Thesis Notes

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Monday, June 15

- Preliminary meeting
- We will begin with ϕ^4 term due to lower energy bound.
- Beginning with code in Python, switch to C/C++ if necessary.

Tuesday, June 16

- Preliminary concepts to understand:
  - scalar field theory on lattice
  - Markov chains and Monte Carlo
  - the gradient flow
  - $O(n)$ symmetry
- General components to research, executed in parallel
  - Reading
  - Mathematical analysis
  - Writing code
  - Present (writing, plot generation,...)
- Things to get out of dissertation (Schaich and Loinaz 2006)
  - Markov chain
  - Cluster algorithms
    - Metropolis is a method for narrowing possibilities by accepting only some changes. It can get stuck in a local mininum, loss of ergodicity. We solve these with cluster algoriths. Wolff grows clus-

ters probabilistically and flips, while Swenson and Yang identifies clusters and flips them probabilistically.

    * Near a phase transition, correlation length grows and changes become less likely to be accepted: need clusters. Clusters dont work far from the phase transition. This is manifested as a sequence of a few metropolis steps and a cluster step.

- Research plan
  - Start with 2D ϕ^4
    * Set up lattice with sign flip for reflection
    * Use Markov chain Monte Carlo to simulate.
    * Measure, magnetization and suseptibility, Binder cumulant
  - Transition to 3D, then maybe transition to C/C++.
  - Implement the gradient flow
  - move to 2-3d nonlinear sigma model.
  - Motivation: the nonlinear sigma model works for QCD given the asymtotic freedom. We may also want to explore topology.

Wednesday, June 17

- Code tips:
  - Try Swendsen-Wang algorithm in addition to Wolff
  - Print out time taken
  - Optimize Hamiltonian
  - Save every tenth measurement or store configurations to calculate path integral. Exclude thermaliztion (first 200)
  - Write in terms of sweeps, not iterations
  - Parallelize (look into checkerboard algorithm)
  - Implement Binder cumulant and suseptibility
  - Store every few states
  - Look into multigrid algorithm
- Reading on Monte Carlo Markov chain and cluster algorithms.

Friday, June 19

- Looking over code
  - Might be too slow, move to C/C++ eventually?
  - Why is the energy increasing with metropolis algorithm?
  - Shift to using action instead of Hamiltonian.
  - Transition from Broken Phase, look at μ_0^2 term.
  - Profile code for possible optimizations.

Monday, June 22

- Coding
  - Add plots to `.gitignore`.
  - Try parallelizing code, using either multigrid or checkerboard algorithm
- Reading
  - Start to focus more on understanding the theory behind research.
  - Read dissertation (Schaich and Loinaz 2006) Chap. 6.5 and 6.6, take notes
    on questions.
  - Newman (Newman and Barkema 1999) (Main textbook for Monte Carlo in
    Statistical Physics)
- Just some things to remember
  - Correlation functions correlate values in statistical systems and relate to propagators in QFT.
  - The problem of renormalization: $a \to 0$ leads to unbounded correlation function. As real physical lengths are measured in terms of the lattice constant, these sometimes tend to infinity.

Wednesday, June 24

- Code
  - Parallelize
  - Transition to numpy
- Theory Question
  - renormalize and regularlize: what do they mean?
  - Look at LePage

Tuesday, June 30

- Code
  - Try `mpi4py`.
  - Move to 3D (this may decrease parallel overhead)
- Reading
  - Continue Reading Collins, others.

Thursday, July 2

- Coding
  - Continue implementing MPI
  - Parallelization may be more apparent in 3D
- Reading
  - Dirac fermions, represented by 4D spinor field (spin up/down, electron/positron)
  - Look at Tong (Chap. 4)
  - Charge (See Tong, Noether's Theorem)
- Next week back: start gradient flow on linear ϕ^4 model

Monday, July 13

- Update from last week
  - Implemented MPI, slowdown may be due to thermal throttling?
  - Questions:
    * Noether's Theorem, 4-current?
    * Star vs. dagger
- Invariance vs covariance
  - Q (charge) is invariant, not covariant. Derivative is 0 (conserved) so no effect of boost. See (StackExchange)[https://physics.stackexchange.com/questions/270296/what-is-the-difference-between-lorentz-invariant-and-lorentz-covariant]
- Operator product expansion
  - Taylor (Laurent in reality) series for operators
  - Used to expand nonlocal (slightly) oeprators using local operators
- TODO:
  - Read conference proceedings, then paper with Orginos
  - Define ρ field (Eq. 2.4), implement it using the exact solution (Eq. 2.5). This will require a FFT

