Critical scaling of quantum systems at phase transitions

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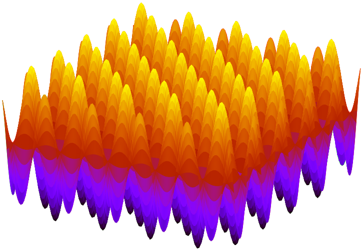
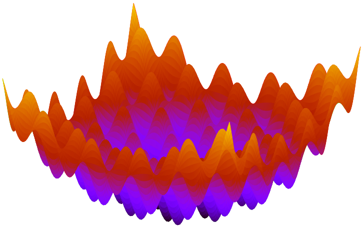
The problem



What we would like condensed matter systems to look like...



...and what they really look like.

Phase transitions

At the change of a parameter, the equilibrium state of some systems qualitatively change.

- Hamiltonian of a many-body system:

$$H(g).$$

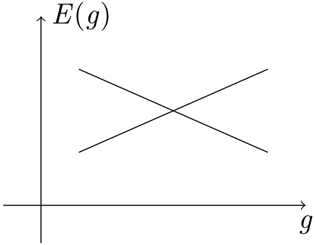
- Free energy density:

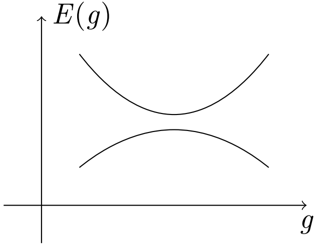
$$f[H] \equiv \frac{1}{V}\mathcal{F}[H] = -\frac{1}{\beta}\ln \mathrm{Tr}\, e^{-\beta H}$$

- At **infinite volume**, for some value of g or β, f becomes non-analytic $\Longrightarrow$ **critical point**.
- **No transition** at finite volume!

Quantum phase transitions

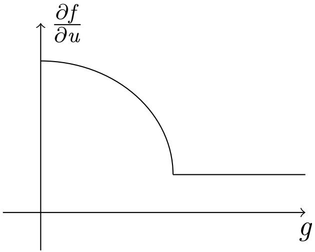
$T = 0$ transitions of quantum systems.

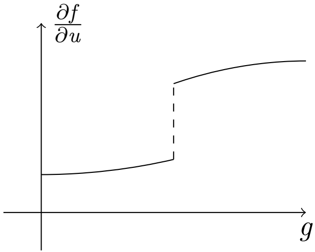




- Change of the properties of the ground state.
- Closing of the energy gap $\Delta(g_c) \Longrightarrow$ **quantum critical point**.
- Infinite volume: **level crossing**.
- Finite volume: **avoided** level crossing.

Order of phase transitions





Continuous

- Ground state properties change **continuously**.
- **Diverging** correlation length $\xi \sim |g - g_c|^{-\nu}$.
- Closing of the gap as $\Delta \sim |g - g_c|^{z\nu} \sim \xi^{-z}$.

Discontinuous or first order

- First order derivatives of $f(g)$ are **discontinuous**.
- **Finite** correlation length at the transition.
- **Phase coexistence.**
- **Sensitivity** to boundary conditions.

How is
the critical behaviour
modified in finite systems?

Finite-size scaling (FSS) at continuous transitions

At the thermodynamic limit, **critical scaling**.
After a blocking transformation by a factor b:

$$\mathcal{F}_{\rm sing}(u_1, u_2, \ldots) = b^{-d}\mathcal{F}_{\rm sing}(b^{y_1}u_1, b^{y_2}u_2, \ldots)$$

Scaling dimensions:
$y_{1,2} > 0$ (relevant perturbations);
$y_{i>2} \leq 0$ (irrelevant).

