Life on the Lattice
Markov Chain Monte Carlo
and all that

David Schaich

Advisor: Prof. Loinaz

Preliminary Thesis Talk

Amherst College

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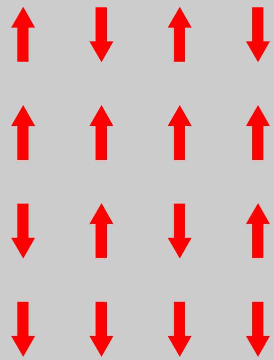
Outline

- Ising Model: A simple model of a magnet
  Phases, phase transitions, and a context for...
- Numerical (lattice) simulations
  The rather large problem of very large numbers
- Markov Chain Monte Carlo
  Efficient 'importance sampling'
- ϕ^4 Theory (time permitting)

Ising Model

Imagine a lattice of 'spins' of magnitude 1 that can only point up (+1) or down (-1).



Spins correspond to magnetic dipoles at temperature T.

Energy: $$E = -\sum_{\langle i,j \rangle} s_i s_j$$ (only nearest neighbors interact)

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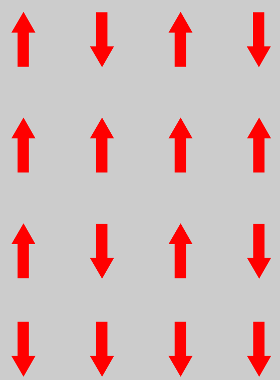


Energy

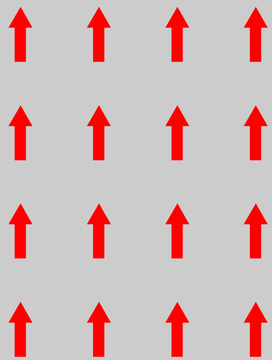
$$E = -\sum_{\langle i,j \rangle} s_i s_j$$

Parallel spins have lower energy, but thermal energy causes fluctuations that randomize the lattice – if the temperature is high enough.

Ising Model Phases

Thus the Ising model has two phases:

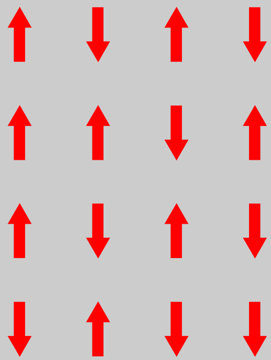
ferromagnetic



- Spins aligned
- Lower energy
- Higher magnetization

Equilibrium for low temperatures

unordered

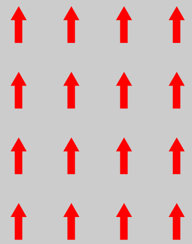


- Spins unordered
- Higher energy
- Lower magnetization

Equilibrium for higher temperatures

Ising Model Phase Transitions

ferromagnetic



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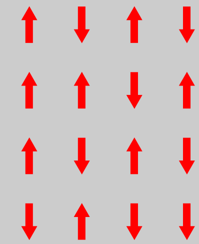
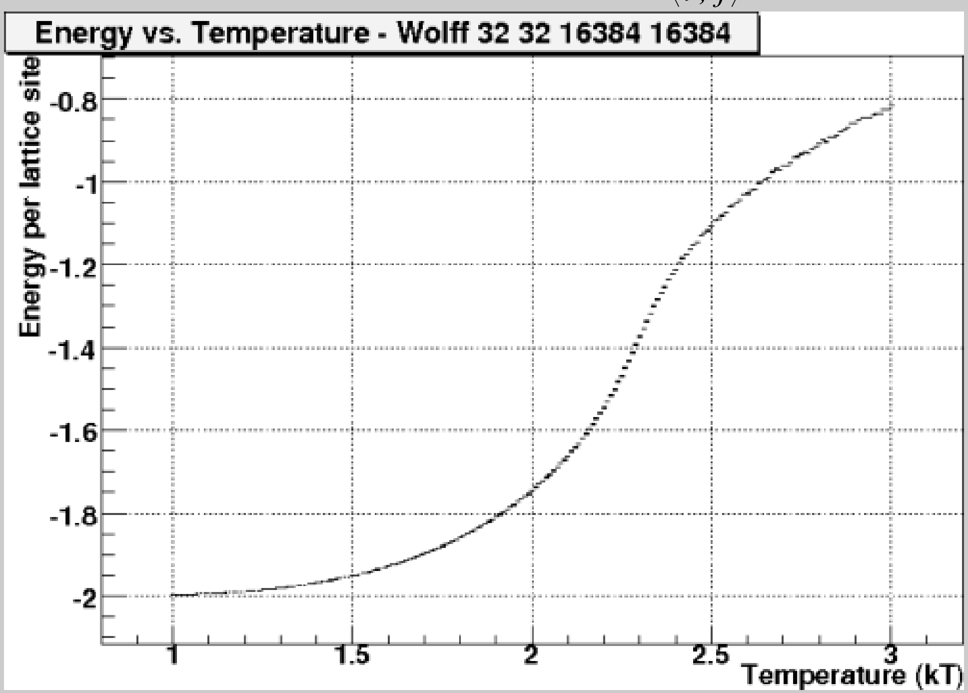
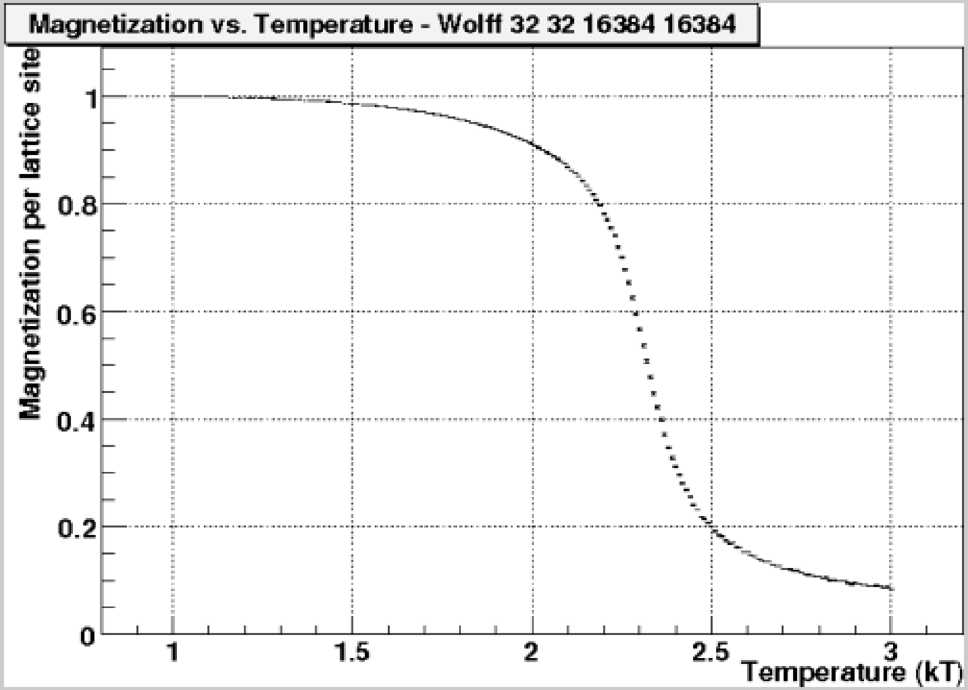