Wednesday, July 15

- Code organization
  - Perhaps implement the nonlinear σ model (at a later date) and the ϕ^4 model as subclasses of a generic lattice class with abstract methods of action, etc.
- Gradient flow
  - Splitting momentum at half of lattice is a-ok.
  - Next, implement observable!
- New terms:
  - autocorrelation times (see Schaich -> MC Textbook -> Wolff): not a QFT concept!

  - Gamma analysis: used to calculate autocorrelation
  - summation window: part of the Gamma analysis
- Three classes of QFTs
  - renormalizable: infinities can be absorbed by a finite number of counterterms
  - nonrenormalizeable: requires infinitely many counterterms
  - super-renormalizeable: there is only one parameter that is divergent

Friday, July 17

- Critical mass problem
  - Check multiple measures (Binder Cumulant, bimodality, etc.)
  - https://journals.aps.org/prd/abstract/10.1103/PhysRevD.58.076003
  - Infinite volume limit?
  - Turn off coupling?
  - Behavior for one node? Two nodes?
  - Metropolis checkerboard? (see (Schaich and Loinaz 2006, pg. 79))
  - Look at Schaich's calculations
  - Note: No true phase transition in finite system since phase transitions are defined by correlation lengths going to infinity

Monday, July 20

- Remarks on critical point graph
  - I should be averaging the measurements from run.
  - Probably will need many more measurements.
  - Spend more time thermalizing
  - Calculate autocorrelation time, use to determine the `record_rate`
  - Production quality: try 10,000 sweeps, with 1000 thermalization
  - Run with slightly larger lattice to verify critical point
- Todo:

  - Flow time dependence (with action)
  - Average all measurements (incorporate this into `recorder.py`)
    * Plot mean and standard error as error bars
  - Autocorrelation times using Gamma analysis
    * Paper has Mathematica notebook link, though it may be broken.
  - Double check that large lattice volumes show correct critical mass.

Wednesday, July 22

- Things I did:
  - Reorganized the `recorder.py` to include measurements and means/errors.
  -
- Questions:
  - Implementing the gradient flow: how does this play into the Monte Carlo simulation?
- TODO:
  - Critical mass
    * Plot histogram for two points of single lattice (thermalized)
    * See if this is affected by a large thermalization, cold start
    * Binder cumulant should be step function
  - Autocorrelation times
    * See Eq. 41
    * Get MatLab code
  - Gradient flow
    * Each measured lattice should be evolved in flow time before recording

Friday, July 24

- Things to do:

  - Gradient flow
  - Try $m_0^2 = -0.8$, see if it become bimodal with large thermalization.
  - Move towards critical value: does τ_{int} increase? (This is what we expect)
  - Perhaps change recording rate?
- Is it time to transcibe the code?
  - Explore efficiency boost
  - C++?
  - Cython?
  - Local cluster?

Monday, July 27

- Shift to utilizing the 0th node for computation.
- Things to note:
  - Histogram in conference proceedings bins single lattice, not average over Markov chain.
- Questions:
  - collecting plots
- To-Do:
  - Run a proper histogram for different thermalizaitons, see if 10^4 is necessary.

Wednesday, July 29

- Plots look good, but are a little wide and not localized on the convergent point
  - Try a cold start
  - Look at 256

  - Average a couple trials
- To-Do:
  - See if I can find the width issue
  - Check autocorrelation times (with/without cluster)
    * close to critical value
  - wait on gradient flow until we are more confident in Markov chain.

Friday, July 31

- Calculate autocorrelation times (as a function of mass), binder cumulant
- Check Wolff algorithm, try Swendsen Wang
- Multigrid algorithm?
- Focus on metropolis algorithm. We don't want to study a cluster algorithm on the backdrop of a broken metropolis algorithm.
- Literature search: must the metropolis algorithm have randomly included sites?

