The fully frustrated XY-model in 2 dimensions

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Summary

M. Hasenbusch, A. Pelissetto, and E. Vicari:

Transitions and Crossover Phenomena in Fully Frustrated XY Systems, cond-mat/0506345, Phys. Rev. B 72 (2005) 184502
Critical behavior of two-dimensional fully frustrated XY systems, cond-mat/0509511, Conference "Counting Complexity"
Multicritical behavior in the fully frustrated XY model and related systems, cond-mat/0509682, J.Stat.Mech. 0512 (2005) P002

- Definition of the model and the observables
- Phase structure?
- Numerical results
- The Monte Carlo algorithm
- Universality, Multi-critical behaviour?

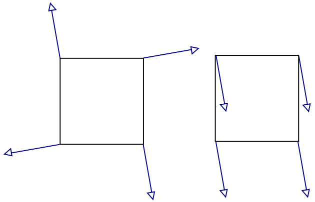
The Hamiltonian of the 2 d fully frustrated XY (FFXY) model:

$$\mathcal{H}_{\mathrm{FFXY}} = -J \sum_{\langle xy \rangle} \cos(\theta_x - \theta_y + A_{xy})$$

where $J > 0$; the angle θ_x is defined on the sites of a regular 2-d lattice. $\langle xy \rangle$ denotes a pair of nearest neighbours on the lattice. The constants A_{xy} satisfy $\sum A_{xy} = \pi$ along a plaquette. The FFXY model is relevant for Josephson-junction arrays in a magnetic field. It should describe the superconduction-to-normal transition at half a flux quantum per plaquette.

Symmetry: $O(2) \times Z_2$

$A = \pi/4$



Possible transitions:

- 2^{nd} order transition, Ising universality class:
  $\xi \propto t^{-\nu}$; $\nu = 1$, $\gamma = 7/4$, $\beta = 1/8$, $\eta = 1/4$

  and Kosterlitz-Thouless
  $\xi \propto \exp(at^{-\nu})$

  at distinct temperatures $T_{KT} \neq T_{c,Ising}$.

- Only one transition; new universality class

year	model	method	transitions	chiral exponents
1983	$\mathrm{FFXY_{sq}}$	MC ($L \leq 32$)		$\approx$ Ising
1984	$\mathrm{FFXY_{tr}}$	MC ($L \leq 32$)	2tr	
1984	$\mathrm{FFXY_{sq}}$	MC ($L \leq 45$)	2tr ($\delta \simeq 0.02$)	
1985	$\mathrm{FFXY_{sq}}$		$\delta \geq 0$	
1985	$\mathrm{FFXY_{sq}}$, CG	RG	1tr	
1985	2cXY	RG	1tr	
1986	$\mathrm{FFXY_{tr}}$	MC ($L \leq 72$)	1-2tr ($\delta \lesssim 0.01$)	$\approx$ Ising
1986	$\mathrm{FFXY_{tr}}$	MC ($L \leq 72$)	1tr	
1986	$\mathrm{FFXY_{sq}}$	MC ($L \leq 100$)	1tr	
1986	2cXY	real-space RG	1tr	
1988	CG	MC ($L \leq 30$)	1tr	
1989	CG	MC ($L \leq 50$)	2tr ($\delta \simeq 0.03$)	
1989	CG	MC ($L \leq 48$)	1tr	
1990	$\mathrm{FFXY_{sq}}$	TM MC ($L \leq 12$)	1tr	$\nu \simeq 1$, $\eta = 0.40(2)$
1991	$\mathrm{FFXY_{sq}}$	MC ($L \leq 40$)	1tr	$\nu = 0.85(3)$, $\eta = 0.31(3)$
1991	$\mathrm{FFXY_{tr}}$	MC ($L \leq 40$)	1tr	$\nu = 0.83(4)$, $\eta = 0.28(4)$
1991	$\mathrm{FFXY_{sq}}$	MC ($L \leq 128$)	1-2tr	$\nu = 1.009(26)$
1991	IsXY ($C = -0.2885$)	MC ($L \leq 32$)	1-2tr	$\nu = 0.84(3)$
1991	FXY_{J_1,J_2}	MC ($L \leq 150$)	1tr	$\nu = 0.9(2)$, $\eta = 0.4(1)$
1992	19-vertex-Is	TM ($L \leq 7$)	1tr	$\nu = 1.0(1)$, $\eta = 0.26(1)$
1992	$\mathrm{FFXY_{sq}}$	MC ($L \leq 240$)	1-2tr ($\delta \gtrsim -0.07$)	$\nu = 0.875(35)$
1992	QLJJ ($E_x/E_y = 1$)	TM QMC		$\nu = 0.81(4)$, $\eta = 0.47(4)$
1992	QLJJ ($E_x/E_y = 3$)	TM QMC		$\nu = 1.05(6)$, $\eta = 0.27(3)$
1993	$\mathrm{FFXY_{sq}}$	TM MC ($L \leq 14$)	1tr	$\nu = 0.80(5)$, $\eta = 0.38(2)$
1994	CG	MC ($L \leq 30$)	2tr ($\delta \simeq 0.04$)	$\nu = 0.84(3)$, $\eta = 0.26(4)$
1994	$\mathrm{FFXY_{sq}}$	MC ($L \leq 48$)	2tr ($\delta \simeq 0.03$)	$\nu = 0.813(5)$, $\beta = 0.089(8)$
1994	19-vertex model	TM ($L \leq 15$)	1tr	$\nu = 0.81(3)$, $\eta = 0.28(2)$
1995	$\mathrm{FFXY_{sq}}$	MC ($L \leq 128$)	2tr ($\delta \simeq 0.013$)	consistent with Ising
1995	IsXY ($C = -0.2885$)	TM MC ($L \leq 30$)	1tr	$\nu = 0.79$, $\eta = 0.40$