For **homogeneous finite systems** of size L, $u_L \sim L^{-1}$ is a new relevant variable:

$$\mathcal{F}_{\rm sing}(u_1, u_2, \ldots, u_L) = b^{-d}\mathcal{F}_{\rm sing}(b^{y_1}u_1, b^{y_2}u_2, \ldots, bu_L)$$

$$\mathcal{F}_{\rm sing}(u_1, u_2) = L^{-d}\mathcal{F}_{\rm sing}(L^{y_1}u_1, L^{y_2}u_2) + \text{corrections}$$

FSS at continuous transitions: results

Quantum Monte Carlo studies of the finite temperature superfluid-Mott insulator transitions of

- $2d$ Bose-Hubbard model.

  [G.Ceccarelli, JN, A.Pelissetto and E.Vicari, Phys. Rev. B **88**, 024517 (2013)]

- $3d$ Bose-Hubbard model.

  [G.Ceccarelli and JN, Phys. Rev. B **89**, 054504 (2014)]

What happens at **first order** transitions?

FSS at first order transitions?

- No diverging correlation length, but coexistence of **large domains** in the same phase $\Longrightarrow$ effective ξ.
- **Sensitivity to boundary conditions!**

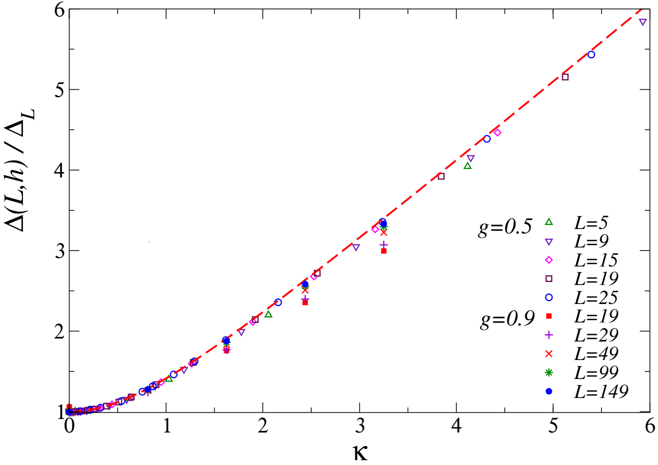
Scaling variable

$$\kappa(L) = \frac{\text{perturbation energy}}{\text{natural energy scale}} = \frac{E_P(L)}{\Delta(L, g_c)}$$

The behaviour of $\Delta(L, g_c)$ may strongly depend on boundary conditions.

FSS at first order transitions: results

Ferromagnetic Ising chain in transverse and parallel field.



[M.Campostrini, JN, A.Pelissetto and E.Vicari, Phys. Rev. Lett. **113**, 070402 (2014)]

FSS at first order transitions

Quantum Potts model

$$H_{\text{Potts}} = -\sum_{i=1}^{L-1}\sum_{k=1}^{q-1}\Omega_i^k\Omega_{i+1}^{q-k} - g\sum_{i=1}^{L}\sum_{k=1}^{q-1}M_i^k$$

$$\Omega = \begin{pmatrix} 1 & & & \\ & \omega & & \\ & & \ddots & \\ & & & \omega^{q-1} \end{pmatrix} \quad M = \begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & & 1 \\ 1 & & & 0 \end{pmatrix} \quad \omega = e^{2i\pi/q}$$

Ferro-para FOQT at $g_c = 1$ for any $q > 4$.

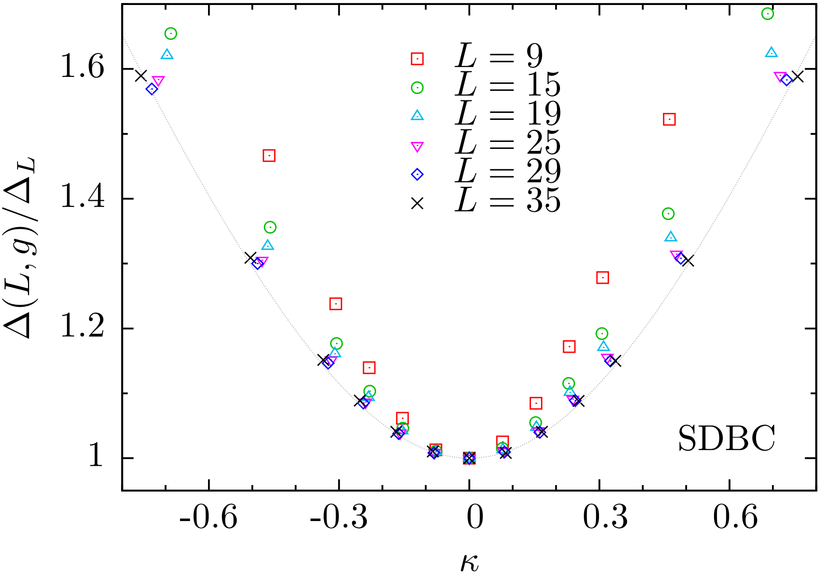
$\Delta \sim \Delta_\infty + cL^{-1}$ for open boundaries.

