Unconventional phase transition in a classical 3-dimensional dimer model

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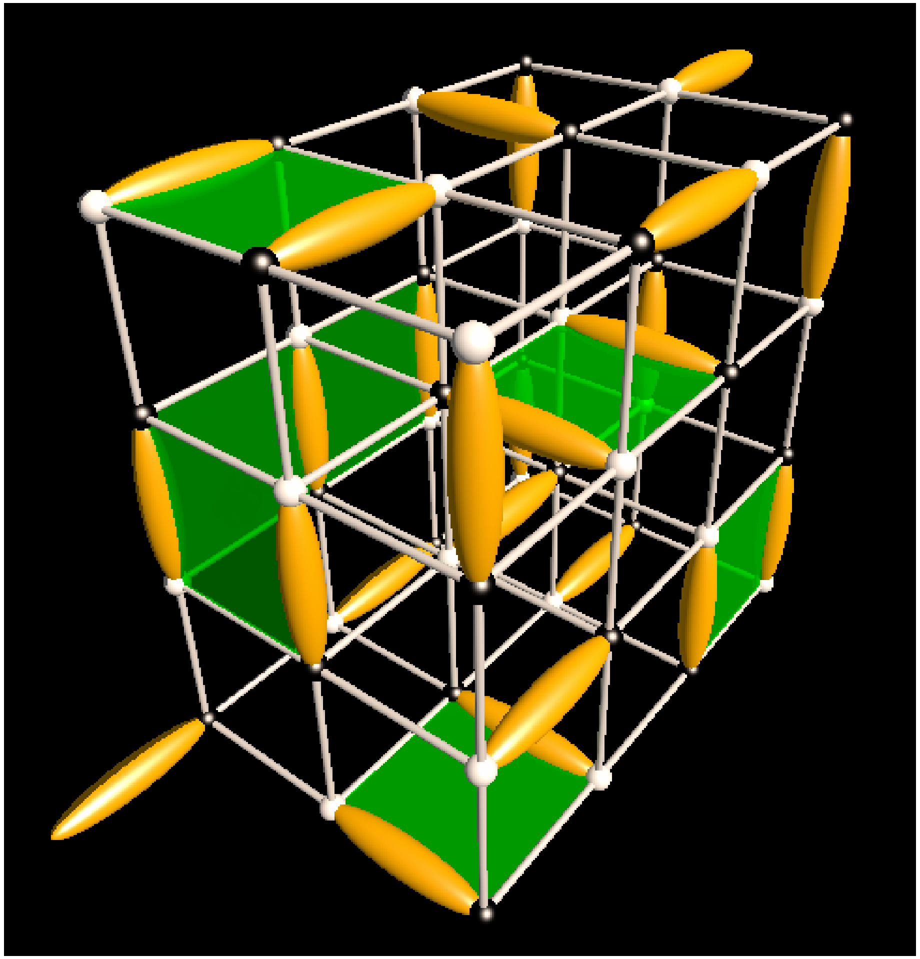
A model with dimers on the cubic lattice



- Fully packed coverings: every site is occupied by one and only one dimer
- 2-dimer interaction which favours parallel dimers on the same square **plaquette**

$$Z = \sum_{c \in \{\text{dimer coverings}\}} e^{-\frac{E(c)}{T}}$$

$$E(c) = -N_{\square}(c)$$

This model presents several phenomena currently studied in D>1 *quantum* systems :

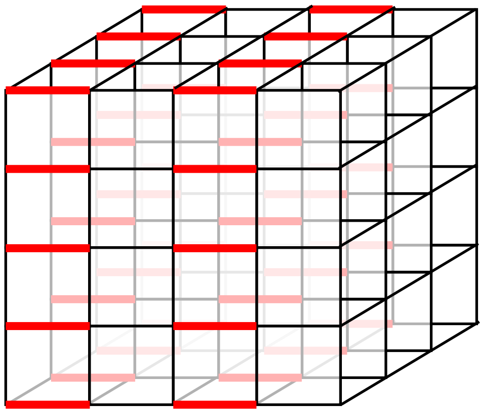
- Physics of constrained models, frustration
- Emergence of gauge degrees of freedom, fractionalization
- Landau-forbidden transitions (Mott insulator/Superfluid) ?

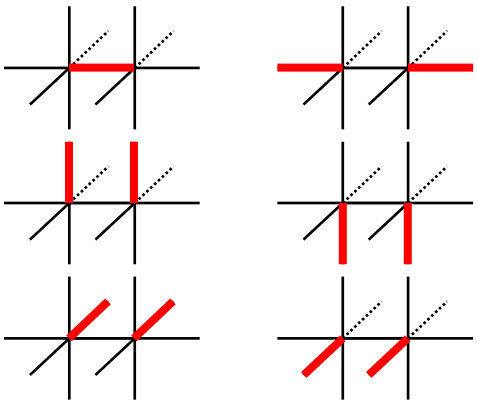
Outline

- Low- and high-T phases: cristal & Coulomb
- 2^{nd} order phase transition, exponents
- Simple (Landau) theories seem to fail to describe the critical point
- Connection with other “Landau forbidden” transitions ?