Thursday, August 6

- Progress:
  - Autocorrelation: see page 6 from Schaich
    * Affected by the measurement rate?
  - Wolff implemented in C, large speed-up
  - Fixed neighbor bug in Wolff algorithm
  - Histogram issue still persists

Friday, August 7

- Binder cumulant shows very different critical mass

- Going forward:
  - Start taking personal notes on the research with sketches, ideas, progress
  - Always calculate all of the observables
- Try the Binder Cumulant without Wolff
- See if the result depends on thermalization
  - This result should not be the same as 0 thermalization.

Wednesdesday, August 12

- There are some major problems with my averaging.
- TODO: implement this fix

Graduate School:

- Aim high
- Best possible school that you're happy at
- Name recognition matters
- If you can afford to do the applications, apply to a lot
- Maybe not scientific instrument lab?
- You will have a choice betweeen famous advisors:
  - Famous: letters and papers will carry weight
  - Not-famous: much less attanetion
- Are you emailing your future advisor?
  - depends on place
  - At MIT, less important to single out a specific professor.
  - At a small school (W&M), you need to identify someone before hand.
    * People can actually change advisors

- Possible schools:
  - UCSD
  - Berkley
  - Rutgers
  - UMD
  - UCSB
  - MIT
  - Yale

Friday, August 14

- First, check previous version and make sure the numbers are not the same.
- Try saving some lattices, then calculating observables in Mathematica

Tuesday, August 25

- Progress:
  - Fixed BC issue by fixing the order of calculations. New order:
    1. calculate volume-average
    2. take any exponents
    3. take the ensemble average
    4. compute any derived quantities
  - This is supported by Eq. 4.19 (Newman and Barkema 1999).
- Future work
  - Calculate errors for derived quantities using `gvar`.
  - Transition to GitHub (ID is `cjmonahan`).
  - Run through measurements that you can think of. Try other measurements (e.g. bimodality) and generate definitive list of plots.
  - Create plots without connected lines

Thursday, August 27

- Problem with Binder-Cumulant: errors are too large.
  - Implement Jackknife method (see (Toussaint 1989)) to measure statistics of variables.
    - Try this on 128 lattice, maybe once overnight
  - Migrate to cluster
  - Or perhaps beforehand, try gradient flow.

Tuesday, September 1

- Questions:
  - Do I apply it to every measurement?
    - Yes
  - Are flow time and Monte Carlo time independent?
    - Not really. This is actually where the gradient flow originates, but its not the point of our research.
  - What is the gradient flow scale?
    - We know that $mass \times length$ is dimensionless, so we can measure the flow time in $mass^{-1}$.
    - In other more realistic theories, we can write the flow time as something physical, like the proton size.
    - In scalar field theory, we can do the same thing, but there is no physical analog.
    - The length scale of flow time should be written in terms of λ or m_0^2, with m_0^2 being the slightly more natural choice.
- Todo:
  - Pick three fixed masses, study the flow time at each.
  - Evolve in flow time for each measurement.
  - Try this at $N = 96$.
  - Add the action as an observable.

Friday, September 4

- Gradient flow should have a 0 imaginary component, so I can take the real component safely, though I should check this.
- Todo:
  - Add momentum constant to Gradient Flow evolution function.
  - Fix flow evolution bug!

Tuesday, September 8

- Issue: Observable values are actually completely flat, may be a memory error in the code. This needs debugging.
- Plot the results on a smaller flow time scale.

Friday, September 11

- Reminder: Must rescale momenta by π/L.
- Problem: Observables look flat
- We won't reproduce Figure 3 from proceedings.
- Continue to nonlinear sigma model.
  - Use (Aoki, Kikuchi, and Onogi 2015) to find other sources
  - Use inspirehep to find other sources.
  - Check out [http://www.scholarpedia.org/article/Nonlinear_Sigma_model]

Friday, September 18

- For Wolff algorithm, chose arbitrary vector to flip along.

Tuesday, September 22

- Converting Cython to C++
  - Converting to flat lattice
  - Swendsen & Wang? we should implement this if Wolff works.
- The nonlinear σ lagrangian:
  - g value is related to $\sqrt{\lambda}$.
  - also does affect system since factor of action is significant in path integral formalism.
  - No mass term.

