

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
 - * Asymptotically 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):

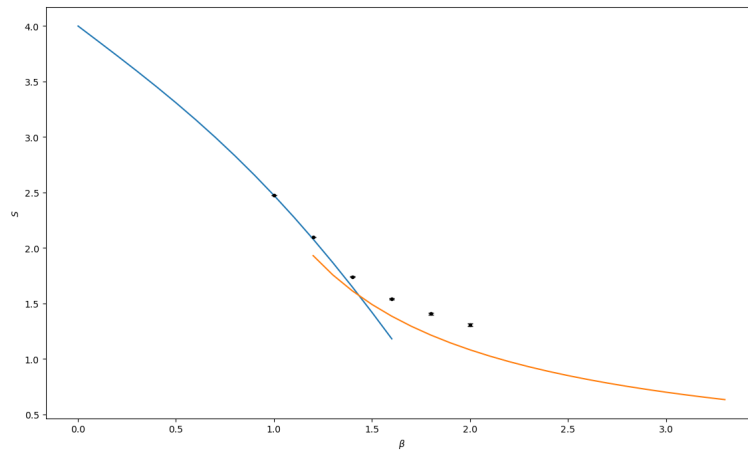


Figure 1: Internal Energy

- 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.

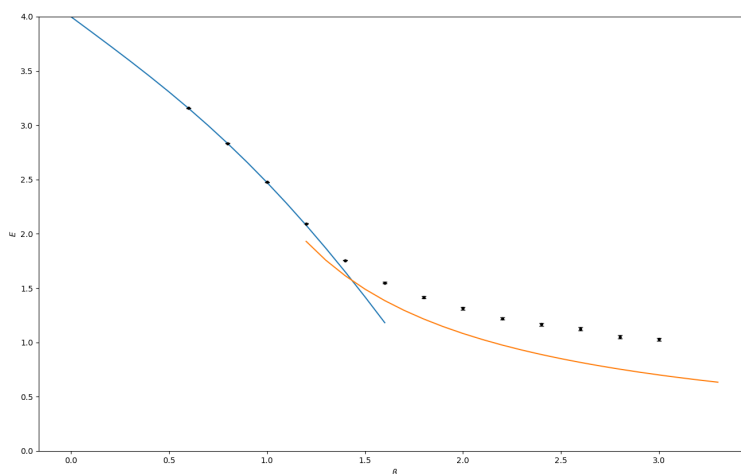


Figure 2: Internal Energy, revised plot

- 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

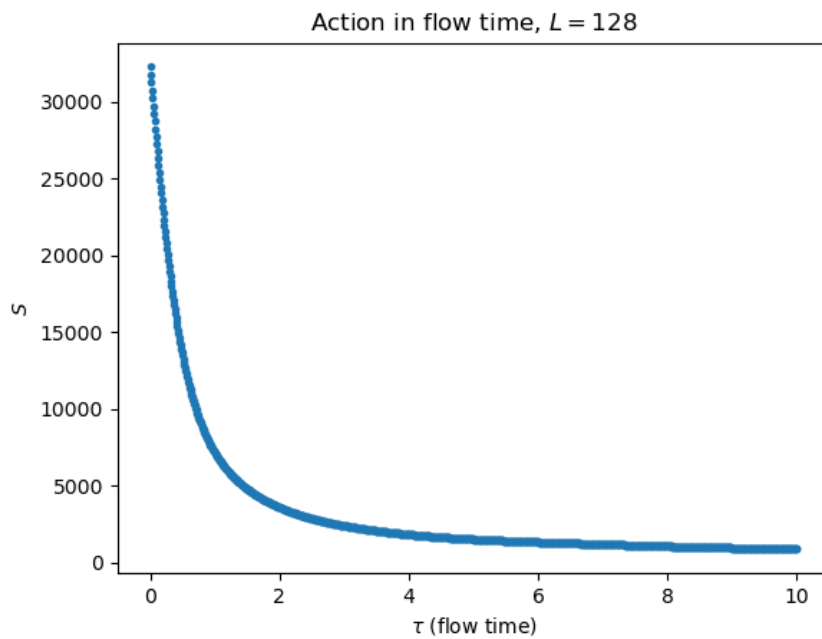


Figure 3: Action in flow time

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

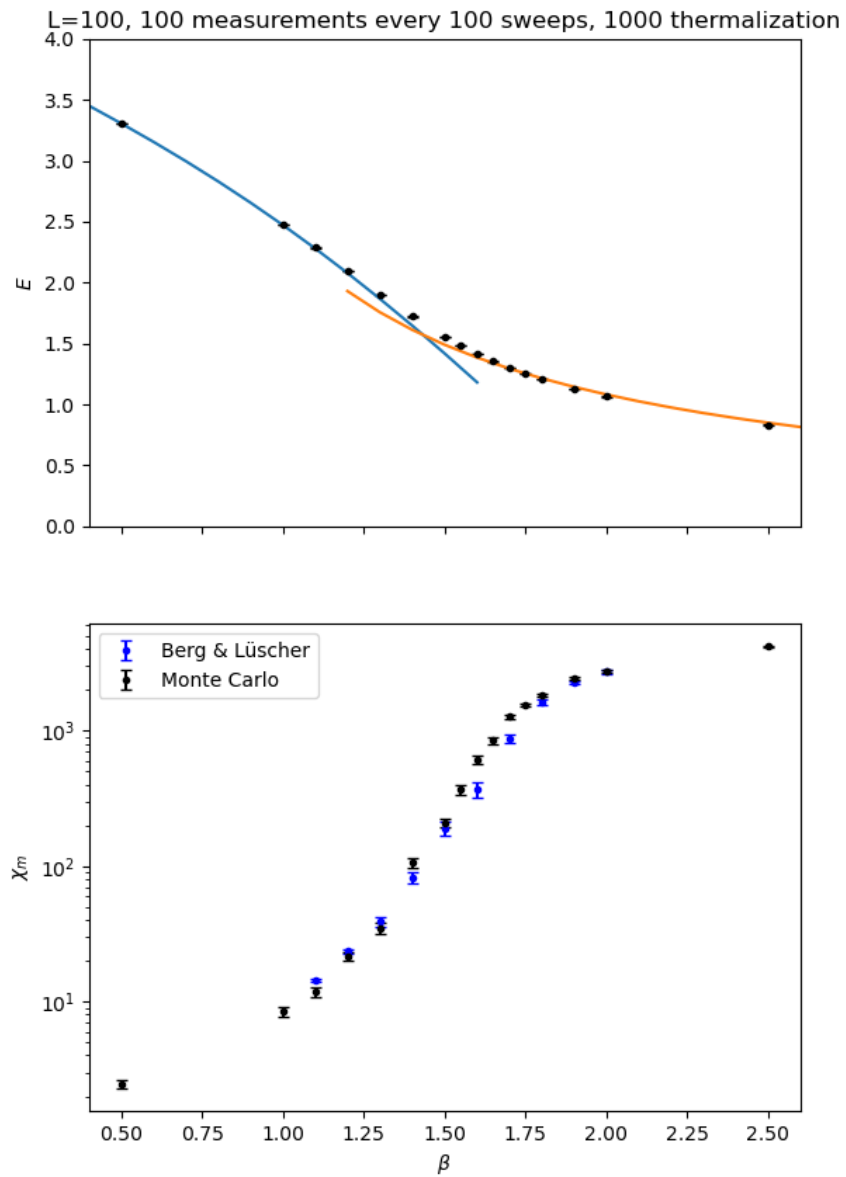


Figure 4: Internal Energy, fixed Wolff algorithm

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?
- Explore (Hasenbusch 1995).

March 10

- Better intuition on topology
- Described gradient flow in the non-linear σ model. Here I use some different notation from Bietenholz since it is more consistent with the rest of my paper. This may be something we want to clear up early on.

Writing:

- Convention:
 1. First priority: internal consistency
 2. Second priority: consistency with literature
 3. Change $\vec{\phi}$ to \vec{e} .
- Index notation to vector notation: make sure you note that you understand. In a way, I am trying to demonstrate mastery and knowledge as well as present research.

Issues with topological charge measurement:

- $\langle Q \rangle_\theta = \sum_{Q'} e^{iQ'\theta} \langle Q \rangle_{\theta=0}^{Q=Q'}$
- Let's try the $\theta = \pi$.
- It's possible that my arbitrary θ formula requires infinite measurements.
- A good exploration of the value of θ and the uncertainty of the calculation may be in order.

Try calculating ξ , then ξ_2 .

Q: What is step scaling?

- A way to change the scale nonperturbatively

March 15

Some notes on topological sector statistics

From (Berg and Lüscher 1981), we can naively extrapolate a formula for $\langle Q \rangle_\theta$ given arbitrary θ :

$$\langle Q \rangle_\theta = \sum_{Q'} e^{iQ'\theta} \langle Q \rangle_{\theta=0}^{Q=Q'} \quad (1)$$

Though this expression accurately estimates $\langle Q \rangle_\theta$ as $N \rightarrow \infty$, the rotational nature of the sum in the complex plane prohibits numerical calculation when θ is not a fraction of 2π . We demonstrate this obstacle by calculating the standard error of the mean for arbitrary θ .