Low temperature crystal

- T→0 : 6 « columnar » ground-states

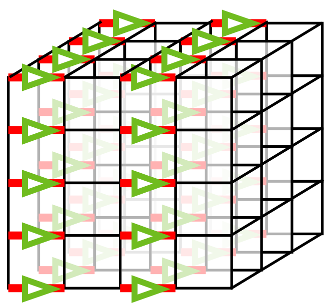


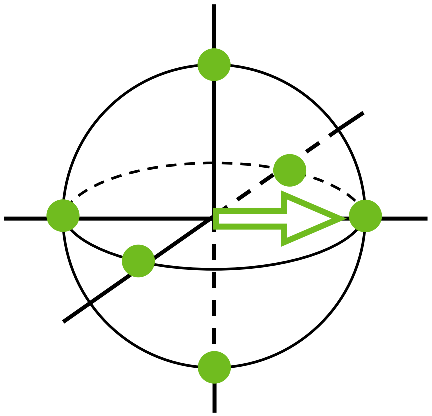


$$d_\alpha(r) = \begin{cases} 1 \text{ if there is a dimer from } r \text{ to } r+\alpha \\ 0 \text{ otherwise} \end{cases}$$

$$\vec{m}(r) = \begin{bmatrix} (-1)^x d_x(r) \\ (-1)^y d_y(r) \\ (-1)^z d_z(r) \end{bmatrix}$$

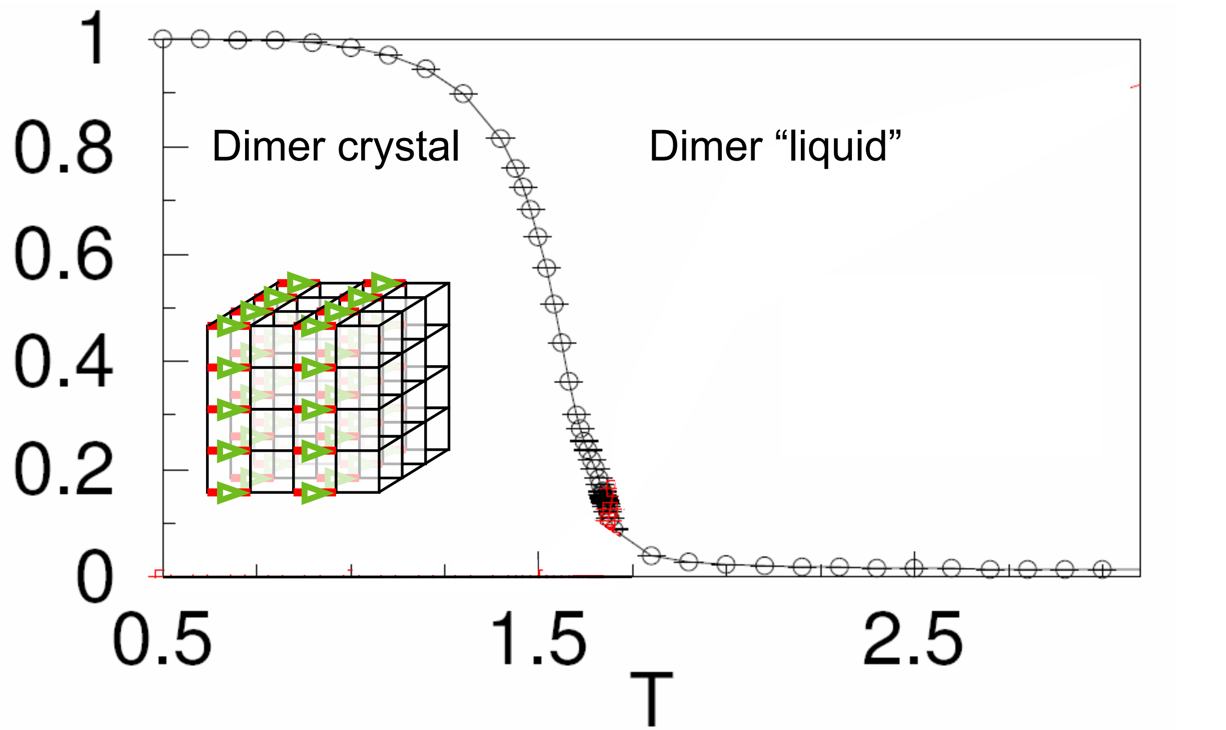
3-component order parameter





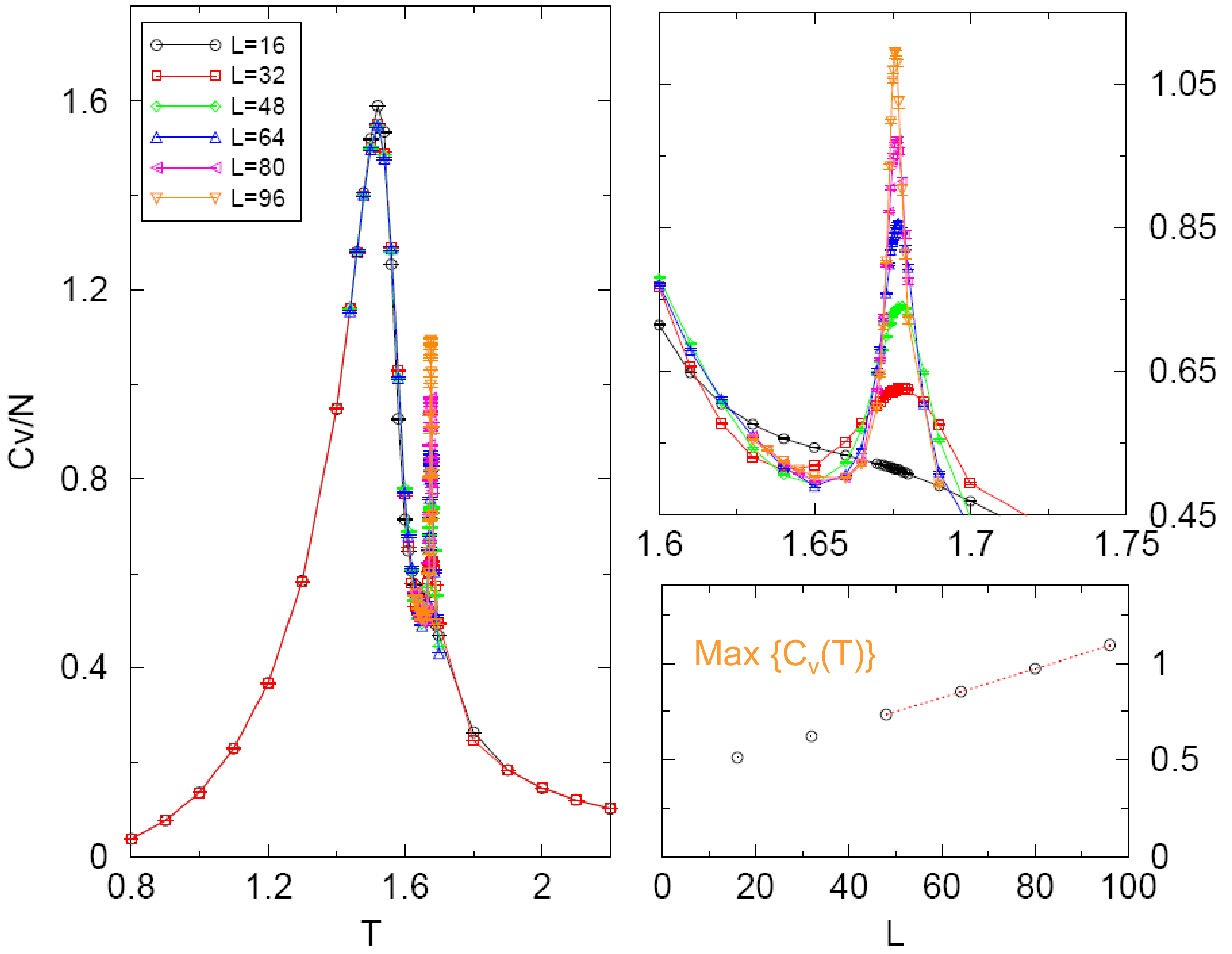
Order parameter of the crystal/columnar phase

