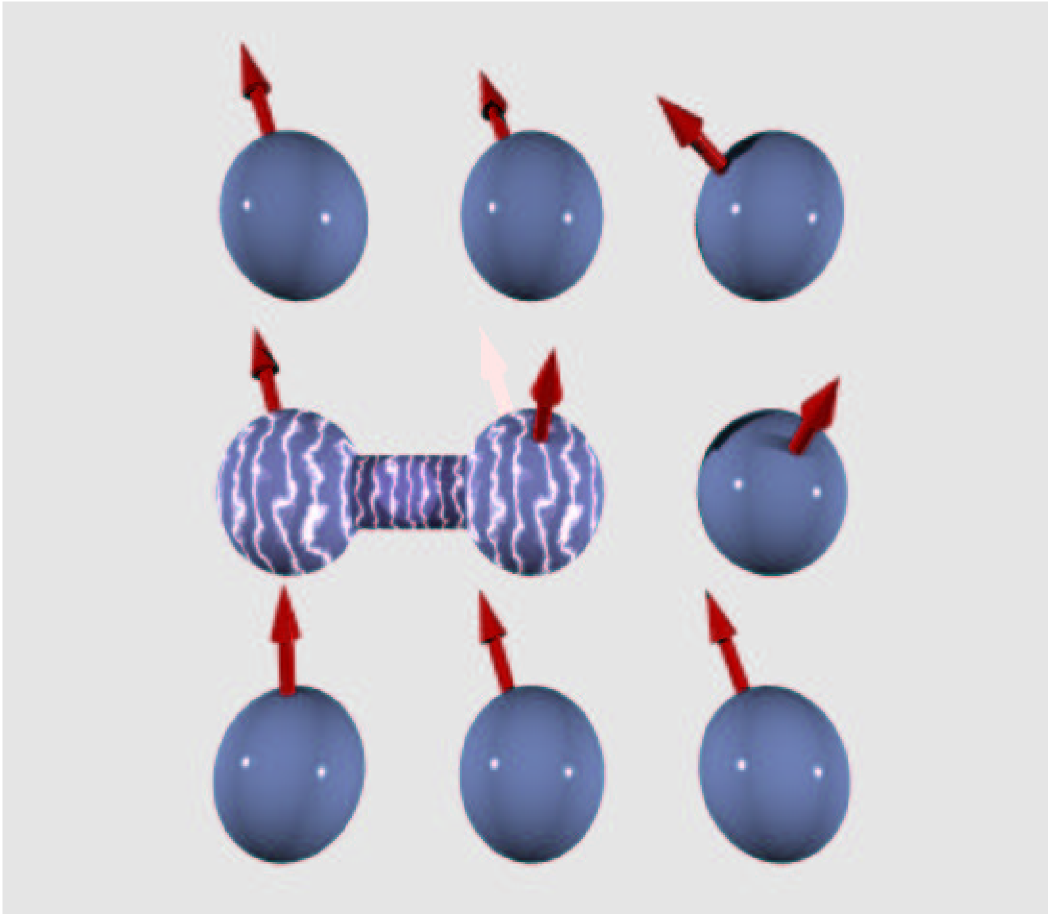

*

The Critical Scaling of the Helicity Modulus of the O(3) classical Heisenberg ferromagnet

Robert G. Brown

Acknowledgements: This work was done with my good friend and colleague, Dr. Mikael Ciftan. We gratefully acknowledge the support of the Army Research Office.

*

Model

Classical Heisenberg ferromagnet (CHF) (the $\mathcal{O}(3)$ model on a $3d$ simple cubic lattice with periodic boundary conditions) in zero external field:

$$\mathcal{H} = -\Sigma_{a<b}^{nn} J_{ab}\mathbf{S}_a \cdot \mathbf{S}_b + \mathcal{H}_{\mathrm{bath}}(\{\mathbf{S}_i\}, T)$$

Goal

To compute and "measure" (with Monte Carlo) the critical exponents of the model, in particular the critical exponent ν_E of the Helicity Modulus $\Upsilon(t)$.

Methods

- **Importance Sampling Monte Carlo (heat bath) "with a twist" to get $\mathbf{E}(\mathbf{L}, \mathbf{T}, \theta_{\mathrm{twist}})$ at high precision for $\mathbf{L} \in [\mathbf{8}, \mathbf{64}...]$.**
- **Finite size scaling used to get critical exponents at $T_c = 1.44295$ (accepted value, ± 0.00005).**
- **Helicity studied by freezing and twisting the (previously periodic) boundary conditions in the (X,Y,1) plane.**

Review of Theory

- **Landau potential for a continuous ferromagnetic model is:**

$$V(S) = \frac{1}{2} r_0 S_\alpha S_\alpha + \frac{1}{4} u_0 S_\alpha S_\alpha S_\beta S_\beta, \tag{1}$$

where S_α are the cartesian components of the coarse grain block spins.