Friday, September 25

-
- Questions:
  - New phi value, guarantee magnitude less than 1 with the other 3 components?
    - Should be using rotation matrices.
    - Take a look at SU(2) Metropolis literature and see how they generate norm-preserving rotation matrices computationally.
  - What exactly are we calculating?
    - Twist-2 operators
    - Condensates
      - VEV in non-perturbative theory.
    - Topology?
    - These could all be topics of our research
  - Prof. Chris: write notes next week about why the nonlinear σ model is "cool."

Wednesday, September 30

- Implement MPI in C++.
- There actually is an application of nonlinear-sigma, in fact multiple.
  - Heisenbuerg Ferro Magnetic, real application to condensed matter.
  - Applications to string theory.
  - Same properties as Yang-Mills Gauge Theories
    * O(2) renormalizable, nontopological solutions of classical EOM at finite action
    * Asymtoticaly free
    * Mass gap in nonperturbative theory
    * Large N limit
    * Dynamical generation of bosons, (like phonons, not explicit in Lagrangian).
  - In $d = 4$, the NLSM is starting point for chiral perturbation theory.

Tuesday, October 6

- Added MPI to C++
  - Some issues with conversion to C array
- Make sure in implementation to keep lattice data continuous.

Wednesday, October 14

- How to debug compilation errors?
  - Can't use print statements like Python.
  - I can use dummy routines to isolate issues.
- Priorities:
  - Ensure that Enrico's project is on the Arxiv while still doing work on my thesis in good faith.

Wednesday, October 21

- Prof. Chris will ask Prof. Orginos about static memory allocation for rank and size.
- Code finally compiles!
- Action looks good but magnetization is incorrect.
  - Get other measurements (suscpetibility, BC, etc.)
  - No need to export lattice average of ϕ^2.

Wednesday, October 28

- Progress
  - Plot with U and χ
  - I think I can statically allocate data in the Sweeper class using an initializer list.
- Do we need MPI?
  - Yes, in 3D it may be necessary since we won't have as many points.
  - Also is necessary for psychological help
  - Also allows adaptive sampling
- Mid Year report due Monday

November 4

- Comparing Python and C++ part. Some issues:
  - Susceptibilities have errors that are too large.
  - Ratio of susceptibilities also wrong, expect a sharper dropoff.
  - Binder Cumulant has wrong final values, susceptibilities.
  - A good future solution is plotting the difference and a horizontal 0 line, also plot error.
  - I should rerun everything with the same data.
  - Also put the data in a nice plot.

    - Make note of the speed up.
- Transition to $O(3)$ model.
- I realized that vectors are continuous memory, almost no slowdown.

November 11

- Updates:
    - Ran calculations again
        * Execution time is actually on a similar order or magnitude
        * MPI on 4 cores actually slows progress
        * A couple of outliers, checked closer, seems right
    - Redeveloped gif debugging tool for C++
        * Shows similar lattice for both methods.
        * Can be ported to $O(3)$ model
- Todo:
    - For difference plot, use larger number of measurements.
    - Still discrepancy with susceptibility error bars
        * See if this changes with lattice size, ensemble size.
        * Jackknife methods
        * Export $\bar{\phi}$ values in python code, compare variances with independent code.
    - Presentation slides by Friday
    - Email Averett about a final draft for the mid-year report.
    - Make changes to the mid-year report

Spring Semester

January 12

- Some clarifying theory questions:
  - Twist-2 operators: not trivial! mass dimension is not just mass of the field.
- **Shift project towards topology**
  - More interesting
  - More applications to condensed matter
  - See references (Bietenholz et al. 2018) and (Mejía-Díaz et al. 2018).
    - Unfortunately, these do exactly what we were planning to do, however they do demonstrate that this research is paper-worthy.
- Todo in the meantime:
  - clean up code
- Writing report:
  - Try to start early
  - Specifically, fix "long-term" issues in mid-year report.

January 21

- New direction, since papers cover what we did:
  - Look at instantons?
- **Topology**
  - What is Q?
    - Global operator
    - χ: topological suscpetibility
- Wedge operator ($\wedge$). - Does it act in real space or spin space? - Must do further research.

