

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 minimum, loss of ergodicity. We solve these with cluster algorithms. 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 don't 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 susceptibility, 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 asymptotic 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 thermalization (first 200)
 - Write in terms of sweeps, not iterations
 - Parallelize (look into checkerboard algorithm)
 - Implement Binder cumulant and susceptibility
 - 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: $a \rightarrow 0$ 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 regularize: 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) operators 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
 - nonrenormalizable: requires infinitely many counterterms
 - super-renormalizable: 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 transcribe 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 between 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
 - * Asymtotically 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 (susceptibility, 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 susceptibility
- 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: susceptibility

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/susceptibility (Fig 2, (Berg and Lüscher 1981))

February 1

- Reproduction of (Berg and Lüscher 1981):

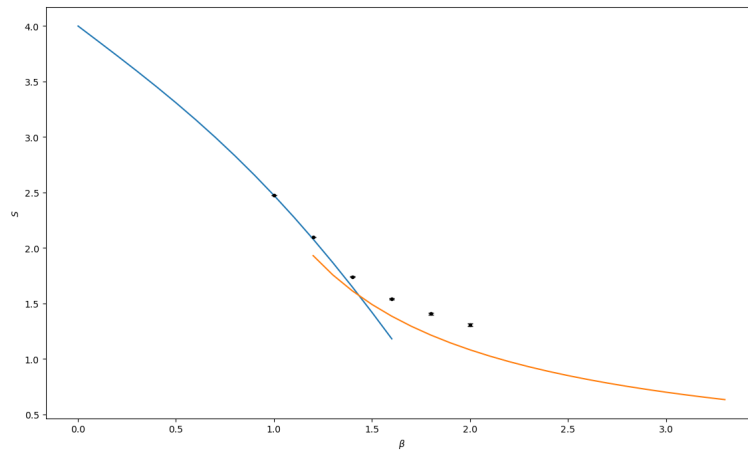


Figure 1: Internal Energy

- 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 Lüscher'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.

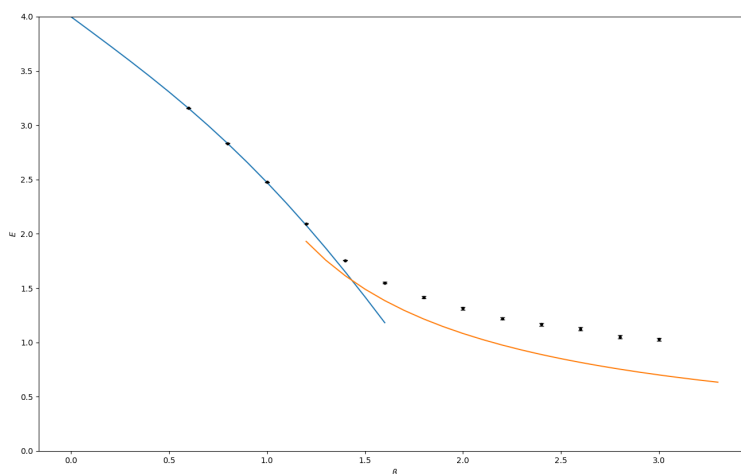


Figure 2: Internal Energy, revised plot

- Mostly the same.
- Todo:

- Try plotting magnetic susceptibility? and compare with Table 1 [berg1981].
- Measure autocorrelation time (for E and/or χ_m). This should go up in strong coupling.
- 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

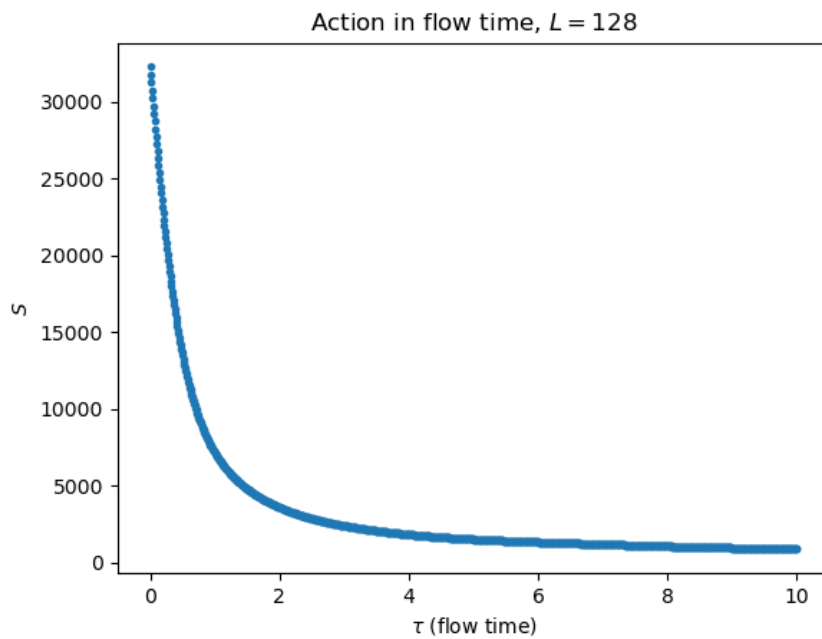


Figure 3: Action in flow time

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 susceptibility.
- 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 $\phi \rightarrow -\phi$ 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