- **Define the block spin $\vec{S}(\vec{r})$ in terms of its mean value (the order parameter) plus a fluctuation:**

$$\vec{S}(\vec{r}) = \vec{m} + \Delta\vec{m} \tag{2}$$

- **Further decompose the fluctuation into a longitudinal and transverse piece:**

$$\vec{S}(\vec{r}) = (m + \Delta m_{||})\vec{n} + \Delta\vec{m}_\perp \tag{3}$$

- **Derive the following general form for the free energy in terms of the transverse coarse grained spin fluctuation gradient $\nabla\vec{m}_\perp(\vec{r})$:**

$$F(\Delta\vec{m}) = \text{longitudinal part} + \frac{1}{2}\int d^d\vec{r}\ b \cdot (\nabla\vec{m}_\perp(\vec{r}))^2. \tag{4}$$

(with phenomenological parameter b, the "spin wave stiffness".

- **One can relate a state of uniform twist angle to the gradient of the transverse spin fluctuation via $\nabla\phi = |\nabla\vec{m}_\perp|/m$. Substituting and differentiating to find the free energy density, one obtains the following two relations:**

$$\frac{dF}{dV} = \frac{1}{2}\Upsilon(T)(\nabla\phi)^2 \tag{5}$$

with

$$\Upsilon(T) = bm^2(T). \tag{6}$$

- **In Landau theory, b approximately constant so $\Upsilon \sim m^2(T)$ as $T \to T_c$ from below. In detailed treatment one gets corrections:**

$$\Upsilon(t) \sim (-t)^{2\beta-\eta\nu} \tag{7}$$

- **Finally, to use finite-size scaling theory (FSST) to extract the critical exponent, we must substitute $-t \to L^{-1/\nu}$, or**

$$\Upsilon(L) \sim (L)^{-2\beta/\nu+\eta} \tag{8}$$

In the last expression, $\Upsilon(L) \approx L^{-2\beta/\nu}$. $2\beta/\nu$ term from m^2 clearly dominant (η is very small, ~ 0.01, for this model, while $\beta \approx 1/3$ and $\nu \approx 2/3$). The helicity modulus should vanish sharply near T_c according to Landau theory.

But...

We cannot directly measure the free energy density dF/dV. We *can* directly measure the enthalpy density E. Following an identical argument:

$$\Delta E(\Theta) \approx \frac{1}{2}\Upsilon_E(T)(\nabla\phi)^2 \tag{9}$$

where $\Delta E(\Theta)$ is the change in internal energy caused by twisting the boundary conditions through the angle $\Theta \leq \pi/2$ with either helicity. From this obvious substitutions yield:

$$\Upsilon_E(T) = \frac{2L^2}{\Theta^2}\Delta E(\Theta) \tag{10}$$

With a page or two of algebra we can show that:

$$\Upsilon_E(t) \sim t^{v_E} \sim t^{-\phi} \tag{11}$$

with the critical exponent

$$v_E = -\phi = 1 - 2\nu - \alpha \tag{12}$$

This is what we wish to measure, in part to *invert* this equation and deduce the values of ν and α.

Note that as before, if we make the finite size scaling hypothesis we will actually measure:

$$\Upsilon(L) \sim (L)^{-v_E/\nu} \sim (L)^{2-\frac{1-\alpha}{\nu}} \tag{13}$$

or

$$-v_E/\nu = 2 - \frac{1-\alpha}{\nu} \tag{14}$$

The enthalpy helicity should thus *diverge* **at T_c.**

It is easy to show that:

$$d - 2 - v_E/\nu \; = \; d - \frac{1-\alpha}{\nu} \tag{15}$$

$$1 - v_E/\nu \; = \; \frac{1}{\nu} \tag{16}$$

$$\nu \; = \; \frac{1}{1 - \frac{v_E}{\nu}} \tag{17}$$

where the second step uses "hyperscaling" (widely believed but by no means proven for this model) to eliminate α for $d = 3$. With this we can compute α and ν given $-v_E/\nu$ and possibly *check* **hyperscaling.**