1996	$FFXY_{\rm sq}$	MC ($L \leq 128$)		$\nu = 0.898(3)$
1996	$FFXY_{\rm tr}$	MC ($L \leq 144$)	2tr ($\delta \simeq 0.02$)	$\gamma = 1.6(3)$, $\beta = 0.11(3)$
1997	Villain $FFXY_{\rm sq}$	MC ($L \leq 256$)	2tr ($\delta \simeq 0.014$)	$\approx$ Ising
1997	Villain $FFXY_{\rm sq}$	spin waves, LT phase	1tr	
1997	$FXY_{\rm zz}$ ($\rho = 0.7$)	MC ($L \leq 36$)	1tr	$\nu = 0.78(2)$, $\eta = 0.32(4)$
1997	$FXY_{\rm zz}$ ($\rho = 1.5$)	MC ($L \leq 36$)	1tr	$\nu = 0.80(1)$, $\eta = 0.29(2)$
1997	FFXY, 2cXY, CG	position-space RG	2tr ($\delta \simeq 0.0005$)	no Ising
1997	SOS-Is	MC ($L \leq 22$)	2tr	$\approx$ Ising
1997	FXY_{J_1,J_2}, CG	RG	1tr	
1998	$FFXY_{\rm sq}$	$NER_{\rm std}$ MC ($L \leq 256$)		$\nu = 0.81(2)$, $\eta = 0.261(5)$
1998	$FFXY_{\rm tr}$	MC ($L \leq 60$)	2tr ($\delta \simeq 0.012$)	$\nu = 0.833(7)$, $\eta = 0.25(2)$
1998	$FFXXZ_{\rm tr}$	MC ($L \leq 120$)	2tr ($\delta \lesssim 0.01$)	consistent with Ising
1998	$FFXY_{\rm sq}$	MC ($L \leq 140$)	1tr	$\nu = 0.852(2)$, $\eta = 0.203(6)$
2000	FXY_{J_1,J_2}	MC ($L \leq 150$)	2tr ($\delta \simeq 0.003$)	$\nu = 0.795(20)$, $\eta = 0.25(1)$
2000	FXY_{nn+nnn}	MC ($L \leq 72$)	2tr ($\delta \lesssim 0.01$)	$\nu = 1.0(1)$
2001	$FFXY_{\rm sq}$	$NER_{\rm std}$ MC ($L \leq 256$)		$\nu = 0.80(2)$, $\eta = 0.276(7)$
2001	FXY_{nn+nnn}	$NER_{\rm std}$ MC ($L \leq 256$)		$\nu = 0.80(3)$, $\eta = 0.282(8)$
2002	FA6SC	MC ($L \leq 192$)	2tr, $\delta \simeq 0.003$	$\approx$ Ising
2002	FFXY		2tr, $\delta > 0$	
2003	LGW ϕ^4	five-loop FT	stable FP	
2003	$FFXY_{\rm sq}$	NER MC ($L \leq 2000$)	2tr ($\delta \simeq 0.010$)	$\nu = 0.82(2)$, $\eta = 0.272(15)$
2003	$FFXY_{\rm tr}$	NER MC ($L \leq 2000$)	2tr ($\delta \simeq 0.008$)	$\nu = 0.84(2)$, $\eta = 0.250(10)$
2005	$FFXY_{\rm sq}$	ED MC ($L \leq 180$)	1tr	$\nu = 0.9(1)$
2005	$FFXY_{\rm sq}$	MC ($L \leq 128$)	2tr, $\delta > 0$	