$\Delta \sim L^{-1}$ for **self-dual** boundaries.

Scaling ansätze

$$\begin{cases} \Delta(L,g) = \Delta(L,g_c)f_\Delta(\kappa), \\ m(L,g) = m_0 f_m(\kappa), \end{cases} \qquad \kappa = \frac{(g-1)L}{\Delta(L,g_c)}.$$

FSS at first order transitions



How does inhomogeneities **change** this?

What's different with inhomogeneities?

External potential U coupled to the system,

$$U(\mathbf{x}) = J \left(\frac{|\mathbf{x}|}{\ell} \right)^p ,$$

with $\ell \equiv$ **trap size**.

- Trap shallow close to the centre:
  As long as $\xi \ll \ell^\theta$, approximately homogeneous.
- For $\xi \gtrsim \ell^\theta$, distortion of universal scaling.

Trap-size scaling at continuous transitions

- Inspired by FSS. $U(\mathbf{x})$ yields a new **relevant field** u_v.
- Must relate the correlation length to the trap size:

$$\xi \sim \ell^{\theta}, \qquad \theta = y_v^{-1} \equiv \textbf{trap exponent} < 1.$$

- Must reduce to FSS in the physical limits.

The TSS limit

$$\begin{cases} |\mathbf{x}| \equiv r \to \infty, \\ \ell \to \infty \end{cases} \qquad \zeta \equiv r\ell^{-\theta} = \text{const.}$$

The modified critical behaviour should appear when $r\ell^{-\theta} \approx 1$.

Trap-size scaling at continuous transitions

The exponent θ

By field theoretical means,

$$\theta = \frac{p}{d - y_\Phi + p}.$$

(y_Φ the scaling dimension of the field to which $U(\mathbf{x})$ couples)

Scaling ansatz

$$\mathcal{F}_{\rm sing}(u_1, u_2, u_v, \mathbf{x}) = b^{-d} \mathcal{F}_{\rm sing}(b^{y_1} u_1, b^{y_2} u_2, b^{y_v} u_v, \mathbf{x}/b)$$

Fixing $u_v b^{y_v} = 1$,

$$\mathcal{F}_{\rm sing}(u_1, u_2, \mathbf{x}) = \ell^{-d\theta} \mathcal{F}_{\rm sing}(\ell^{y_1\theta} u_1, \ell^{y_2\theta} u_2, r\ell^{-\theta})$$

[Campostrini, Vicari, Phys.Rev.Lett. **102**, 240601 (2009)]

Trap-size scaling at first order transitions

- **Proceed in analogy** with the continuous case.
- First order transitions are characterised by **extremal** effective critical exponents.