- **General research question**: How do I go about figuring out mathematical expressions.
  - Keep Googling phrases!
    - try the arxiv!
  - Find other papers with the same expression.
  - Compare different definitions from different papers.
  - Ask someone.
- How to determine gradient flow in $O(3)$ model?
  - Runge-Kutta: check out Numerical Recipe
  - Try $O(4)$ approx.
- Todo:
  - First order: gradient flow and topological charge
  - Second order: susceptibilty

January 27

- Parallel Runge-Kutta method
  - Prof. Chris will ask Prof. Orginos
  - Go ahead and implement serial algorithm, then check if adaptive step size changes efficiency significantly.
  - Implement second-order Runge-Kutta and compare efficiency/accuracy.
  - Matrix options: look at parallelism across the method.
- What statistics to use
  - Maybe use the term "observable"
  - Magnetization may be important, as with action and susceptibility
  - Topological density
  - For topological charge see (Berg and Lüscher 1981)
- Todo:
  1. Runge-Kutta gradient flow

2. Adaptive step size
3. Check internal energy from (Berg and Lüscher 1981)
4. Then, consider topological charge/suscpetibility (Fig 2, (Berg and Lüscher 1981))

February 1

- Reproduction of (Berg and Lüscher 1981):

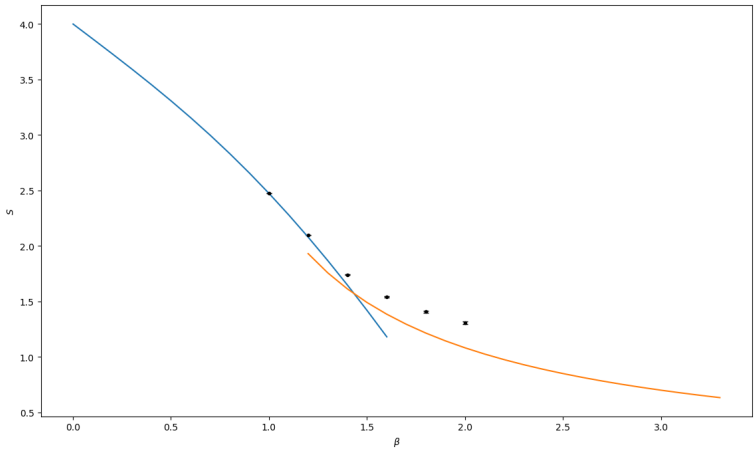

Figure 1: Internal Energy

- Gradient flow:
  - Action increases with flow time
  - May be due to normalization.
- Orginos: Runge-Kutta parallel python code. May be a shortcut to calculate the gradient flow :(Lüscher 2010): - Used with $SU(3)$ but not $O(3)$. - Could be mapped but the mathematics are very difficult (see general technique in (Munthe-Kaas 1999)). - Note that Bietenholz does not use L"uscher's method.

- Internal Energy:
  - Run 100x100 and compare with specific β values from Table 1 (Berg and Lüscher 1981).
  - Try some more β values, including 2 that are smaller than 1.
  - Small fixes: start y-axis at 0, change S to E.
  - Try decreasing record rate (maybe its the autocorrelation value)?

  Scan past what you're supposed to read.

February 3

- New internal energy plot:
  - 100×100
  - 100 measurements 200 sweeps apart, 2000 sweep thermalization. Wolff cluster every 5 sweeps.

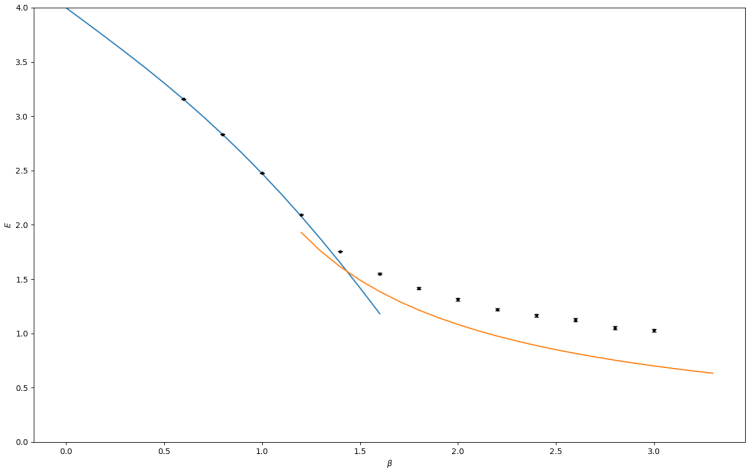

Figure 2: Internal Energy, revised plot

- Mostly the same.
- Todo:

```
- Try plotting magnetic susceptibility? and compare with Table 1 [@berg1981].
- Measure autocorrelation time (for $E$ and/or $\chi_m$). This should go up in strong co
```

