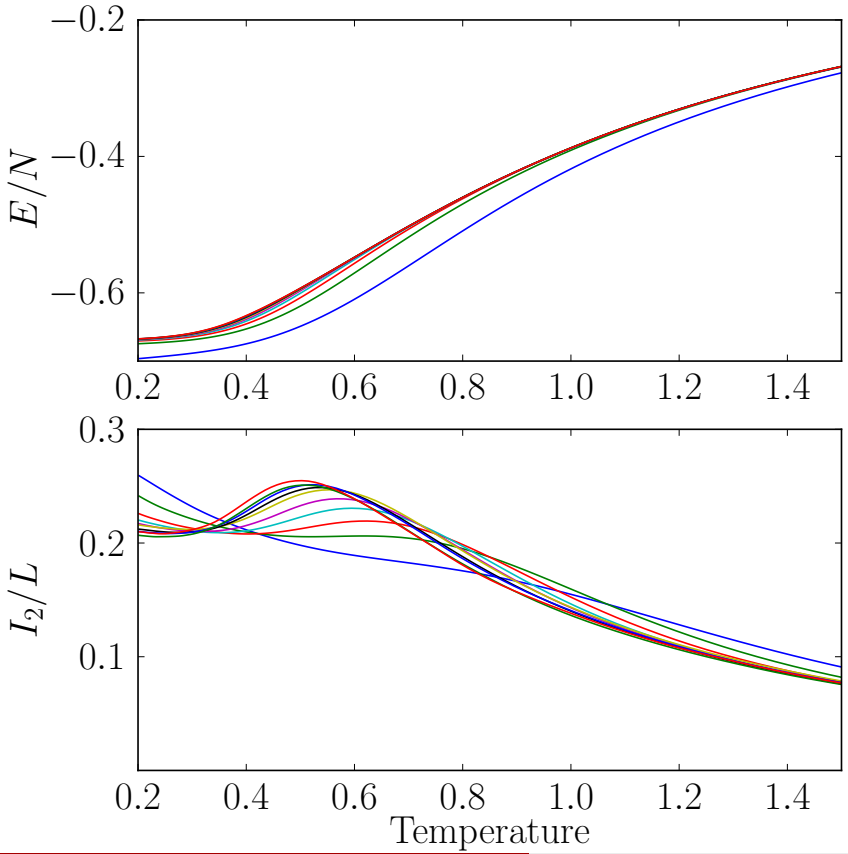
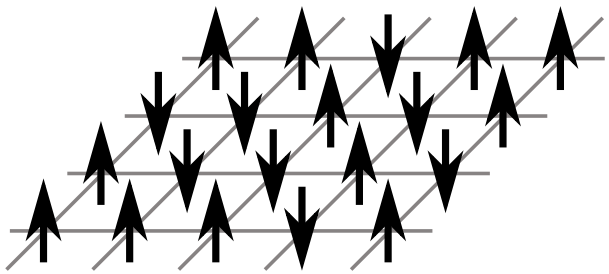
2D Heisenberg (Delta = 1)



$$H = -\sum_{<ij>}\left(\Delta S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y\right)$$



