# Thesis Notes

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## Monday, June 15

- Preliminary meeting
- We will begin with  $\phi^4$  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 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  $\phi^4$ 
  - \* 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 thermalization (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  $\mu_0^2$  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  $\phi^4$  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) opprators using local operators
- TODO:
  - Read conference proceedings, then paper with Orginos
  - Define  $\rho$  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  $\sigma$  model (at a later date) and the  $\phi^4$  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.

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- 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

- $\bullet~$  Things to do:
  - Gradient flow
  - Try  $m_0^2 = -0.8$ , see if it become bimodal with large thermalization.
  - Move towards critical value: does  $\tau_{int}$  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 thermalizations, see if 10<sup>4</sup> 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, Sept 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 graident 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  $\lambda$  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, Sept 4

 $\bullet$  Gradient flow should have a 0 imaginary component, so I can take the real component safely, though I should check this.

To do: - Add momentum constant to Gradient Flow evolution function. - Fix flow evolution bug!

## References

- "1.27 at DuckDuckGo." n.d. Accessed September 1, 2020. https://duckduckgo.com/?q=1.27&t=osx&ia=web.
- 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.
- Horgan, R. R. 2014. Statistical Field Theory.

Introduction to QCD and the Standard Model. n.d.

Kleinert, Hagen. 2016. Particles and Quantum Fields.

- Kleinert, Hagen, and Verena Schulte-Frohlinde. 2001. Critical Properties of  $\phi^4$ -Theories.
- Loinaz, Will, and R. S. Willey. 1998. "Monte Carlo Simulation Calculation of Critical Coupling Constant for Continuum  $\phi_2^4$ ." *Physical Review D* 58 (7): 076003. https://doi.org/10.1103/PhysRevD.58.076003.
- 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.
- 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/ptv 044.
- Mélin, R. 2000. "Spin-Resolved Andreev Reflection in Ferromagnet-Superconductor Junctions with Zeeman Splitting." *EPL (Europhysics Letters)* 51 (2): 202. https://doi.org/10.1209/epl/i2000-00532-1.
- 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.
- 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.
- 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," nos. AZPH-TH-89-72 (December): 12 p. https://cds.cern.ch/record/204810.
- 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.