$$m = \frac{2}{V} \left\| \sum_r \vec{m}(r) \right\|$$



- About the simulations
  - “Directed loop” Monte-Carlo algorithm [Syljuasen & Sandwik PRE 2002; Sandvik 2003]
    Non-local updates ⇒ efficient thermalization even when the correlation length is large.
  - Large system sizes L≤96 ($N=L^3 \leq 884.736$ sites)
  - ALPS numerical libraries
  - ~200.000 CPU hours

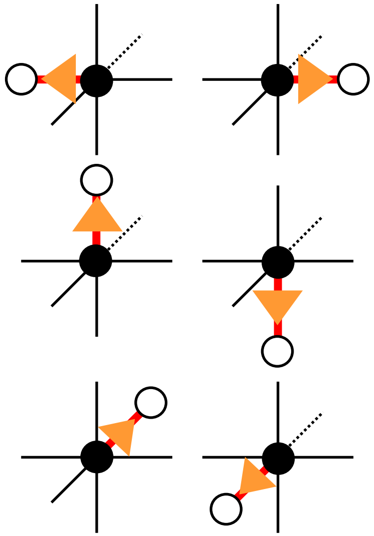
Specific heat



Coulomb phase at high temperatures

- Fictitious « magnetic field »

Huse, Krauth, Moessner & Sondhi, PRL 2003
Hermele *et al.*, PRB 2004;
Isakov *et al.*, PRL 2004;
Henley, PRB 2005



Bi-partite lattice

$\Rightarrow$ 

$$\vec{B}(r) = (-1)^{x+y+z} \begin{bmatrix} d_x(r) \\ d_y(r) \\ d_z(r) \end{bmatrix}$$

$$\text{div}\, \vec{B}(r) = (-1)^{x+y+z}$$

≈ 0 when coarse grained

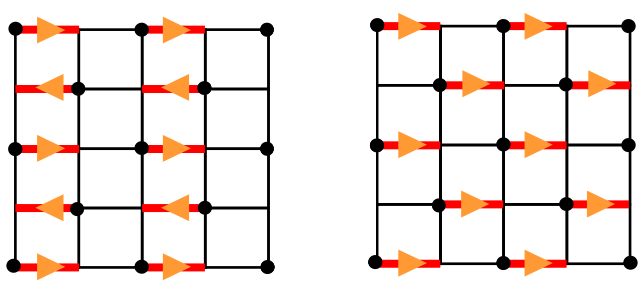
$$\Rightarrow \vec{B} \approx \vec{\nabla} \times \vec{A}$$

$$S_{eff} = \frac{K}{2} \int d^3 r \left(\vec{\nabla} \times \vec{A} \right)^2$$

$\Downarrow$

Dipolar correlations

$$\left\langle B^\alpha(r) B^\beta(0) \right\rangle \approx \frac{1}{2\pi K} \frac{3 r^\alpha r^\beta - r^2 \delta^{\alpha\beta}}{r^5}$$