Energy: $e = \frac{E}{N} = \frac{-1}{N} \sum_{\langle i, j \rangle} s_i s_j$

Magnetization: $m = \frac{M}{N} = \sum_{i=0}^{N-1} s_i$



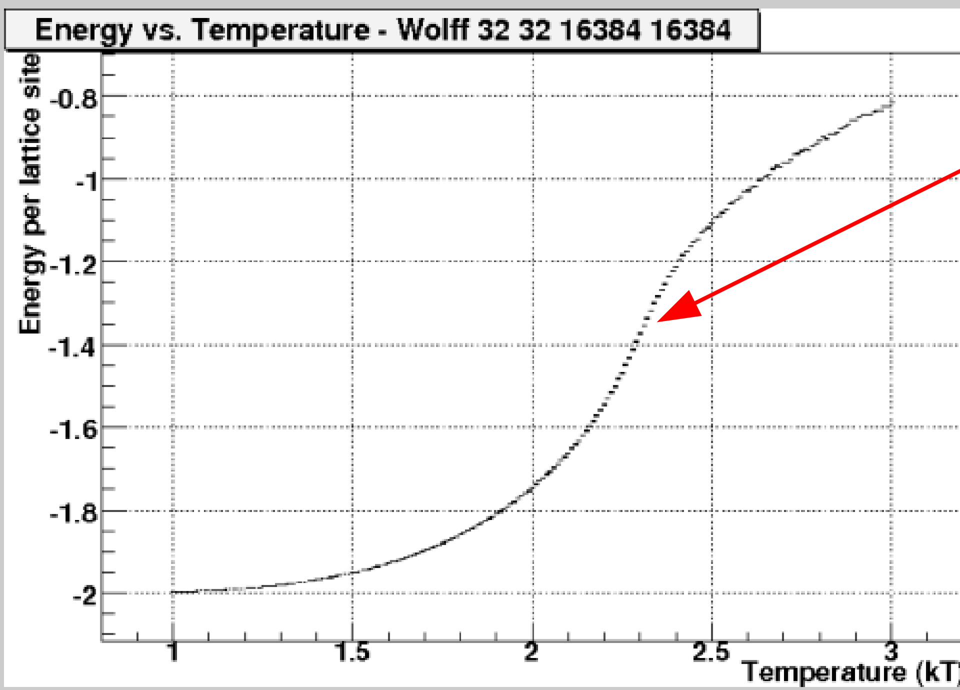


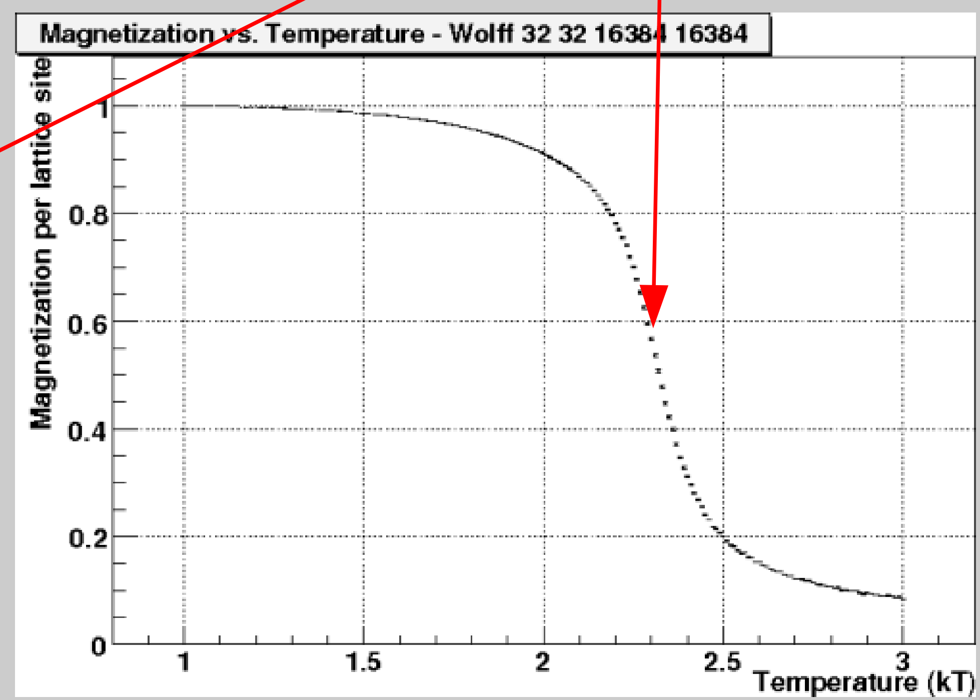
Ising Model Phase Transitions

Phase transition becomes sharp as lattice size L➞∞
(equivalent to lattice spacing a➞0).