Preliminary Results

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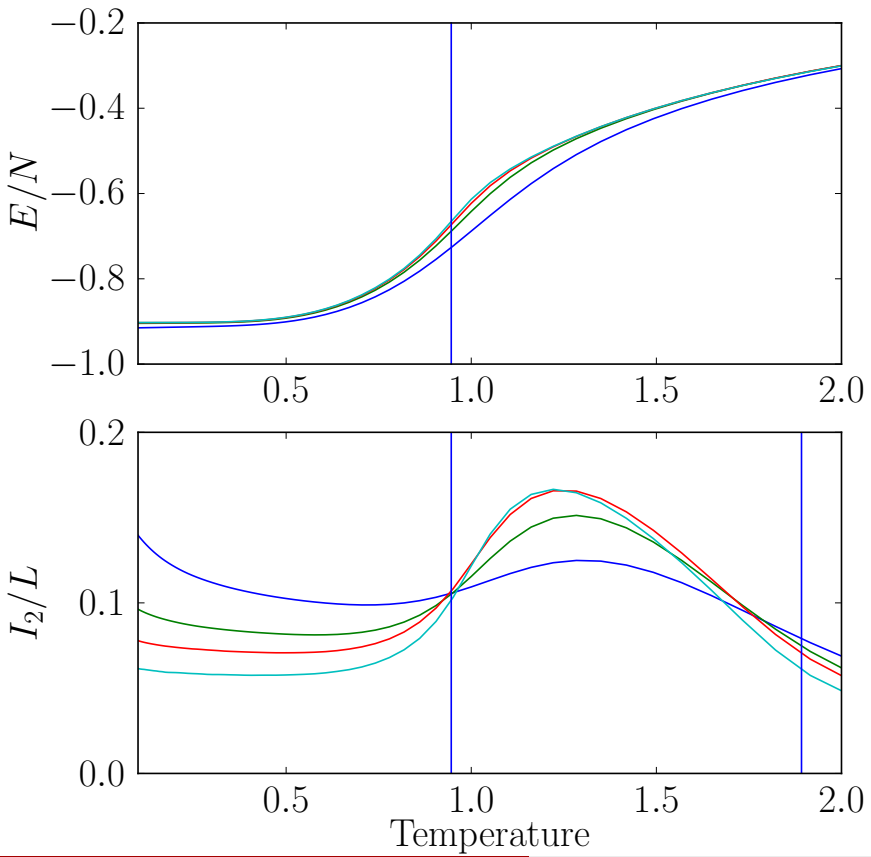
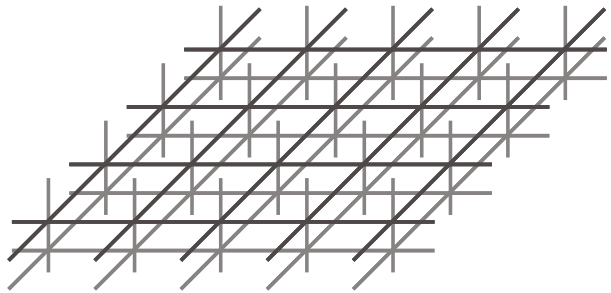
3D Heisenberg (Delta=1)



$$H = -\sum_{<ij>}\left(\Delta S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y\right)$$

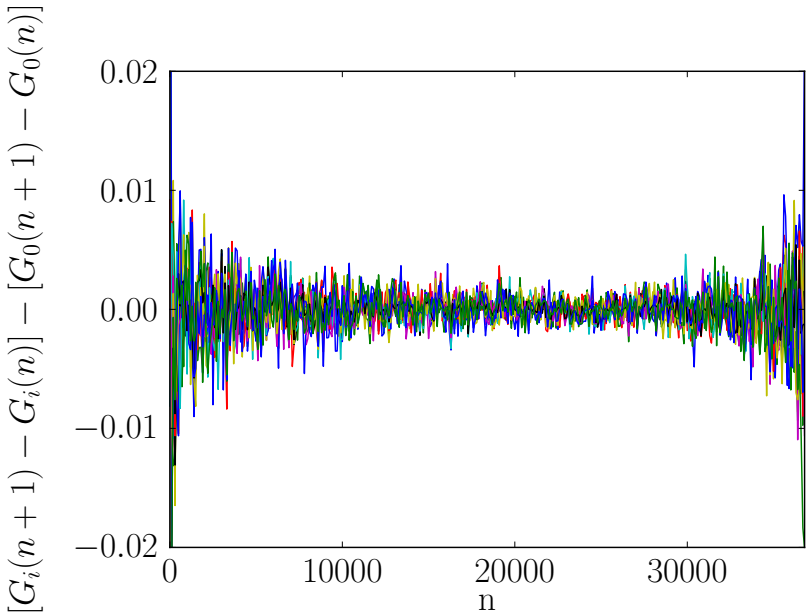


Noise in Wang-Landau

Noise in $dG(n)/dn$
$G(n) = \log(g(n))$

When examining the distribution of $g(n)$ from separate simulations, we found it was not $g(n)$ that was being converged, but rather $dg(n)/dn$.

This means for large n, $g(n)$ has a larger variance, since we pin $g(n)$ at the known point $g(0)$.



Advantage of the Wang-Landau algorithm

We have implemented quantum Wang-Landau for the modified simulation.

The benefits are

- only one simulation is required rather than many
- no (explicit) cumulative integration error
- results may be improved building on old data easily

The difficulties are

- single simulation takes longer
- harder to measure non-energy related observables

Summary

We have implemented Wang-Landau for quantum systems with modified boundary conditions.

We will use it to explore the qualities of entanglement entropy in quantum systems.

Thanks to my supervisor, Roger Melko, NSERC / Vanier CGS for funding this work and SHARCNET for computing resources.