Measuring $\Upsilon(T, L)$ with Monte Carlo

- **Calculations were performed on several generations of "brahma" (our beowulf compute cluster, also ganesh and rama).**
- **Heat bath only (cluster method a bit difficult if boundary layers are "frozen").**
- **Equilibrate $L \times L \times L$ lattice with periodic boundary conditions.**
- **"Freeze" (x,y,1) layer of spins.**
- **Rotate (x,y,1) spins through angle θ and store them in (x,y,L+1) layer (replacing PBC's in z-direction with frozen *twisted* PBC's).**
- **Re-equilibrate only the (x,y,2) to (x,y,L) spins with the heat bath (with PBC's in the x and y directions).**
- **Sample**
- **Repeat (easiest to restore PBC's, re-equilibrate, repeat).**
- **Sweep angles $\theta \in [0, \pi/2]$, $L \in [8, 48]$ at T_c.**
- **Fit $\frac{E}{L^3} = \frac{1}{2}\Upsilon(L)(\nabla\phi)^2$ where $\nabla\phi = \theta/L$.**
- **Fit $\Upsilon(L) = L^{x/\nu}$**
- **Obtain ν, α from hyperscaling.**

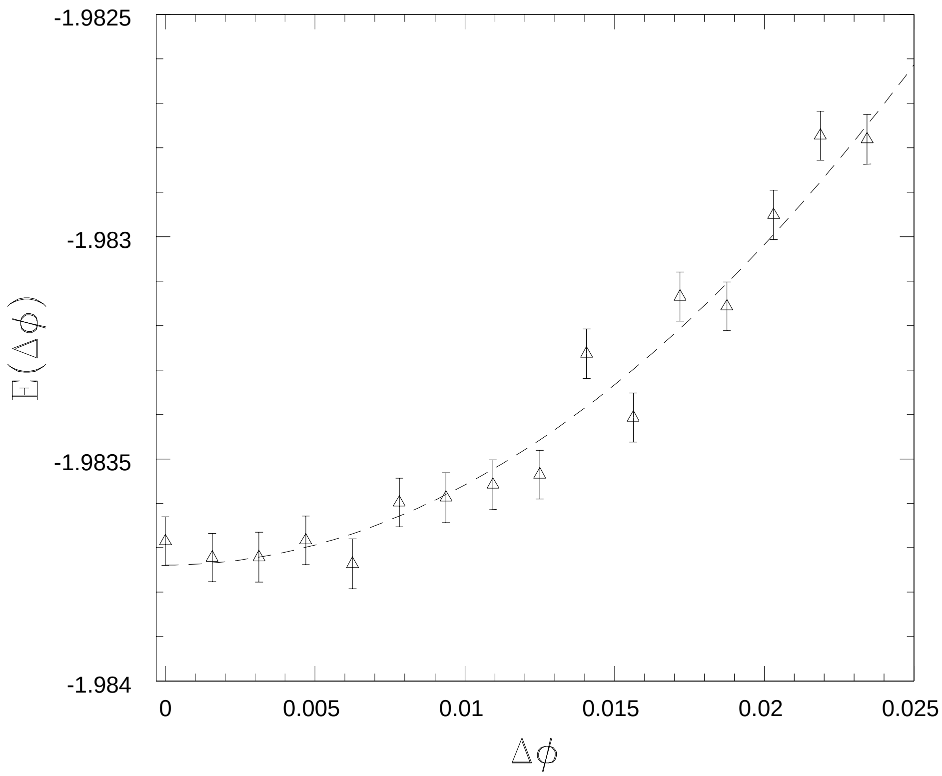

Figure 1: E per spin as function of interlayer twist angle $\Delta\phi$ for $L = 64$ (in progress). This is fit to obtain the helicity.