Point at which phase transition occurs is 'critical temperature'

$$T_c = \frac{2}{\ln(1+\sqrt{2})} = 2.269$$





Numerical Simulations

How to calculate those pretty graphs on the previous slide?

Idea #1: Set up each possible configuration, calculate the desired quantity and weigh it by its Boltzmann probability

$$\langle Q \rangle = \frac{\sum_i Q_i e^{-E_i/kT}}{\sum_i e^{-E_i/kT}} \qquad \text{(See Physics 30)}$$

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Problem #1: This isn't practical.

Example: Even a very small (16x16) Ising lattice has $\sim 2^{256}$ ($\sim 10^{77}$) configurations, which will take at least $\sim 10^{60}$ years to fully calculate.

It gets even worse for moderately-sized (512x512) lattices ($\sim 10^{78,900}$ years) or small thermodynamic systems ($\sim 10^{10^{23}}$ years)

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(See Physics 30)

Problem #2: This is just silly

Generally only a *very* small proportion of the possible states actually matter. It's a waste of time to worry about the others.

Importance Sampling

Idea #2: Only sample the important states: instead of considering every state and then weighing by its Boltzmann factor, only worry about those states with sufficiently large probabilities.

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Complication: How to determine which states matter without checking all of them?

Markov Processes

Markov processes are ways to generate a random set of states according to the Boltzmann probabilities. (Proof left to reader)

But what are Markov processes?

Markov Chain Monte Carlo

Given an initial state X, a Markov process randomly generates a new state Y with 'transition probability' $P(X \rightarrow Y)$.

This series of states produced by the Markov process is known as a 'Markov chain.'

Because of its use of randomness, this approach is known as the 'Markov Chain Monte Carlo (MCMC) method' in honor of the famous casino center in Monaco.

To reproduce the Boltzmann distribution, the Markov process needs to satisfy three conditions.

Markov Chain Monte Carlo

Three conditions guarantee Boltzmann distribution:

1) $P(X \rightarrow Y)$ can depend only on X and Y – in particular, none of the previous states can influence the transition probability to the next state (hence 'chain').

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3) The probability of going from X to Y must be the same as the probability of going from Y to X:

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$$p_X P(X \rightarrow Y) = p_Y P(Y \rightarrow X) \Rightarrow \frac{P(X \rightarrow Y)}{P(Y \rightarrow X)} = \frac{p_Y}{p_X} = \exp\left[\frac{-(E_Y - E_X)}{kT}\right]$$

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ϕ^4 Theory (in 2-D)

Lagrangian (density):

$$\mathscr{L} = \frac{1}{2}(\partial_\alpha \phi)^2 + \frac{1}{2}\mu^2\phi^2 + \frac{\lambda}{4}\phi^4$$

($\phi \in \mathbb{R}$)

Discretized ϕ^4 Theory (in 2-D)

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Discretized action (energy): $E = -\sum_{\langle i,j \rangle} \phi_i \phi_j + \sum_n [(2 + \frac{\mu_{0L}^2}{2})\phi_n^2 + \frac{\lambda_L}{4}\phi_n^4]$