High Temperature expansion

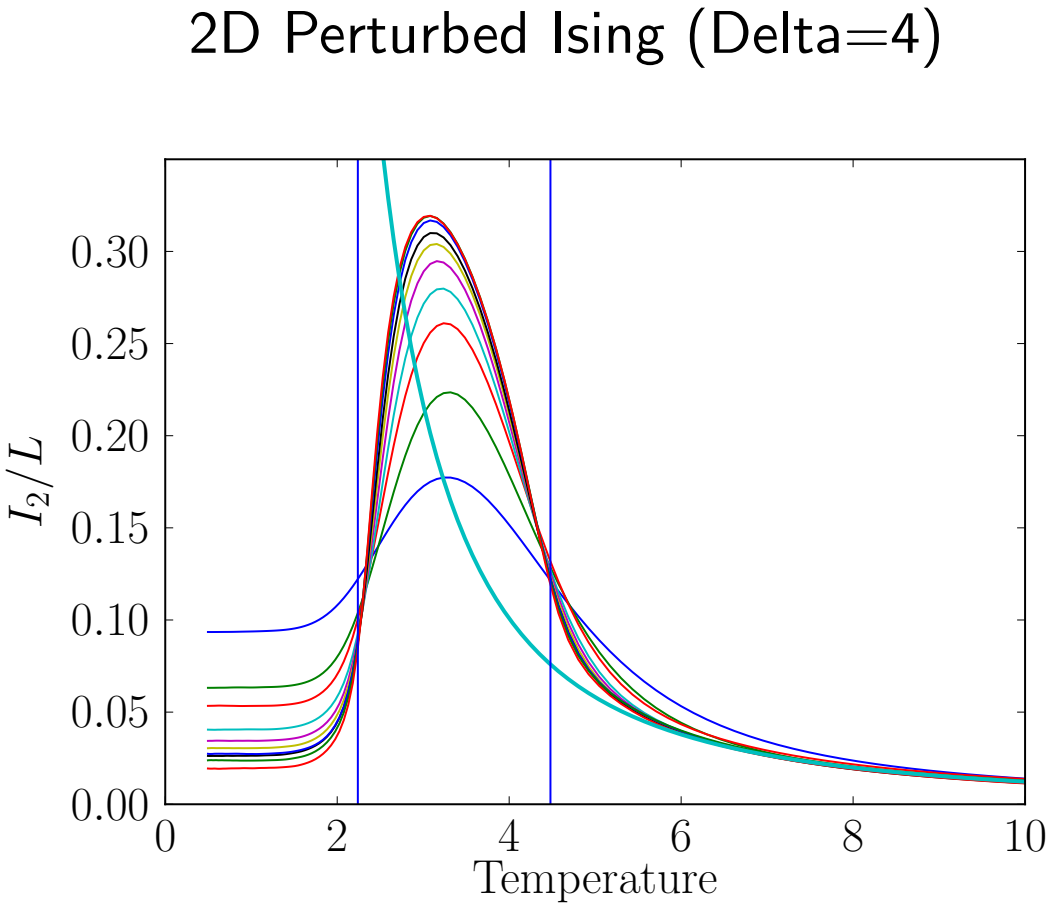
The important term in the entropy has the form

$$a_2(\beta) = (\frac{\beta}{4})^2 \frac{2A_2}{2} - (\frac{\beta}{4})^3 A_3 + (\frac{\beta}{4})^4 \Big[14(\frac{A_4}{24} - \frac{A_2^2}{8}) + 10(\frac{B_4 - A_2^2}{2} + C_4) \Big]$$

Where A_2, A_3, A_4, B_4 and C_4 all have dependance on Δ, the ising component of the XXZ model.