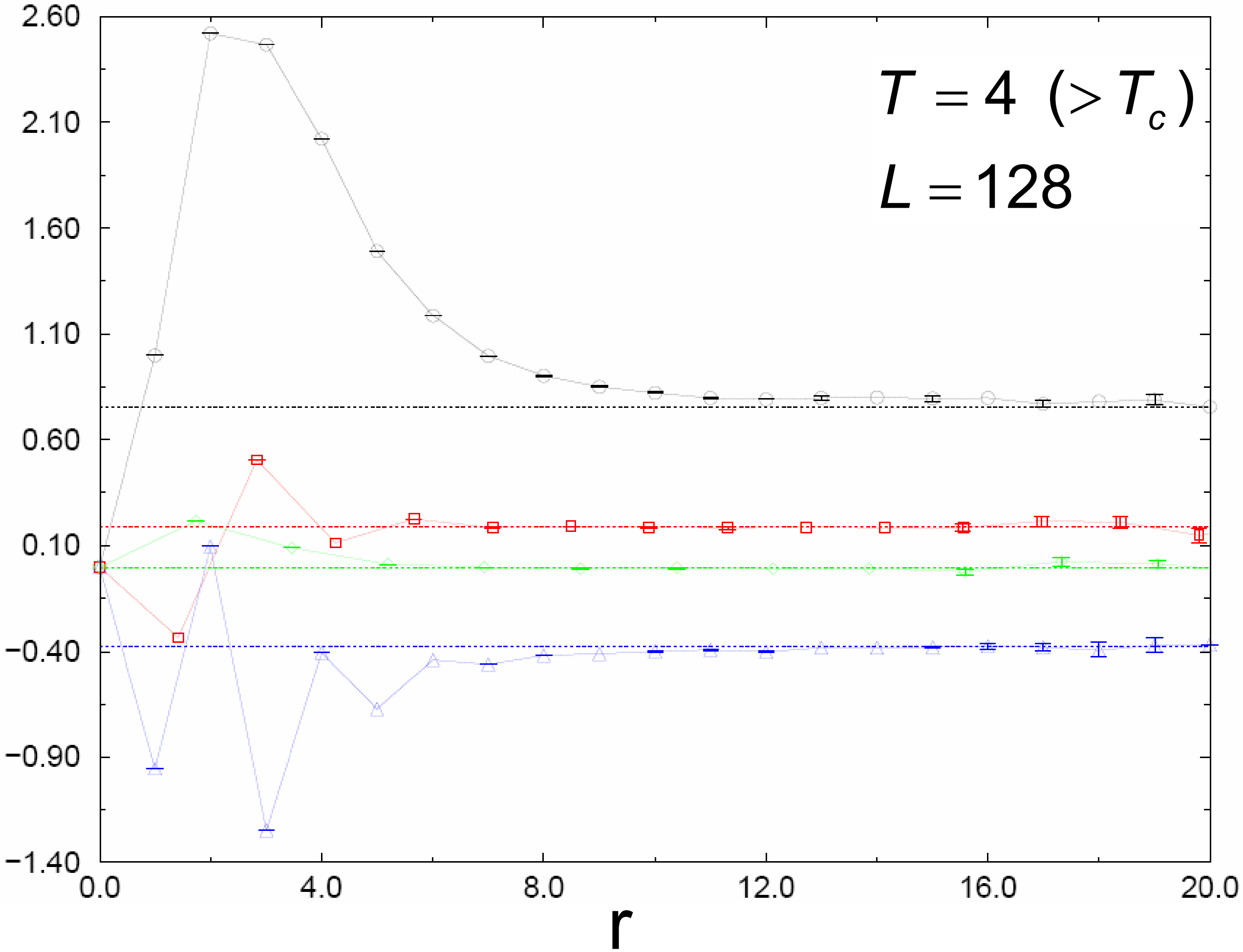
Crystal $\Rightarrow$ no average magnetic field
Staggered $\Rightarrow$ maximum magnetic field

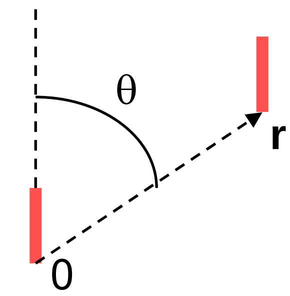
(dipolar) Dimer-dimer correlations in the Coulomb phase

See also Huse *et al.* 2003

2 parallel bonds :

$$\left\langle d^z(0)d^z(r)\right\rangle^c \cdot r^3 \xrightarrow[r\to\infty]{} 3\cos^2\theta - 1$$