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The discretized theory is characterized by two independent dimensionless parameters that depend on the lattice spacing a:

$$\mu_{0L}^2 = \mu_0^2 a^2$$

$$\lambda_L = \lambda a^2$$

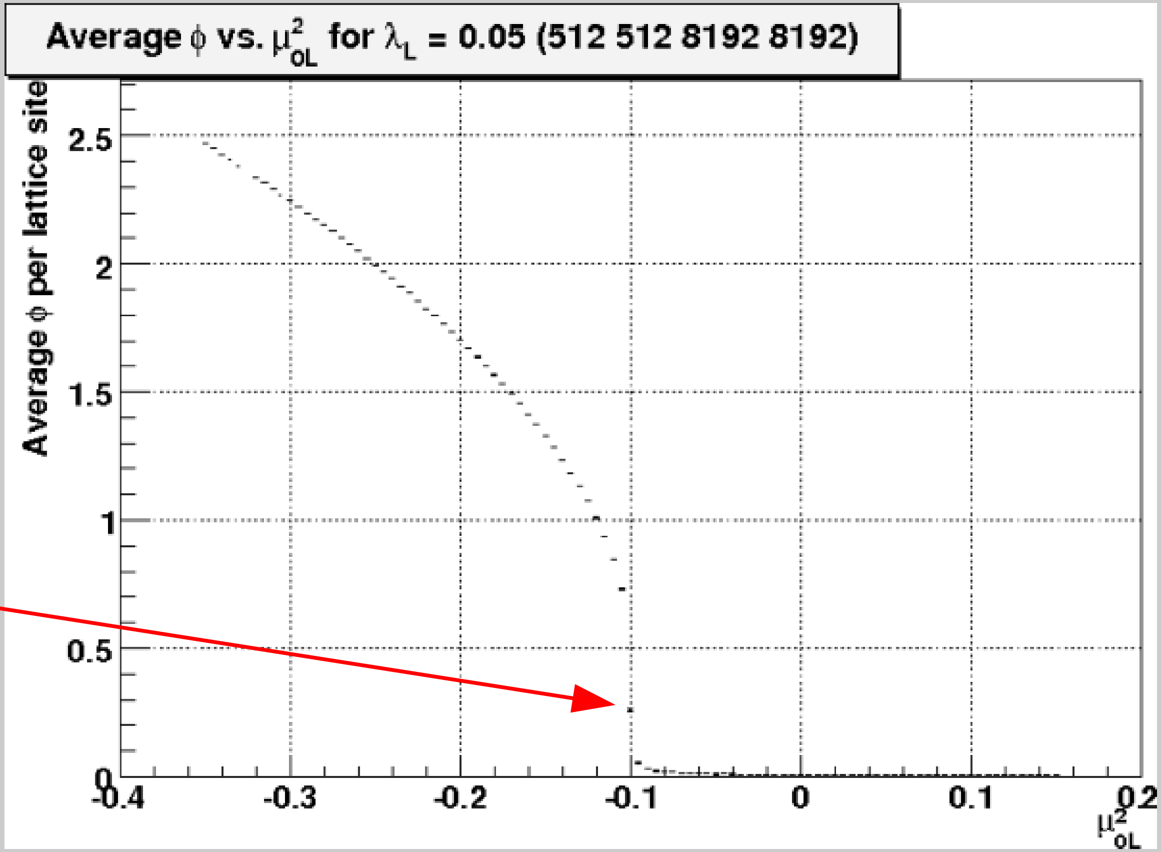
(both $\mu_0{}^2$ and λ have dimensions of mass squared)

Discretized ϕ^4 Theory Phase Transition

$$E = -\sum_{\langle i,j \rangle} \phi_i \phi_j + \sum_n [(2 + \frac{\mu_{0L}^2}{2}) \phi_n^2 + \frac{\lambda_L}{4} \phi_n^4]$$

As with the Ising model, ϕ^4 theory also exhibits a phase transition, with a critical μ^2_{0L} for each $\lambda_L > 0$.

$$[\mu_{0L}^2]_{crit} = -0.10$$



Discretized ϕ^4 Theory Continuum Limit

$$E = -\sum_{\langle i,j \rangle} \phi_i \phi_j + \sum_n \left[\left(2 + \frac{\mu_L^2}{2}\right) \phi_n^2 + \frac{\lambda_L}{4} \phi_n^4 \right]$$