We assume that the standard deviation of each topological sector is equivalent to the standard deviation of the entire ensemble σ . Given the formula for standard error of the mean $\text{StdErr}(Q) = \sigma/\sqrt{N}$, we can determine the error of each topological sector to be $\text{StdErr}_{Q=Q'}(Q) = \sqrt{N/N_{Q'}} \text{StdErr}(Q)$. Using a Pythagorean sum, we can write the standard error of Q_θ from Eq. 1 as

$$\text{StdErr}(Q_\theta) = \sqrt{\sum_{Q'} \frac{N}{N_{Q'}}} \text{StdErr}(Q_{\theta=0}).$$

From this formula, it is clear that the standard error becomes infinite when any topological sector contains no configurations. This result prohibits numerical calculations of the topological charge (or any observable) in the $\theta \neq 0$ case unless $\theta = 2\pi/n$ where $n \in \mathbb{Z}$. Even when the number of topological sectors is finite, the statistical errors are significantly larger. If we assume each topological sector is equally large, the standard error reduces to

$$\text{StdErr}(Q_\theta) = n \text{StdErr}(Q_{\theta=0})$$

where n is the number of topological sectors.

Meeting Wednesday? (it is a Spring Break Day)

References

- Alles, B., and A. Papa. 2007. “Numerical Study of the Mass Spectrum in the 2d $O(3)$ Sigma Model with a Theta Term.” *arXiv:0711.1803 [Hep-Lat]*, November. <http://arxiv.org/abs/0711.1803>.
- Aoki, Sinya, Kengo Kikuchi, and Tetsuya Onogi. 2015. “Gradient Flow of $O(N)$ Nonlinear Sigma Model at Large N .” *Journal of High Energy Physics* 2015 (4): 156. [https://doi.org/10.1007/JHEP04\(2015\)156](https://doi.org/10.1007/JHEP04(2015)156).
- Azcoiti, Vicente, Giuseppe Di Carlo, Eduardo Follana, and Matteo Giordano. 2012. “Critical Behaviour of the $O(3)$ Nonlinear Sigma Model with Topological Term at $\Theta=\pi$ from Numerical Simulations.” *Physical Review D* 86 (9): 096009. <https://doi.org/10.1103/PhysRevD.86.096009>.
- Balog, J., F. Niedermayer, M. Pepe, P. Weisz, and U.-J. Wiese. 2012. “Drastic Reduction of Cutoff Effects in 2-d Lattice $O(N)$ Models.” *Journal of High Energy Physics* 2012 (11): 140. [https://doi.org/10.1007/JHEP11\(2012\)140](https://doi.org/10.1007/JHEP11(2012)140).
- Berg, B, and Martin Lüscher. 1981. “Definition and Statistical Distributions of a Topological Number in the Lattice $O(3)$ σ -Model.” *Nuclear Physics B* 190 (2): 412–24.
- Bietenholz, Wolfgang, Philippe de Forcrand, Urs Gerber, Héctor Mejía-Díaz, and Ilya O. Sandoval. 2018. “Topological Susceptibility of the 2d $O(3)$ Model Under Gradient Flow.” *Physical Review D* 98 (11): 114501. <https://doi.org/10.1103/PhysRevD.98.114501>.
- Bögli, M., F. Niedermayer, M. Pepe, and U.-J. Wiese. 2012. “Non-Trivial θ -Vacuum Effects in the 2-d $O(3)$ Model.” *Journal of High Energy Physics* 2012 (4): 117. [https://doi.org/10.1007/JHEP04\(2012\)117](https://doi.org/10.1007/JHEP04(2012)117).

- Del Debbio, Luigi, Leonardo Giusti, and Claudio Pica. 2005. “Topological Susceptibility in the SU(3) Gauge Theory.” *Physical Review Letters* 94 (3): 032003. <https://doi.org/10.1103/PhysRevLett.94.032003>.
- Hasenbusch, M. 1995. “An Improved Estimator for the Correlation Function of 2d Nonlinear Sigma Models.” *Nuclear Physics B - Proceedings Supplements* 42 (1-3): 764–66. [https://doi.org/10.1016/0920-5632\(95\)00375-J](https://doi.org/10.1016/0920-5632(95)00375-J).
- Horgan, R R. 2014. *Statistical Field Theory*.
- Hoshen, J., and R. Kopelman. 1976. “Percolation and Cluster Distribution. I. Cluster Multiple Labeling Technique and Critical Concentration Algorithm.” *Physical Review B* 14 (8): 3438–45. <https://doi.org/10.1103/PhysRevB.14.3438>.
- Introduction to QCD and the Standard Model*. n.d.
- Ioffe, B. L. 2003. “Condensates in Quantum Chromodynamics.” *Physics of Atomic Nuclei* 66 (1): 30–43. <https://doi.org/10.1134/1.1540654>.
- Kleinert, Hagen. 2016. *Particles and quantum fields*.
- Kleinert, Hagen, and Verena Schulte-Frohlinde. 2001. *Critical Properties of ϕ^4 -Theories*.
- Körner, Daniel. n.d. “Non-perturbative renormalization on the lattice,” 124.
- Loinaz, Will, and R. S. Willey. 1998. “Monte Carlo Simulation Calculation of Critical Coupling Constant for Continuum ϕ_2^4 .” *Physical Review D* 58 (7): 076003. <https://doi.org/10.1103/PhysRevD.58.076003>.
- Lüscher, Martin. 2010. “Properties and Uses of the Wilson Flow in Lattice QCD.” *Journal of High Energy Physics* 2010 (8): 71. [https://doi.org/10.1007/JHEP08\(2010\)071](https://doi.org/10.1007/JHEP08(2010)071).
- Makino, H., F. Sugino, and H. Suzuki. 2015. “Large-N Limit of the Gradient Flow in the 2d O(N) Nonlinear Sigma Model.” *Progress of Theoretical and*