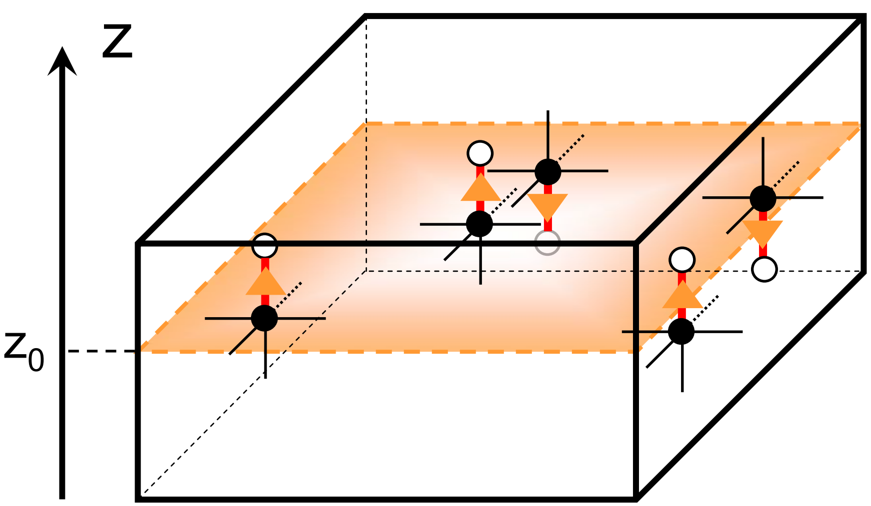
$\cos\theta = 1$

$\cos\theta = \frac{1}{\sqrt{2}}$

$\cos\theta = \frac{1}{\sqrt{3}}$

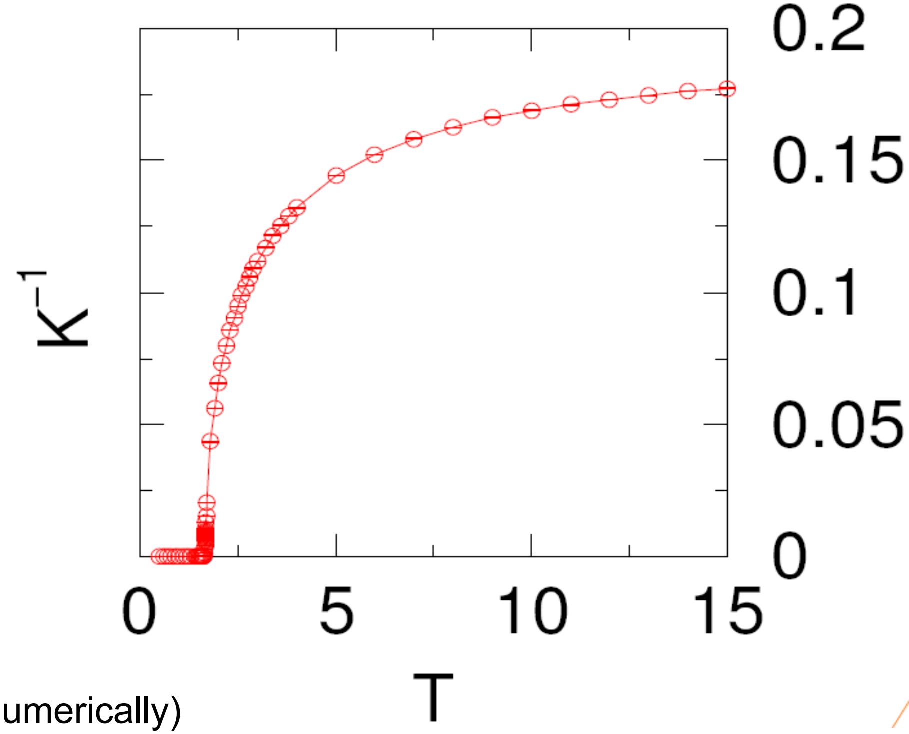
$\cos\theta = 0$

Total magnetic flux (dimer winding number)



$$\phi^z(z_0) = \int dxdy \;\; B^z(x,y,z_0)$$
$$= N_{d\uparrow} - N_{d\downarrow}$$
$$= \text{indep. of } z_0$$

$$S_{eff} = \frac{K}{2}\int d^3r \left(\vec{\nabla}\times\vec{A}\right)^2$$
$$\Rightarrow \left\langle \left(\phi^z\right)^2 \right\rangle = K^{-1}\cdot L$$



- NB: Another characterization of the Coulomb phase:
  1/r interaction between 2 “test” monomers (checked numerically)

A second order phase transition

- Transition temperature
  - $T_c^{Cv} = 1.676(1)$
  - $T_c^{\langle \phi^2 \rangle} = 1.6745(5)$
  - $T_c^{Columnar} = 1.67525(50)$
- From Energy histograms/cumulant : 2nd order transition
- Critical exponents
  - From $\langle \Phi^2 \rangle$
  - From $\langle m^2 \rangle$ & $\langle m^4 \rangle$ (Binder cumulant)
  - From C_v

$$\left.\begin{aligned} \nu &= 0.51(3) \\ \alpha &= 0.56(7) \\ \eta &= -0.02(5) \end{aligned}\right.$$

⇨ Compatible with tricritical universality class $\nu = \alpha = 1/2$; $\eta = 0$

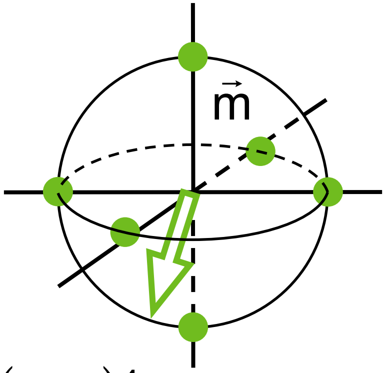
[φ^6 theory for an O(n) model in d≥3]

- NB: 2D version of the model → Kosterlitz-Thouless transition

  between a dimer crystal and a « rough » (critical) phase [Alet *et al.* PRL 2005]

"Landau-Ginzburg" approach from the crystal phase

- Write an effective theory for a slowly varying order parameter m(r)
  O(3) action + anisotropies
  (to reduce the symmetry to the discrete group of the cube)



$$S_{\text{Crystal}}[\vec{m}] = \int d^3r \ \rho(\nabla \vec{m})^2 + t\vec{m}^2 + g\vec{m}^{2^2} + u \sum_{\alpha=x,y,z} (m^\alpha)^4 + \dots$$

- Problems:
  - No conserved flux (absence of empty sites not taken into account)
  - Erroneously produces a massive phase at high temperature (no Coulomb phase)
  - Transition would be 1st order

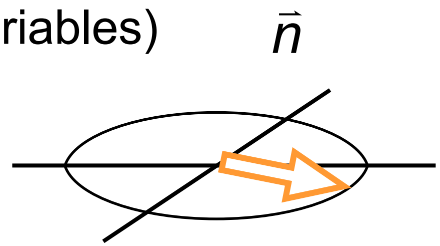
  [Carmona *et al.*, PRB (2000)]

"Landau-Ginzburg" approach from the Coulomb phase

- No broken symmetry at high temperature...
  No order parameter in the original (dimer) variables
- Move to ***dual*** variables ⇒ this introduces an O(2) symmetry
  [Banks, Myerson & Kogut, 1977]

This symmetry is spontaneously broken in the Coulomb phase
Coulomb phase ⇔ ordered "XY ferromagnet" (in dual variables)
n(r): magnetization density of this dual XY model

$$S_{\text{Coulomb}}[\vec{n}] = \int d^3 r \; \rho(\nabla \vec{n})^2 + t\vec{n}^2 + g\vec{n}^4 + \dots$$



- Problems:
  - Does not predict a dimer crystal for $T<T_c$ but a "paramagnetic" phase (in the dual variables). It corresponds to a non-physical state with B~0 everywhere (no dimer…)
  - Different exponents for the transition
    [Campostrini et al., PRB 2001]