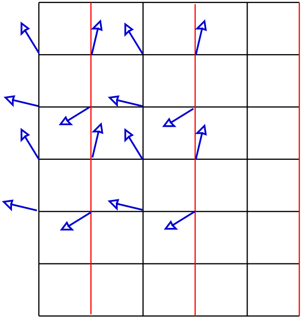
The FFXY model

Square lattice of the size L^2 , periodic boundary conditions, lattice spacing $a = 1$

$$\mathcal{H}_{\mathrm{FFXY}} = -\sum_{\langle xy \rangle} j_{xy}\, \vec{s}_x \cdot \vec{s}_y$$

Spin $\vec{s}_x$ with two real components, $\vec{s}_x \cdot \vec{s}_x = 1$

$j_{xy} = 1$ for links $\langle xy \rangle$ in 1-direction, $j_{xy} = 1$ and $j_{xy} = -1$ for links in 2-direction, in 1-direction alternating

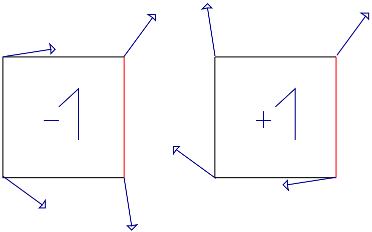


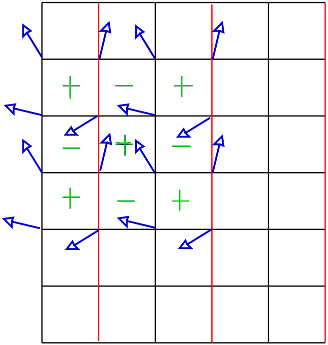
Boltzmann-factor: $\exp(-\beta \mathcal{H}_{\mathrm{FFXY}})$

Chirality

$$\chi_n = \mathrm{sign}\left[\sum_{\langle xy\rangle\in\Pi_n} \sin(\theta_x - \theta_y + A_{xy})\right] = \mathrm{sign}\left[\sum_{\langle xy\rangle\in\Pi_n} j_{xy}\sin(\theta_x - \theta_y)\right]$$

where Π_n is a plaquette and n the site of the dual lattice in the centre of this plaquette.