High Temperature expansion

Comparison to high temperature expansion



High Temperature expansion

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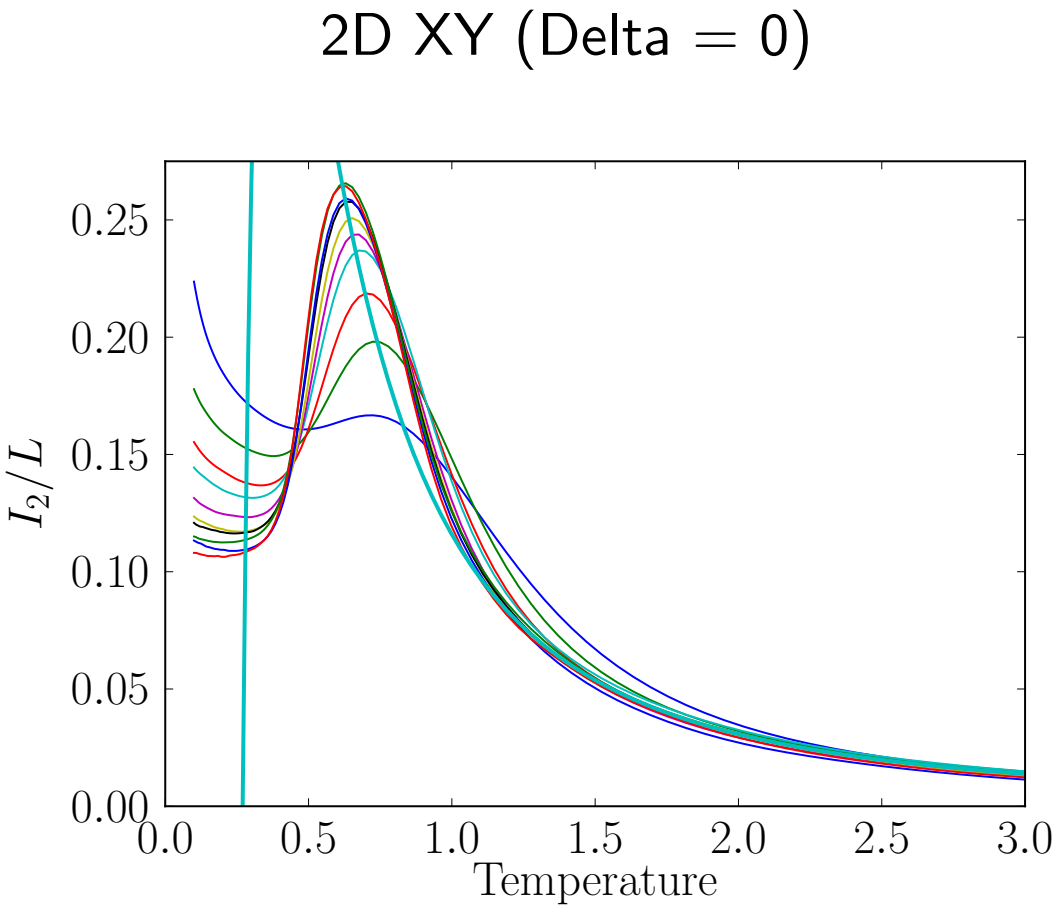
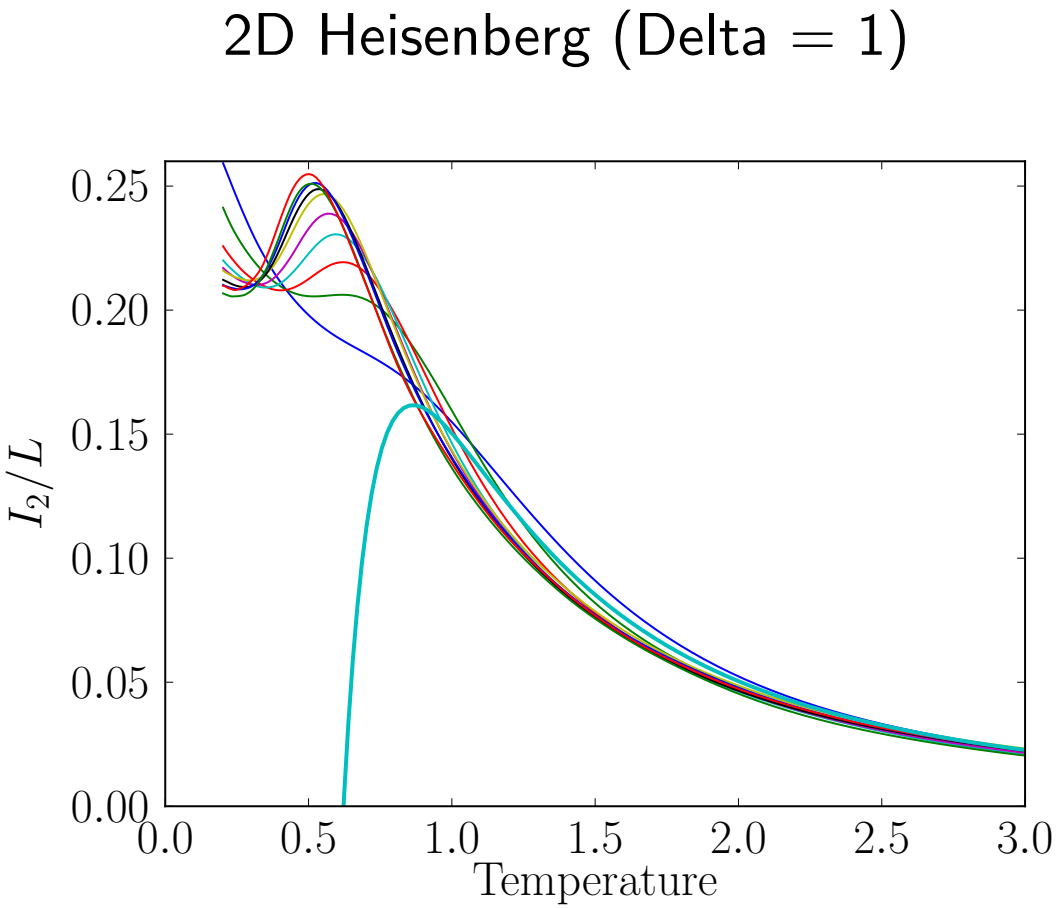