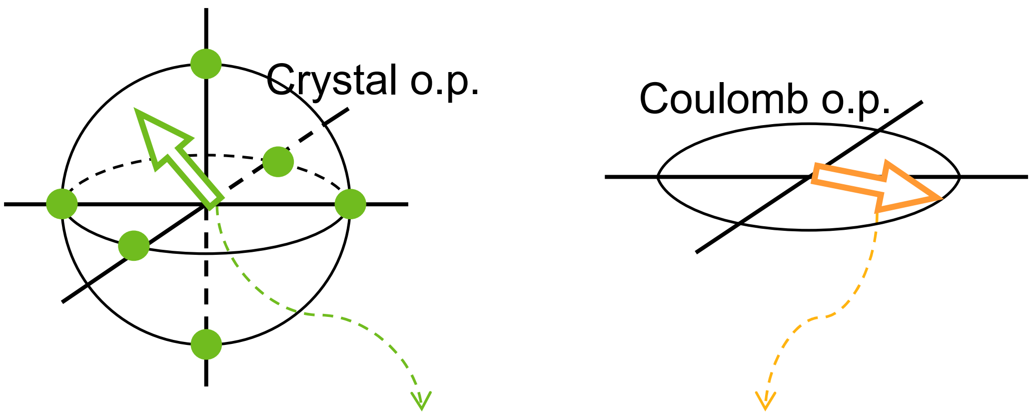
$$\nu_{\text{3DXY}} = 0.67155(27) \qquad \nu = 0.51(3)$$

$$\alpha_{\text{3DXY}} = -0.0146(8) \quad \neq \quad \alpha = 0.56(7)$$

$$\eta_{\text{3DXY}} = 0.0380(4) \qquad \eta = -0.02(5)$$

"Landau-Ginzburg" with *both* order parameters

- Write down all possible terms involving n and m allowed by symmetries



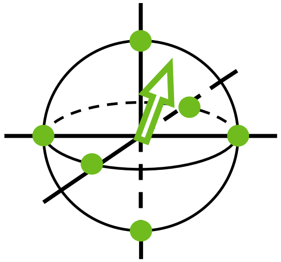
m and *n* transform according to different symmetries
⇒ energy-energy-like couplings only

$$S = S_{Crystal}\left[\vec{m}\right] + S_{Coulomb}\left[\vec{n}\right]$$
$$+ \int d^3 r \left\{ (\cdots)\, \vec{n}^2 \cdot \vec{m}^2 + (\cdots)\, \vec{n}^2 \left(\nabla \vec{m}\right)^2 + (\cdots)\, \vec{m}^2 \left(\nabla \vec{n}\right)^2 + \cdots \right\}$$

- Problems / questions:
  - Mixes direct and dual variables (sometimes lead to wrong results)
  - *Generically* not a direct second order transition
    (unless the parameters are fine-tuned to a multi-critical point)
  - If this is the correct point of view, what is the reason for such a fine tuning ?

CP^1 representation of the crystal order parameter

- Split $\vec{m}$ in two spinors



$$\vec{m} = \sum_{\alpha=\uparrow,\downarrow} \bar{z}_\alpha \vec{\sigma}_{\alpha\beta} z_\beta$$

$z_\uparrow, z_\downarrow$: 2 complex numbers

$\sigma^x, \sigma^y, \sigma^z$: Pauli matrices

$\vec{m}^2 = |z_\uparrow|^2 + |z_\downarrow|^2$

- Coupling between the vector potential A_μ and the *spinor* $(z_\uparrow, z_\downarrow)$

$$L = L_{Crystal}\left[\vec{m} = \bar{\mathbf{z}}\vec{\sigma}\,\mathbf{z}\right] + \sum_{\substack{\alpha=\uparrow,\downarrow \\ \mu=x,y,z}} \left|\left(\nabla_\mu - iA_\mu\right)z_\alpha\right|^2 + \frac{K}{2}\underbrace{\left(\varepsilon_{\mu\nu\rho}\nabla_\mu A_\nu\right)}_{B}{}^2$$

$\langle \mathbf{z} \rangle = 0 \Rightarrow$ Coulomb phase

$\langle \mathbf{z} \rangle \neq 0 \Rightarrow$ Crystal phase.

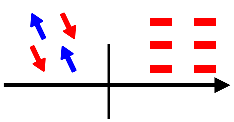
Higgs mechanism $\Rightarrow$ gapped gauge fluctuations

Gauge transformation

$$\begin{cases} \begin{bmatrix} z_\uparrow(r) \\ z_\downarrow(r) \end{bmatrix} \rightarrow e^{i\theta(r)} \begin{bmatrix} z_\uparrow(r) \\ z_\downarrow(r) \end{bmatrix} \\ A_\mu \rightarrow A_\mu + \nabla_\mu \theta \end{cases}$$

- Previously proposed to describe "Landau-Forbidden" 2nd order phase transition

  This effective action does *not* involve any of the two order parameters m or n.

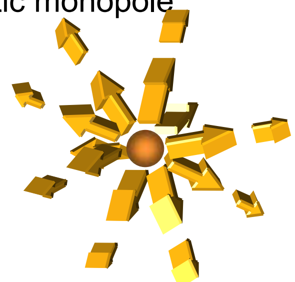
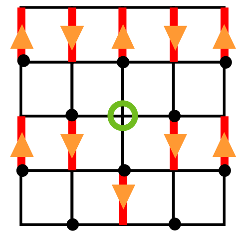
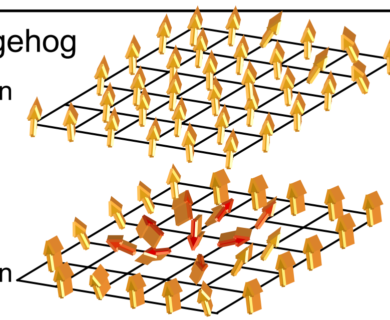


  - Motrunich & Vishwanath, PRB 2004: Heisenberg spin model with suppressed topological defect (hedgehog)
  - Senthil *et al.*, Science 2004, PRB 2004: Néel/BVS transition in 2D spin-1/2 quantum antiferromagnets

- Ingredient: absence of topological defects (mag. Monopoles)

O(3) sigma model with hedgehog suppression

Motrunich & Vishwanath (2004)