Staggered magnetisation:

$$\mu_c = \frac{1}{L^2} \sum_n (-1)^{(n_1+n_2)} \chi_n$$

correlation function:

$$G(m-n)_c = (-1)^{(m_1+m_2+n_1+n_2)} \chi_n \chi_m$$

Spin-Quantities

The ground state is invariant under shifts by $k(2,0) + l(0,2)$ where k, l are integer.
Therefore we define the spin-magnetisation as

$$\mu_s = \frac{4}{L^2} \sum_{x=(2k,2l)} \vec{s}_x$$

The spin-correlation function

$$G_s(x) \equiv \langle \vec{s}_0 \cdot \vec{s}_x \rangle$$

only for $x = (2k, 2l)$

Dimensionless Quantities

The susceptibility χ and the (second moment) correlation length ξ:

$$\chi \equiv \sum_x G(x) \qquad \xi^2 \equiv \frac{1}{4\sin^2(q_{\min}/2)} \frac{\widetilde{G}(0) - \widetilde{G}(q)}{\widetilde{G}(q)}$$

where $\widetilde{G}(q)$ The Fourier transform of the two-point function is $G(x)$, with $q = (q_{\min}, 0, 0)$ and $q_{\min} \equiv 2\pi/L$

We consider RG-invariant ratios (correlation length over the linear lattice size, Binder cumulant)

$$R \equiv \frac{\xi}{L} \qquad B = \frac{\langle (\mu^2)^2 \rangle}{\langle \mu^2 \rangle^2}$$

Helicity modulus

Consider neighbours (x, y) with $x_1 = L$, $y_1 = 1$ and $x_2 = y_2$. In the Hamiltonian, replace the term $\vec{s}_x \cdot \vec{s}_y$ by

$$\vec{s}_x \cdot R_\varphi \vec{s}_y = s_x^{(1)} \left(s_y^{(1)} \cos\varphi + s_y^{(2)} \sin\varphi \right) + s_x^{(2)} \left(s_y^{(2)} \cos\varphi - s_x^{(1)} \sin\varphi \right)$$

R_φ is a rotation by the angle φ. The helicity modulus is defined as:

$$\Upsilon \equiv - \left. \frac{\partial^2 \ln Z(\varphi)}{\partial \varphi^2} \right|_{\varphi=0}$$

Estimate of the transition temperature:
Binder crossing method.
At the transition, in the limit $L \to \infty$ RG-invariant quantities take a universal value.
For the Ising model on the L^2 lattice with periodic boundary conditions: (Salas und Sokal 2000)

$$\begin{aligned} \xi_{2nd}/L &= 0.9050488292(4) \\ U &= 1.167923(5) \end{aligned}$$

critical exponent of the correlation length:

$$\left.\frac{\partial R}{\partial \beta}\right|_{\beta_c} \propto L^{1/\nu} \; (1 + cL^{-\omega} ...)$$

Strategy to determine the nature of the transition

Finite size scaling (FSS) method:

We keep $\xi_{2nd,c}/L = 0.9050488292$ fixed.

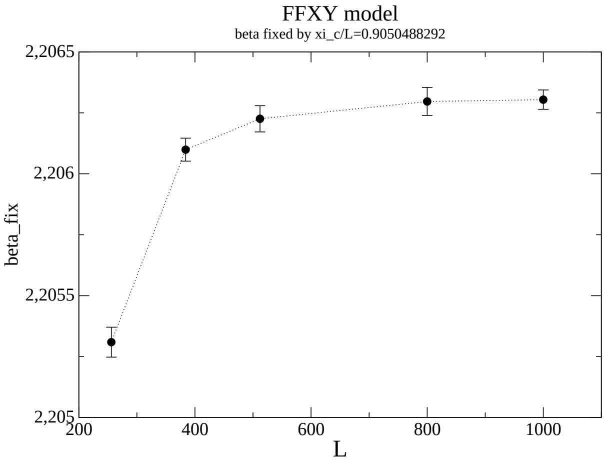
I.e. all quantities are evaluated for the vcalue of β, where $\xi_{2nd,c}/L$ takes the value 0.9050488292.
In practice: Simulation at $\beta \approx \beta_c$, then reweighting, (Swendsen Ferrenberg).