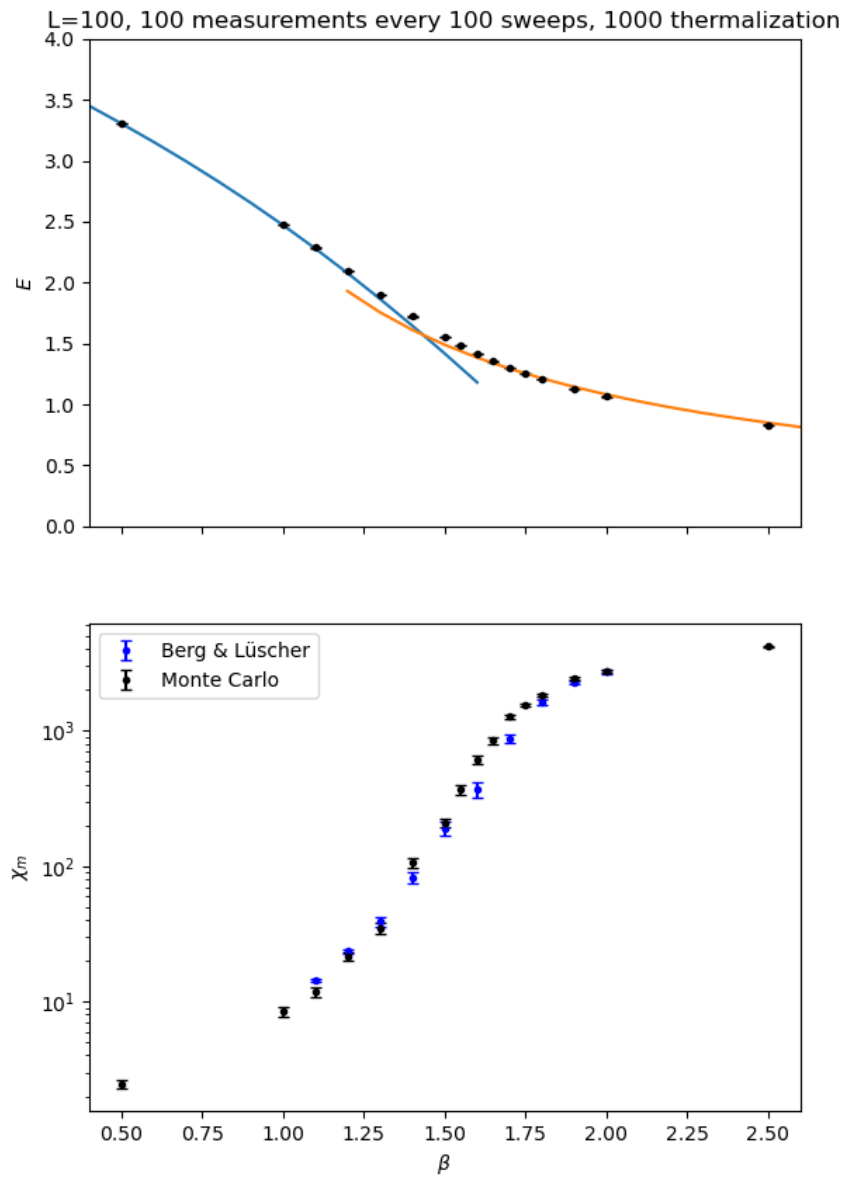


Figure 4: Internal Energy, fixed Wolff algorithm

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 Taylor 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

- 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} .
 - We can bring the tolerance back to a normal regime
 - *standard error vs. standard mean*
- Read (Bögli et al. 2012), looks like this only applies to $\theta = \pi$.
 - They consider $\theta = \pi/2$
- Several unanswered questions:
 - Is this a problem with the definition of topological charge? Could we look at another definition?
 - We can look at the results around $\theta = 0$.
 - We may need a different gradient flow for a θ term.
 - *What is the gradient flow with a θ term?*
- Try to reproduce the Bietenholz plot

- Derive around θ .
- Set up an outline of the report. Pick a good Latex template that is in accordance with department regulations.

March 3

- Standard error vs Standard deviation: things are correct.
- Outline:
 - OK to copy some things from the mid-year report.
- Take the continuum limit
 - Check Bietenholz for how they take the continuum limit, I will have to scale β and perhaps τ .
- Problem with the gradient flow: Q is not continuous so it is not differentiable.
 - Let's assume the gradient flow remains the same. In that case, check the results with Bietenholz.

March 8

- No from Berkeley, probably between Yale, UMD and *maybe* Cornell.
- Question about final report: how much to include regarding ϕ^4 model?
 - Double check page minimum
 - No more than 1/3 regarding ϕ^4 model.
- Data progress:
 - Long simulation, 2 days, up to $L = 270$.
 - Convergence plot
 - Calculate jackknife errors on $\langle Q \rangle|_{\theta=0}$
 - * Perform this on each sector?
 - Should we use **plug in formula**

- Explore (Hasenbusch 1995).

References

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