Gauge theory	Dimer model	O(3) Heisenberg model without hedgehog
Magnetic field $B^z(r)$	dimer $(-1)^{x+y+z} d_z(r)$	Spin chirality $\vec{n}_r \cdot \left(\vec{n}_{r+x} \times \vec{n}_{r+y}\right)$
Magnetic monopole 	Monomer 	Hedgehog 
Broken symmetry phase (Higgs)	Dimer crystal [discrete broken symmetry]	Ferromagnet [O(3) broken symmetry]
Coulomb phase	"Dipolar" dimer liquid	"Dipolar" paramagnet
	$\nu = 0.51(3)$ $\eta = -0.02(5)$ $\alpha = 0.56(7)$ $\beta \approx 0.25$	? $\nu = 1 \pm 0.2$ $\eta \approx 0.6$ $\alpha < 0$ $\beta = 0.8 \pm 0.05$

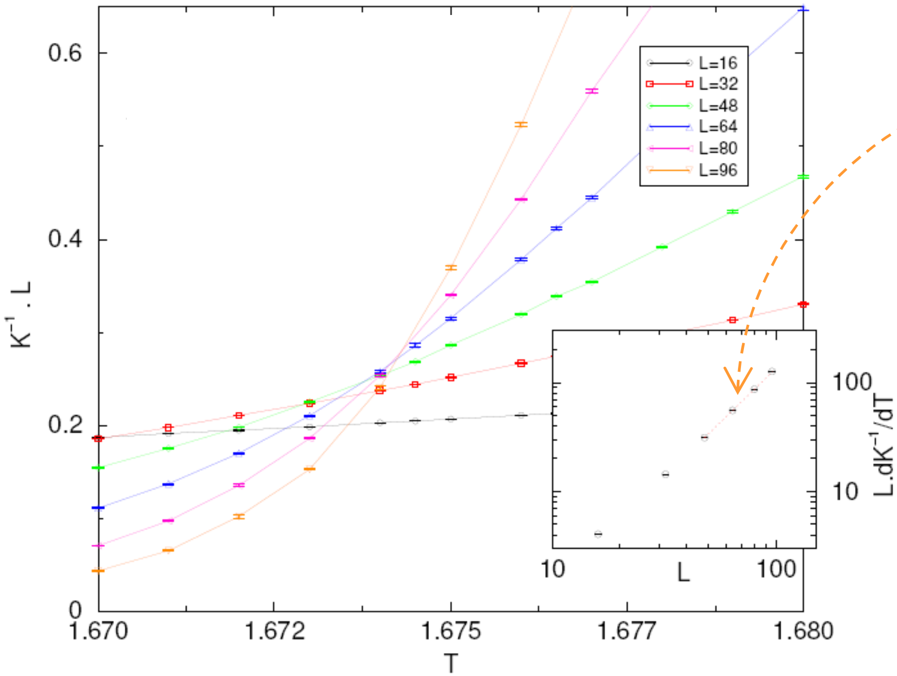
Conclusions

cond-mat/0603499
(to appear in PRL)

- Very simple microscopic model
- 2 phases (dimer crystal and Coulomb liquid) which are qualitatively well understood
- High precision Monte-Carlo simulations
- *Apparently* simple transition: mean-field tricritical exponents ?
- But this is quite unexpected/unconventional
  - A simple approach based on the order parameters of the ordered phase(s) would generically predict a *first-order* transition.
  - Strong similarities with other “Landau-forbidden” transitions studied recently [Motrunich & Vishwanath; Senthil *et al.;* Bergman, Fiete & Balents] A gauge-theory description of the critical point is likely.
- New universality class ?
- To do/in progress: put monomers, change the interaction, change the lattice, formulate the model in terms of [O(2)] vortex lines, …

Appendix 1: How are the critical exponents measured ?

- Example of the correlation length exponent ν



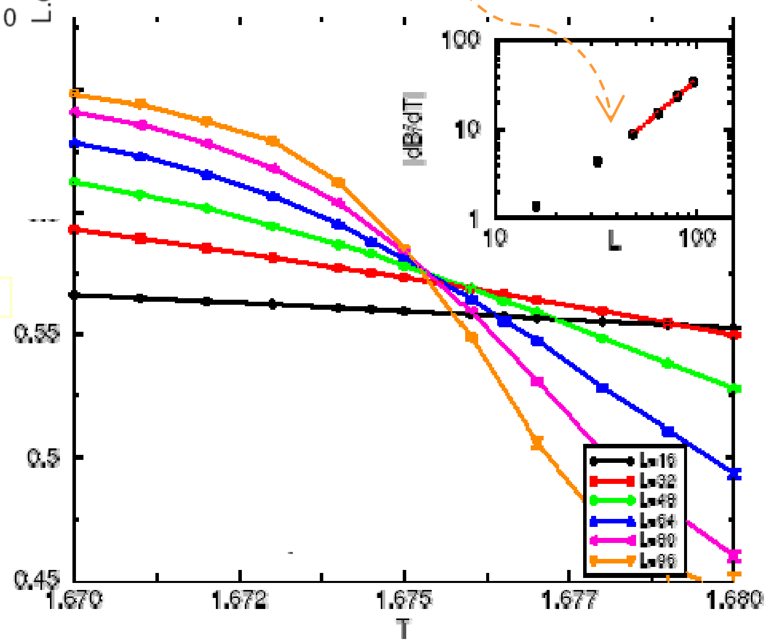
$$\log\left[\left.\frac{d\langle\phi^2\rangle}{dT}\right|_{T=T_c}\right] \sim \frac{1}{\nu}\log L$$