$\lim_{L\to\infty} \xi_{2nd,s}/L$ finite $\Rightarrow$ New universality class

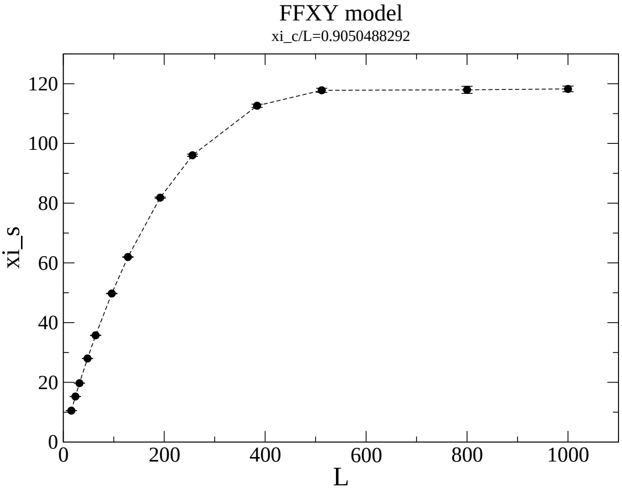
$\lim_{L\to\infty} \xi_{2nd,s}$ finite $\Rightarrow$ Two separate transitions
Ising-Universality: $\lim_{L\to\infty} B_c = 1.167923$, $\lim_{L\to\infty} \nu_{eff} = 1$
Fit $\partial R/\partial\beta = aL^{1/\nu_{eff}}$ for lattices between L and $2L$

Critical temperature

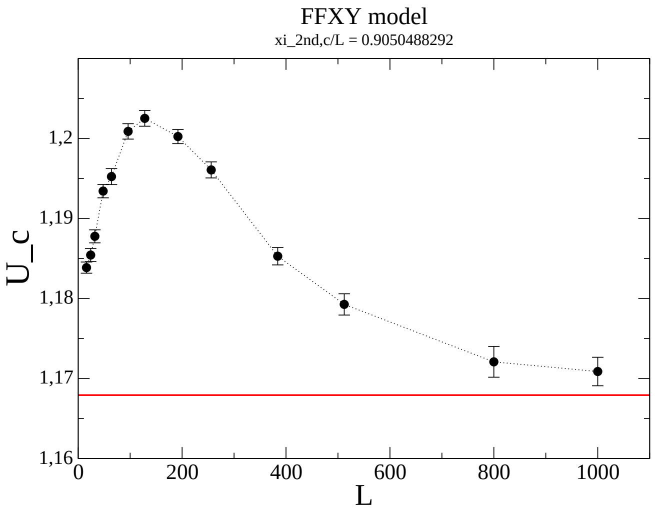
$\beta_c = 2.0632(5)$



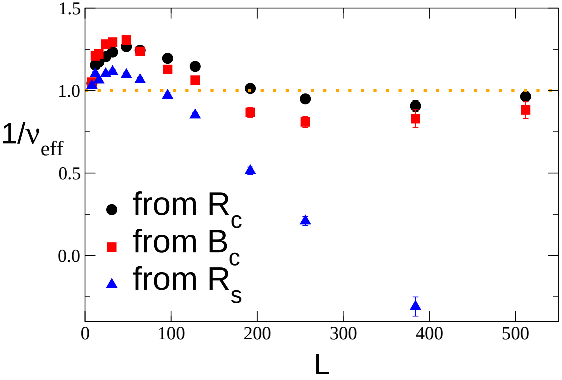
Spin-correlation length



Chiral Binder cumulant



Effective exponent of the correlation length



Kosterlitz-Thouless transition

On the squared L^2 lattice with periodic boundary conditions at the KT-transition:

$$\Upsilon = 0.63650817819... + \frac{0.318899454...}{\ln L + C_\Upsilon} + ...,$$
$$R = 0.7506912... + \frac{0.212430...}{\ln L + C_R} + \; ...,$$

where C_R and C_Υ are non-universal.
corrections: $\ln \ln L / \ln^2 L$.

We simulate at $\beta = 2.24$, 2.242.
Υ and R_s as function of β by linear interpolation.