However, we're interested in the continuum theory (a→0). Since the dimensionless parameters depend on the lattice spacing, this presents a problem:

$$\lim_{a \to 0} \mu_{0L}^2 = \lim_{a \to 0} \mu_0^2 a^2 = 0$$

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Solution:

Introduce dimensionless **critical coupling constant**:

$$[\lambda / \mu^2]_{crit} = \lim_{a \to 0} [\lambda_L / \mu_L^2]_{crit}$$

The continuum theory is characterized by this single parameter.

(μ^2_{L} is the renormalized version of $\mu^2_{0\mathrm{L}}$ – no time to cover that subject)

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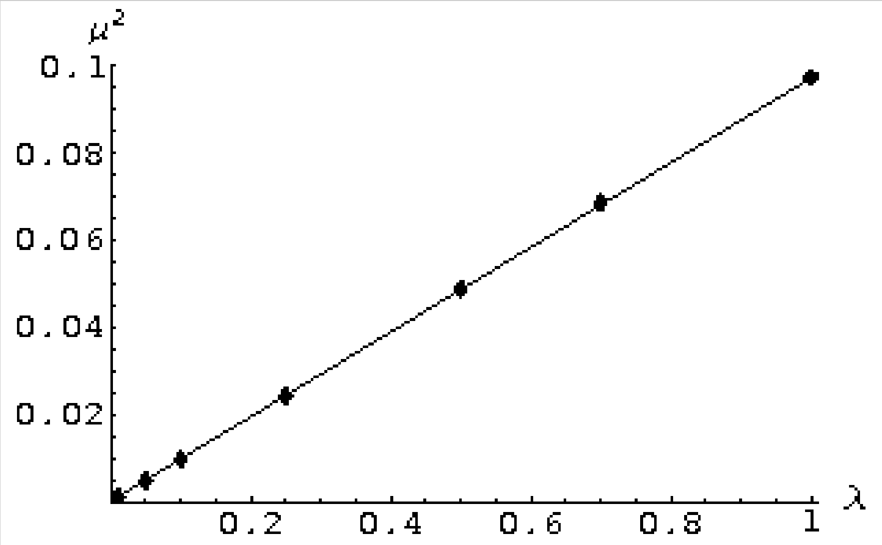
Preliminary Results



Critical coupling constant is inverse of slope:

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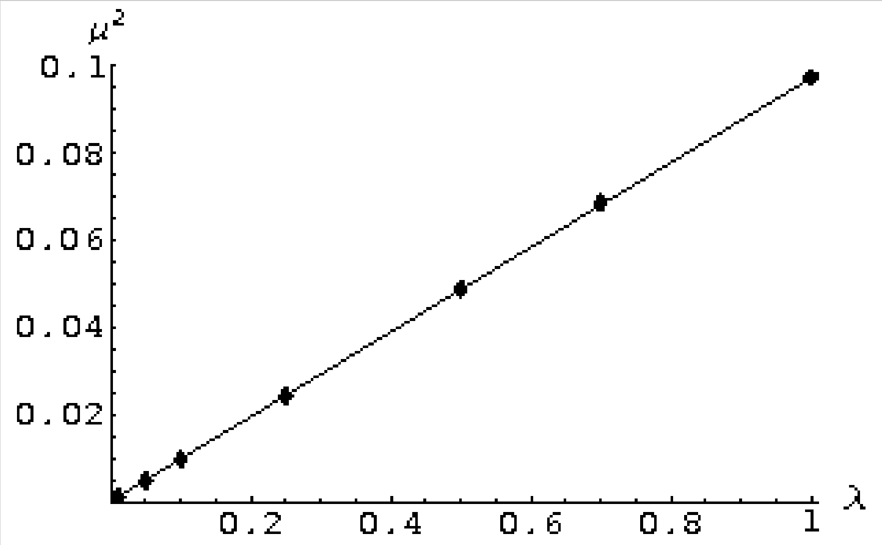