$$\log\left[\left.\frac{dB}{dT}\right|_{T=T_c}\right] \sim \frac{1}{\nu}\log L$$

$$\langle\phi^2\rangle \sim f_1\left(L^{1/\nu}\cdot(T-T_c)\right)$$

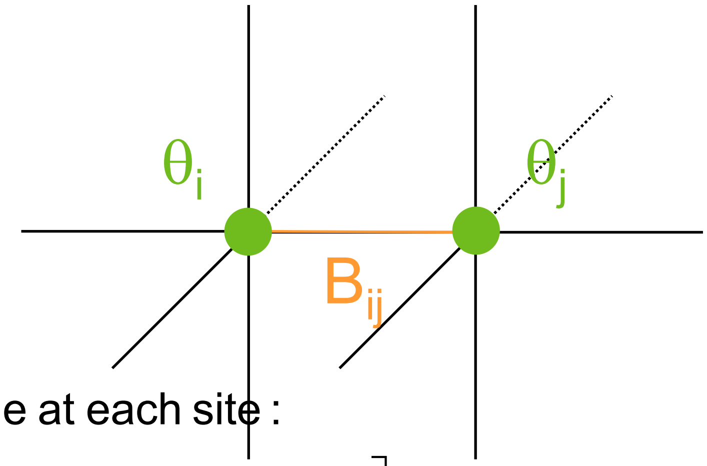
$$B = 1 - \frac{\langle m^4\rangle}{3\langle m^2\rangle^2}$$

$$\sim f_2\left(L^{1/\nu}\cdot(T-T_c)\right)$$



⇨ $\nu = 0.51(3)$ from *both* sides of the transition

Appendix 2: Coulomb ↔ XY duality



$$Z_{\text{Coulomb}} = \sum_{\substack{B_{ij}=-\infty\cdots\infty \\ \text{div}B=0}} \exp\left[-\frac{K}{2}\sum_{\langle ij\rangle} B_{ij}^2\right]$$

div$B$=0 constraint ⇒ integrate an angular variable at each site :

$$= \left(\prod_i \int_0^{2\pi} \frac{d\theta_i}{2\pi}\right) \sum_{B_{ij}=-\infty\cdots\infty} \exp\left[-\frac{K}{2}\sum_{\langle ij\rangle} B_{ij}^2 - i\sum_{\langle ij\rangle} B_{ij}\left(\theta_i-\theta_j\right)\right]$$

Poisson summation : $B \in Z$ replaced by $x \in R$ & $m \in Z$

$$= \left(\prod_i \int_0^{2\pi} \frac{d\theta_i}{2\pi}\right) \sum_{m_{ij}=-\infty\cdots\infty} \left(\prod_{\langle ij\rangle} \int_{-\infty}^{\infty} dx_{ij}\right) \exp\left[-\frac{K}{2}\sum_{\langle ij\rangle} x_{ij}^2 - i\sum_{\langle ij\rangle} x_{ij}\left(\theta_i-\theta_j+2\pi m_{ij}\right)\right]$$

Gaussian integrals over dx_{ij} :

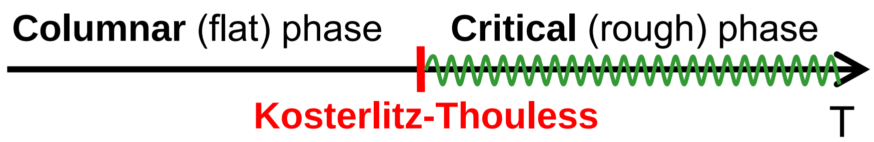
$$\sim \left(\prod_i \int_0^{2\pi} \frac{d\theta_i}{2\pi}\right) \sum_{m_{ij}=-\infty\cdots\infty} \exp\left[-\frac{2}{K}\sum_{\langle ij\rangle} \left(\theta_i-\theta_j+2\pi m_{ij}\right)^2\right]$$

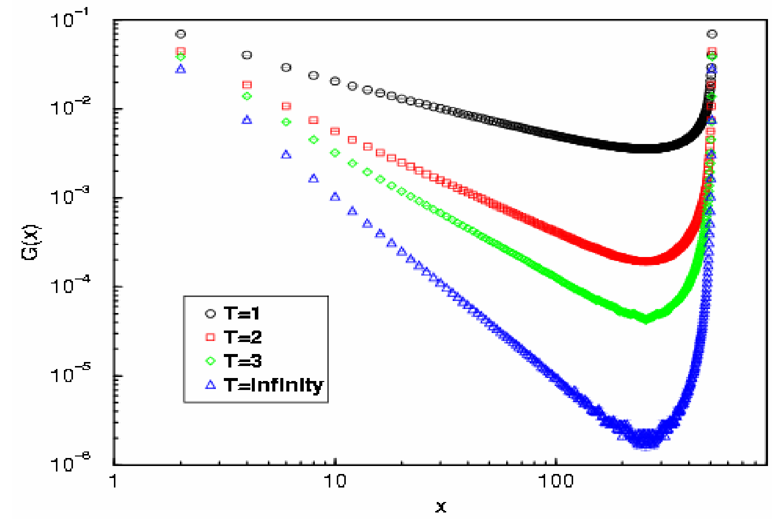
= XY model (with Villain potential) at temperature T ~ K

Appendix 3: 2D dimer model (compared with 3D)

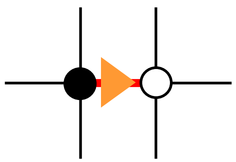
Alet *et al.*, PRL 2005

- Analogous phase diagram





- As in 3D :



$$\mathrm{div}\,\vec{B}(r) = (-1)^{x+y}$$

$$\approx 0 \text{ when coarse grained}$$

$$\Rightarrow \vec{B} \approx \vec{\nabla} \times \vec{A}$$

- But the vector potential is in fact just a (one-component) height field

$$\vec{A} = \begin{bmatrix} 0 \\ 0 \\ h(r) \end{bmatrix}$$

Sine-Gordon model

$$S = \int d^2 r\, g\pi \left|\nabla h(r)\right|^2 + V\cos(8\pi h(r))$$