Estimates for β_{KT}:

L_1	L_2	using R_s	using Υ
128	256	2.236(5)	2.2405(12)
256	512	2.2400(10)	2.2415(5)
512	1024	2.2409(3)	2.2415(5)

$\beta_{KT} = 2.2415(5)$

$\delta = (\beta_c - \beta_{KT})/\beta_c = 0.0159(2)$

" Critical slowing down"

At the critical temperature, the autocorrelation time increases as

$$\tau \propto L^z$$

with the lattice size. I.e. the effort grows as L^{d+z}

For the Ising or the standard-XY model:

algorithm	z
local Metropolis	≈ 2
overrelaxation	≈ 1
cluster	≈ 0

local updates

Metropolis algorithm:

- proposal $\vec{s}_x'$ for one site x $P(\vec{s}_x \to \vec{s}_x') = P(\vec{s}_x' \to \vec{s}_x)$
- $\vec{s}_x'$ is accepted with the propability
  $A = \min[\exp(-\beta(\mathcal{H}' - \mathcal{H})), 1]$ else $\vec{s}_x$ stays.

Demons $d_x \in [0, \infty)$ with a distribution $\propto \exp(-\sum_x d_x)$ are introduced as auxilliary fields. This way the acceptance step can be replaced by:

If $d_x' = d_x - \beta(\mathcal{H}' - \mathcal{H}) \geq 0$ then $\vec{s}_x$ and d_x are replaced by $\vec{s}_x'$ and d_x', else the old values are kept. (M. Creutz)

☺ No random number, no $\exp()$ ☹ Not ergodic

Heatbath for the demons: $d_x = -\ln(z_x)$, where z_x is uniformly distributed in $(0,1]$

Proposal for the Metropolis or demon algorithm:

- $\vec{s}_x{}' = R(\alpha)\vec{s}_x$, where α is uniformly distributed in $[-s,s]$.

Heatbath for the demons: $d_x = -\ln(z_x)$, where z_x is uniformly distributed in $(0, 1]$

Proposal for the Metropolis or demon algorithm:

- $\vec{s}_x{}' = R(\alpha)\vec{s}_x$, where α is uniformly distributed in $[-s, s]$.
- Metropolis reflection (MR) (Grosse Pawig, Pinn)

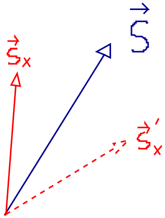
$$\vec{s}_x' = 2(\vec{r} \cdot \vec{s}_x)\vec{r} - \vec{s}_x$$

For all sites the same: $\vec{r} = (\cos(\alpha), \sin(\alpha))$,

☺ No random number, no cos(),sin()
At the chiral transition: Acceptance 25%

microcanonical overrelaxation (OR):

$$\vec{s}_x{}' = \frac{2\vec{s}_x \cdot \vec{S}}{S^2}\vec{S} - \vec{s}_x$$



where $\vec{S} = \sum_{y.nn.x} j_{xy} \vec{s}_y$

☺ No random number, no exp() ☹ Not ergodic

For the standard XY model, using the optimal ratio of Metropolis and OR sweeps the dynamical critical exponent is $z \approx 1.2$ (Gupta et. al 1988).

complete cycle

- Heatbath of the demons
- $5 \times$ ([DMR+OV] sweep $+ \; n_{or} \times$ OR sweeps)

$n_{or} = 3$ at the chiral transition
$n_{or} \propto L$ for $\beta \geq \beta_{KT}$

Implementation

- Programming language C
- Random number generator: Ranlux (Lüscher 1994).
- Parallelisation with MPI (Message Passing Interface)
  The lattice is split along one direction
- For non-trivial loop-unrolling in the other direction: In the case of the OR-update, the for-loop runs from $x_1 = 0$ up to $x_1 = L/2 - 1$. Along with the update of (x_0, x_1) also $(x_0, x_1 + L_1/2)$ is done. Speed up of 30%

On a server with 4 1.8GHz Opteron CPUs a full update-cycle (with one heat-bath of the demons and 5 ((DMR + OR) + 3 OR) sweeps) 0.26s for a 1000^2 lattice. I.e. about 1 s on an Opteron with one core.

Autocorrelation times

Integrated autocorrelation times for the chiral susceptibility. The τ's are measured in units of local update cycles.