- Gradient flow:
  - after decreasing dt step size, action now makes sense:
  - Implement adaptive step size if it becomes a problem.
  - Todo:
    - Begin to study other observables (E, χ_m)
- Afterwards: work on topological susceptibility
- No meeting on Monday

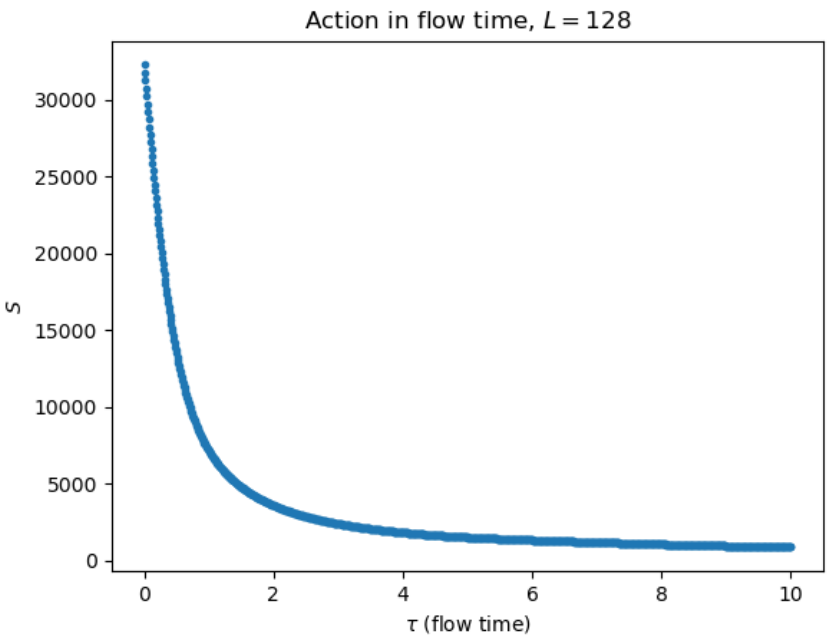

Figure 3: Action in flow time

February 10

- UF Acceptance!

- New computer, runs simulations faster.
- New result with χ_m shows discrepancy at phase transition:
  - Try removing Wolff algorithm
  - Perhaps magnetic susceptibility is related to Wolff cluster size? (see Newman and Barkema (1999) , p. 102)
    * See Hasenbusch (1995)
  - Check out change in lattice size
  - Interesting point: the internal energy differs at a different region from the magnetic susceptibilty.
- Gradient Flow
  - Normalize χ_m in terms of L^4.
  - Run in strong correlation regime.

February 15

- After adjusting Wolff algorithm, plot looks better.
  - I was taking flipping $\phi \to -\phi$ instead of just flipping along projection vector.
  - Also, there was an issue in ΔS.

Todo: - Gradient flow: - Run in strong correlation regime. - Autocorrelation time: - Reproduce autocorrelation with internal energy and put figure in notes. - Implement the local topological density.

- Don't worry too much about the exact solution.

February 17

- *Note that a large β indicates weak coupling*

Todo: - Check that β is correct (see above point). - Take real ensemble statics on