- Experimental Physics* 2015 (4): 43B07–0. <https://doi.org/10.1093/ptep/ptv044>.
- Makino, Hiroki, and Hiroshi Suzuki. 2015. “Renormalizability of the Gradient Flow in the 2d $O(N)$ Non-Linear Sigma Model.” *Progress of Theoretical and Experimental Physics* 2015 (3): 33B08–0. <https://doi.org/10.1093/ptep/ptv028>.
- Mejía-Díaz, Héctor, Wolfgang Bietenholz, Krzysztof Cichy, Philippe de Forcrand, Arthur Dromard, Urs Gerber, and Ilya O. Sandoval. 2018. “Topological Susceptibility Under Gradient Flow.” *EPJ Web of Conferences* 175: 11024. <https://doi.org/10.1051/epjconf/201817511024>.
- Michael, C. 1986. “Fast Heat-Bath Algorithm for the Ising Model.” *Physical Review B* 33 (11): 7861–62. <https://doi.org/10.1103/PhysRevB.33.7861>.
- Monahan, Christopher. 2016. “The Gradient Flow in Simple Field Theories.” In *Proceedings of The 33rd International Symposium on Lattice Field Theory — PoS(LATTICE 2015)*, 052. Kobe International Conference Center, Kobe, Japan: Sissa Medialab. <https://doi.org/10.22323/1.251.0052>.
- Monahan, Christopher, and Kostas Orginos. 2015. “Locally Smeared Operator Product Expansions in Scalar Field Theory.” *Physical Review D* 91 (7): 074513. <https://doi.org/10.1103/PhysRevD.91.074513>.
- Morningstar, Colin. 2007. “The Monte Carlo Method in Quantum Field Theory.” *arXiv:hep-Lat/0702020*, February. <http://arxiv.org/abs/hep-lat/0702020>.
- Munthe-Kaas, Hans. 1999. “High Order Runge-Kutta Methods on Manifolds.” *Applied Numerical Mathematics* 29 (1): 115–27. [https://doi.org/10.1016/S0168-9274\(98\)00030-0](https://doi.org/10.1016/S0168-9274(98)00030-0).
- Newman, M. E. J., and G. T. Barkema. 1999. *Monte Carlo Methods in Statistical Physics*. Oxford: Oxford University Press.
- Schaich, David A, and William Loinaz. 2006. “Lattice Simulations of Nonperturbative Quantum Field Theories.” Amherst College.

- Solbrig, Stefan, Falk Bruckmann, Christof Gattringer, Ernst-Michael Ilgenfritz, Michael Müller-Preussker, and Andreas Schäfer. 2007. “Smearing and Filtering Methods in Lattice QCD - a Quantitative Comparison.” *arXiv:0710.0480 [Hep-Lat]*, October. <http://arxiv.org/abs/0710.0480>.
- Tong, David. 2007. *Quantum Field Theory*. University of Cambridge Part III Mathematical Tripos.
- . 2017. *Statistical Field Theory*. University of Cambridge Part III Mathematical Tripos.
- Toussaint, D. 1989. “Error Analysis of Simulation Results: A Sample Problem,” no. AZPH-TH-89-72 (December): 12 p. <https://cds.cern.ch/record/204810>.
- Wang, Jian-Sheng. 1989. “Clusters in the Three-Dimensional Ising Model with a Magnetic Field.” *Physica A: Statistical Mechanics and Its Applications* 161 (2): 249–68. [https://doi.org/10.1016/0378-4371\(89\)90468-8](https://doi.org/10.1016/0378-4371(89)90468-8).
- Wolff, Ulli. 2007. “Monte Carlo Errors with Less Errors.” *Computer Physics Communications* 176 (5): 383. <https://doi.org/10.1016/j.cpc.2006.12.001>.