L	β	measurements	CPU-time/days	$\tau_{\chi,chiral}$
256	2.2053	22000	8	$500 \times 1.76(10)$
384	2.2062	56600	68	$700 \times 2.67(13)$
512	2.2063	39500	120	$1000 \times 3.31(18)$
800	2.2066	20500	304	$2000 \times 3.63(31)$
1000	2.2063	35700	826	$2000 \times 6.2(5)$

Fit: $\tau_{\chi,chiral} = 0.022(8) \times L^{1.91(6)}$ with $\chi^2/\text{d.o.f.} = 0.99$.

Futher Models

Ising-XY model

$$\mathcal{H}_{\mathrm{IsXY}} = -\sum_{\langle xy \rangle} \left[\frac{J}{2}(1+\sigma_x\sigma_y)\,\vec{s}_x\cdot\vec{s}_y + C\sigma_x\sigma_y \right]$$

where $\sigma_x \in -1, 1$, $\vec{s}_x$ is a unit vector with two real components.

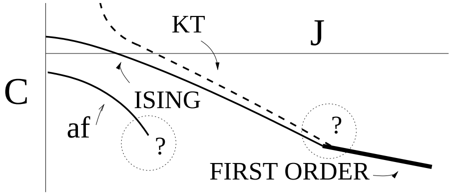
ϕ^4-model on the lattice.

$$\begin{aligned}\mathcal{H}_\phi &= -J\sum_{\langle xy \rangle, i} \vec{\phi}_{i,x}\cdot\vec{\phi}_{i,y} + \sum_{i,x}\left[\phi_{i,x}^2 + U(\phi_{i,x}^2-1)^2\right] \\ &\quad +2(U+D)\sum_x \phi_{1,x}^2\phi_{2,x}^2\end{aligned}$$

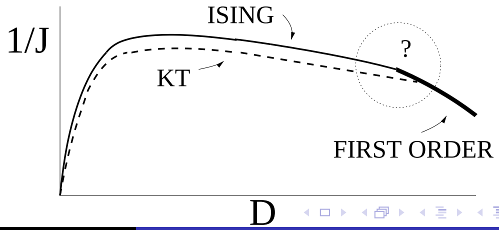
where $i=1,2$ and $\vec{\phi}_{i,x}$ have two real components.