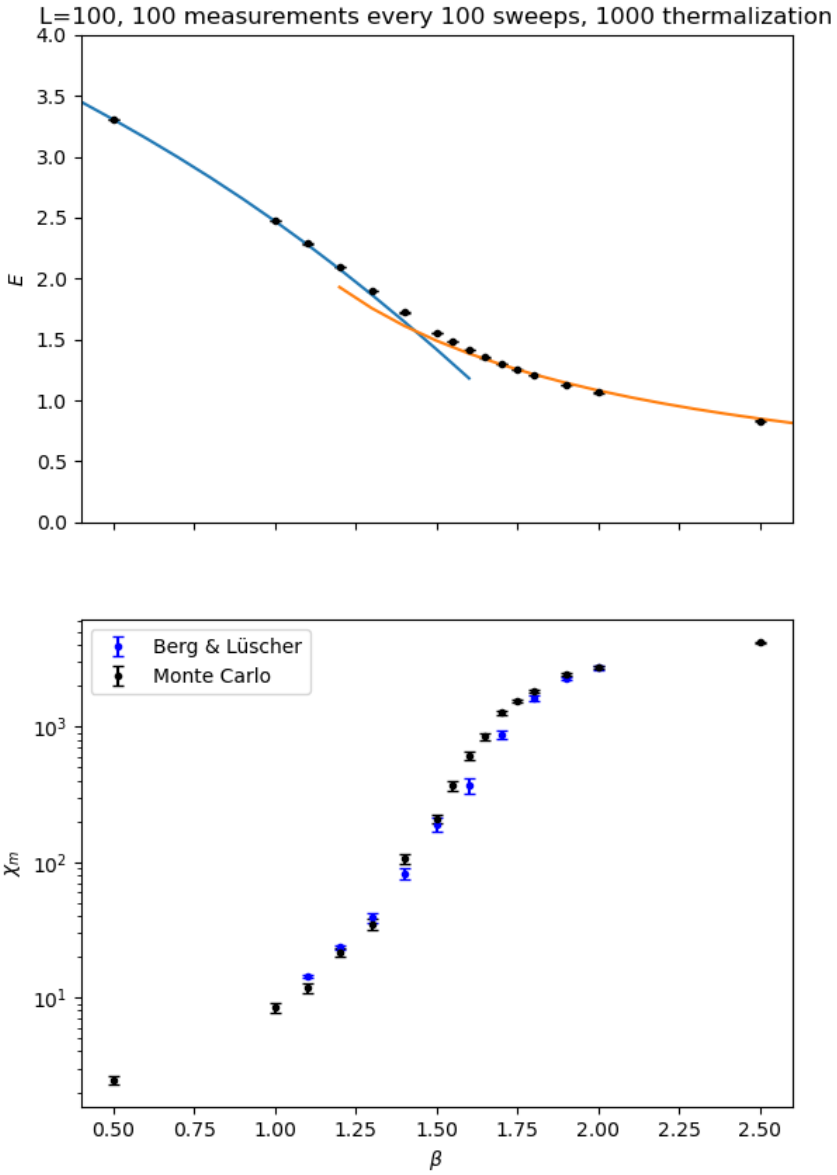

Figure 4: Internal Energy, fixed Wolff algorithm

topological charge to check if $\langle Q \rangle = 0$ and measure error. - Run this along the same lines as Bietenholz. - Figure out difference in topological susceptibilities. - Something weird with autocorrelation, maybe measure every 5 sweeps? This is because the time units are not real. - Also run without cluster update.

February 22

- Honors Committee
  - Prof. Chris
  - Enrico
  - Perhaps Stathopoulos from Computer Science
  - Contact Prof. Averett about this.
  - Deadline is this Friday
- Honors deadline is coming up!
  - Have an outline in March.
- Yale Acceptance
  - Yale feels like an old-school physics department
  - Both have a lot of resources.
- TODO:
  - Recreate Fig. 4 up to 54, plotted in terms of t_0. (Check table 1)
  - Read Bietenholz conclusions for ideas of extensions
    - Look at θ term numerically.
      - Two methods for fixing the "sign problem":
      - Reweighting, or we can use the Tyalor expansion method.
      - Use the Taylor expansion method.
  - In the context of Lattice field theory, Q is the main topological quantity.
  - Spend some time learning topological quantities.
  - Two timescales: April 23rd and later for paper
    - Since I *could* write this up, I have some time to do some reading.
  - Email Stathopoulos

February 24

- Some errors in the Q value:
  - Try a more statistics and lower tolerance
  - Overall pretty good.
- Where to go next:
  - (Bögli et al. 2012) studies $\theta \neq 0$ case, which Bietenholz only lightly touches.
  - Read (Bögli et al. 2012).

March 1

- Progress:
  - Compiled on cluster
  - Ran with 10^5 measurements and lower tolerance, same result ($Q \neq 0$ within errors).
    - Seems like errors are too small and Jackknife value are proportional to $\sqrt{N}$.
  - Read (Bögli et al. 2012), looks like this only applies to $\theta = \pi$.

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