High Temperature expansion

Comparison to high temperature expansion

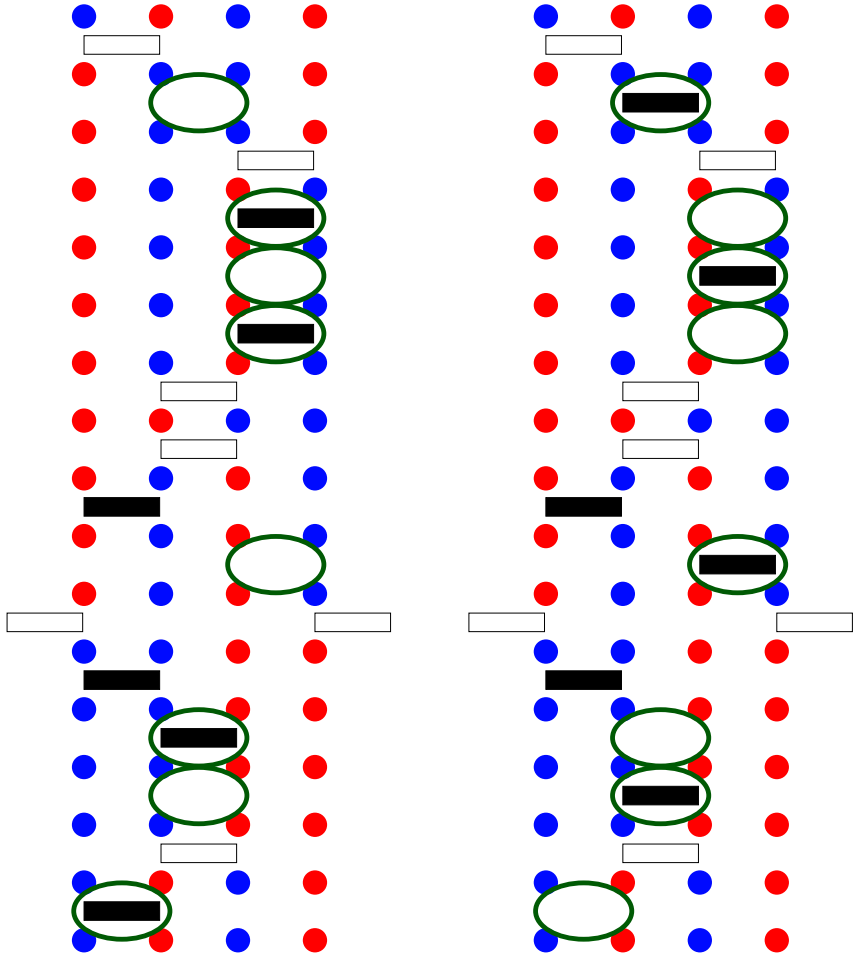


The Stochastic Series Expansion

Diagonal Update

This update iterates through the list of operators and

- If a diagonal operator is present, tried to remove it
- If there is no operator, tries to add a diagonal operator



The Stochastic Series Expansion

Directed Loop

This update generates a loop through the legs of the operators

- When encountering an operator, uses probability to choose the path
- Loop closes when it encounters it's own starting point

This move updates spins and operator types.