Phase diagram

Ising-XY



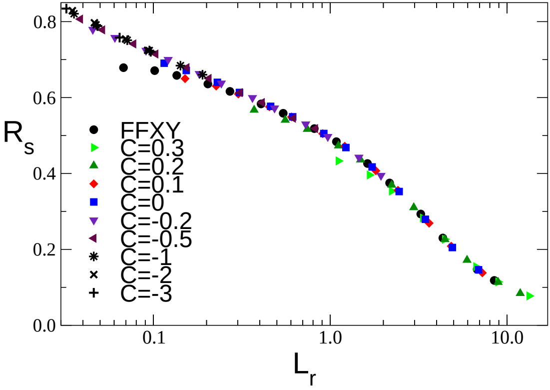
ϕ^4, $U = 1$

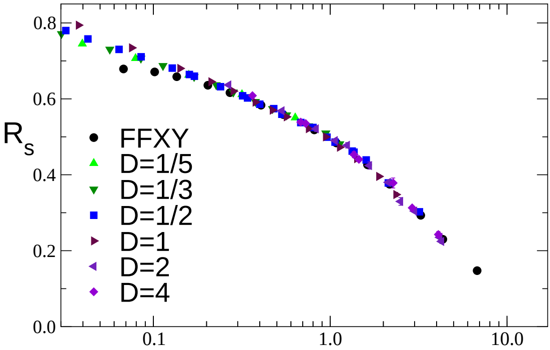


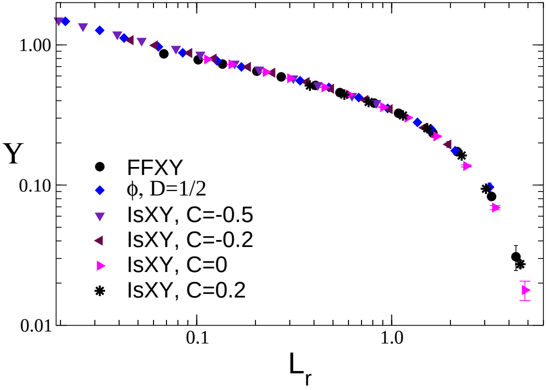
Universality of the FSS behaviour

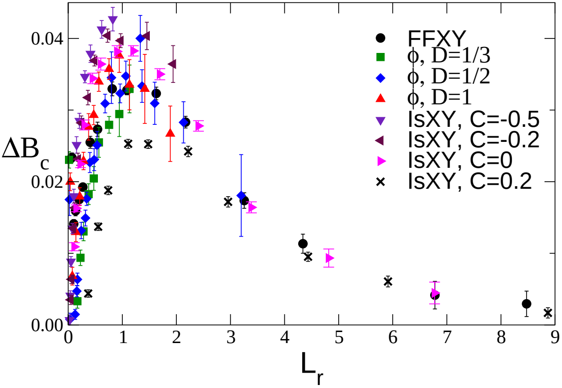
Rescaling of the lattice size, the FSS curves of various model fall on top of each other; in following plots:

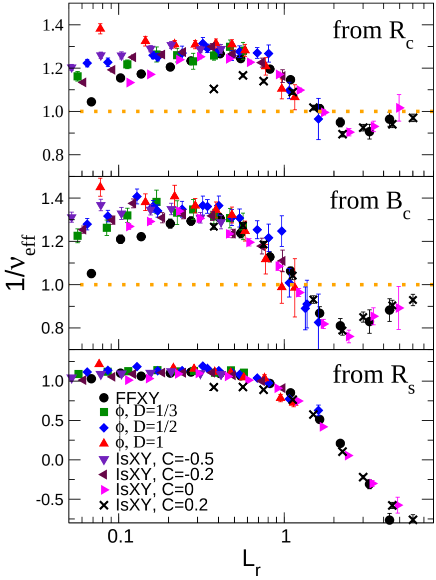
$$L_r = L/\xi_s^{(c)}$$


0.8
0.6
0.4
0.2
0.0
R_s
FFXY
C=0.3
C=0.2
C=0.1
C=0
C=-0.2
C=-0.5
C=-1
C=-2
C=-3
0.1
1.0
10.0
L_r


0.8
0.6
0.4
0.2
0.0
R_s
FFXY
D=1/5
D=1/3
D=1/2
D=1
D=2
D=4
0.1
1.0
10.0


Y
1.00
0.10
0.01
0.1
1.0
L_r
FFXY
ϕ, D=1/2
IsXY, C=-0.5
IsXY, C=-0.2
IsXY, C=0
IsXY, C=0.2


FFXY
ϕ, D=1/3
ϕ, D=1/2
ϕ, D=1
IsXY, C=-0.5
IsXY, C=-0.2
IsXY, C=0
IsXY, C=0.2
ΔB_c
L_r
0.00
0.02
0.04
0
1
2
3
4
5
6
7
8
9


from R_c
from B_c
from R_s
1.4
1.2
1.0
0.8
0.5
0.0
-0.5
1/ν_eff
FFXY
φ, D=1/3
φ, D=1/2
φ, D=1
IsXY, C=-0.5
IsXY, C=-0.2
IsXY, C=0
IsXY, C=0.2
0.1
1
L_r

Summary

- The FFXY model undergoes two separate transitions. The transition temperatures are close to each other. At the higher transition temperature there is a second order transition with a breaking of the Z_2 symmetry, this transtition belongs to the Ising universality class. At the lower transition temperature there is a KT-transition of the continuous degrees of freedom.
- The spin correlation length at the chiral transition is large: $\xi_s \approx 118$. Hence lattice sizes of $L \approx 1000$ are needed, to identify the natur of the transitions.
- Other models with the same symmetries show a similar FSS-behaviour. Multi-critical behaviour?