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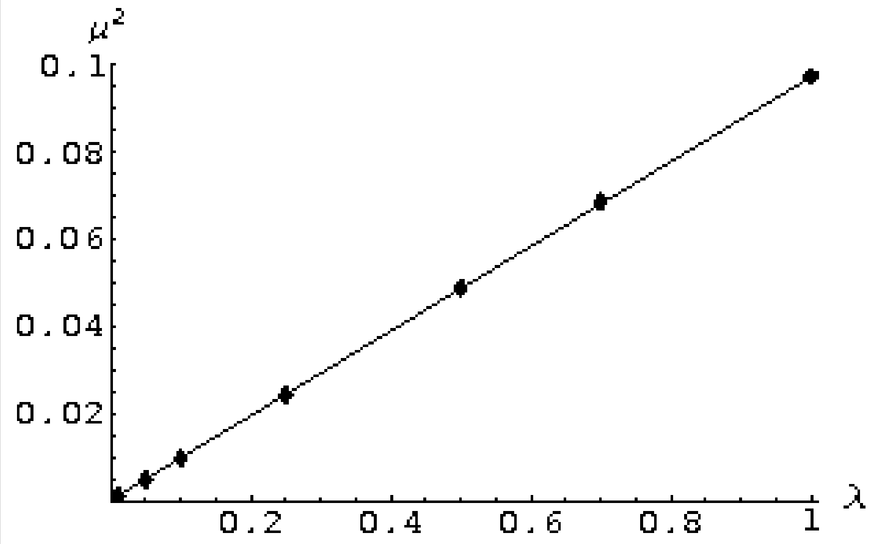

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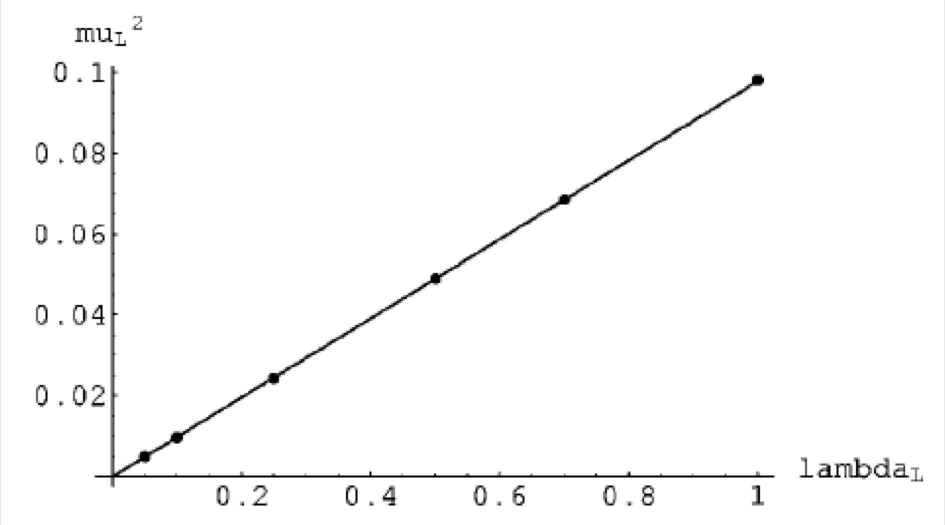
Published Results:



$$[\lambda/\mu^2]_{crit} = 10.26^{+.08}_{-.04}$$

W. Loinaz & R. S. Willey, Phys. Rev. D. **58**, 076003 (1998).

Future Plans

- Polish up result on previous slide
- Calculate critical coupling constant for four-dimensional ϕ^4 theory
- Calculate soliton masses in two-dimensional ϕ^4 theory
- Time permitting, calculate soliton masses in four-dimensional ϕ^4 theory and other simple nonperturbative field theories

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