Results

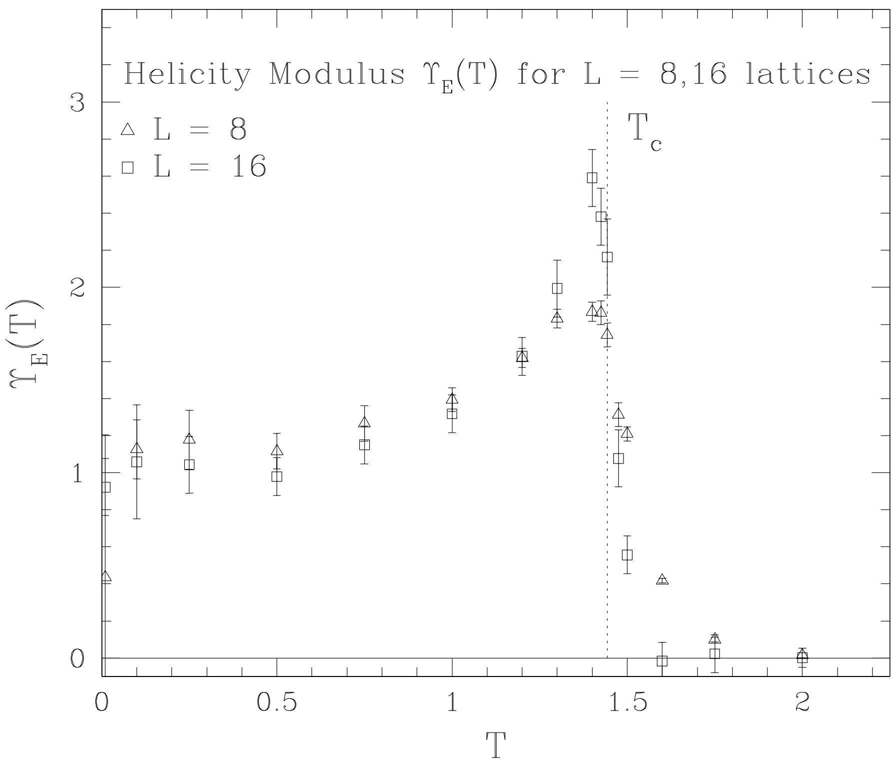

Figure 2: $\Upsilon(T)$ for $L = 8$ and $L = 16$, evaluated at low precision to get trend only.

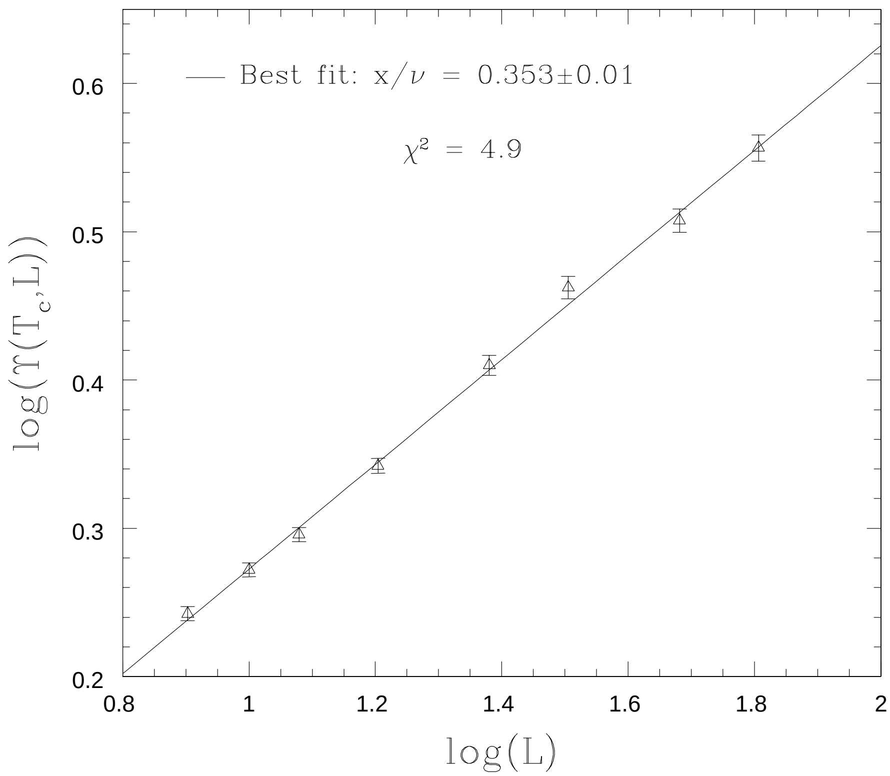

Figure 3: The helicities for various L at T_c. The nonlinear least squares fit of this yields $x/\nu = -v_e/\nu$.

Best result to date: $x/\nu = 0.353 \pm 0.02$

Conclusions

- **The** *only* **direct measurement of this quantity to date.**
- $\nu = \frac{1}{1-\frac{\nu_E}{\nu}} = \frac{1}{1.353} = 0.739 \pm 0.01$. **This is quite large compared to most other Monte Carlo results (which tend to yield** $\nu \approx 0.705 \pm 0.01$**) but is not inconsistent with the most recent renormalization predictions.**
- **The hyperscaling relation itself then yields** $\alpha = -0.222$. **This is a weakly singular quantity and is** *very difficult to measure*. **This is a major motivation of this work.**
- **For this particular talk, we emphasize that there are easily more than 30 "GFLOP-years" of effort in this result (whatever you consider a GFLOP to be). (32x400x3 = 38400) + (16x1300x2 = 41600) + (32x1600x1 = 51200) = 131.200 GHz-years, supercomputing indeed. Impossible without the beowulf/cluster model.**