  [B.Nienhuis and M.Nauenberg, Phys. Rev. Lett. **35**, 477 (1975)]

θ exponent

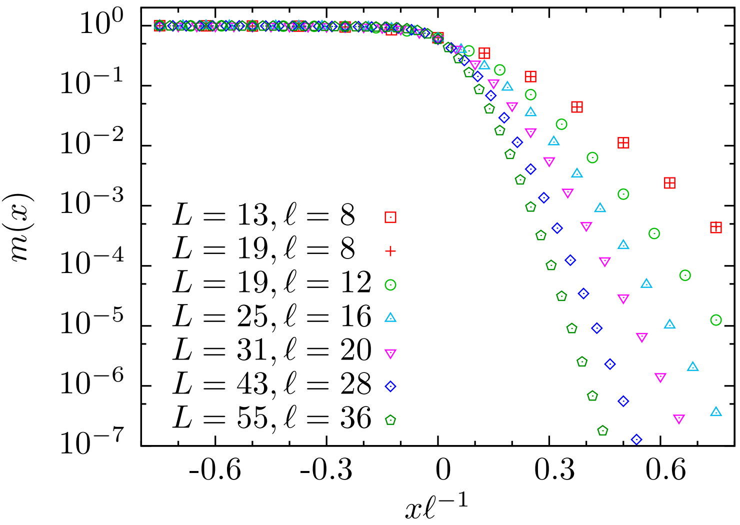
- Conjecture

$$\theta = \frac{p}{y_g + p},$$

  with $y_g = D \equiv d + z$. (z the dynamic critical exponent).
- Verify a posteriori.

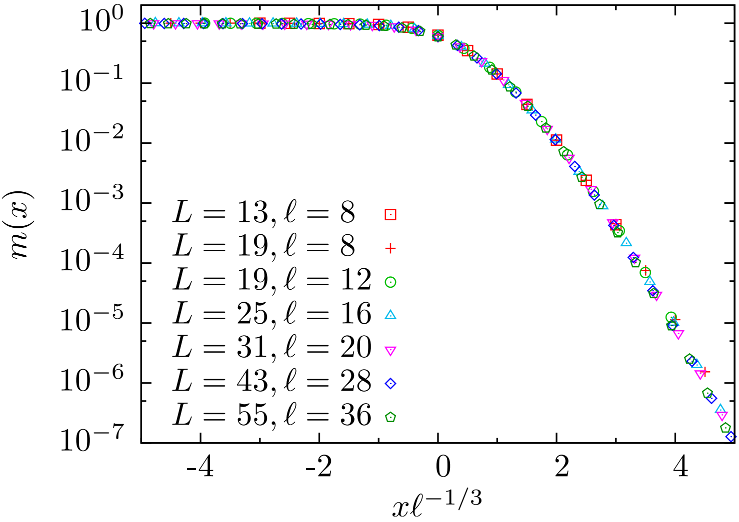
Trap-size scaling at first order transitions

Quantum Potts, $p = 1$, $z = 1$.



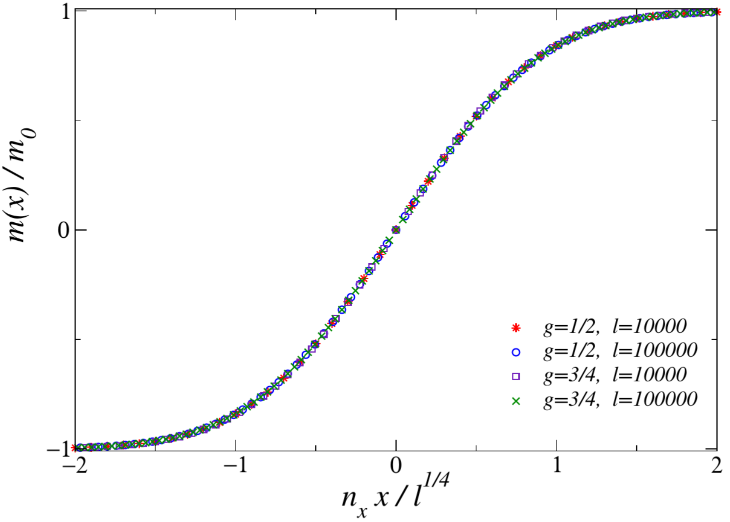
Trap-size scaling at first order transitions

Quantum Potts, $p = 1$, $z = 1$.



Trap-size scaling at first order transitions

Ferromagnetic Ising chain, $p = 1$, $z = 2$.



Conclusions

- Critical phenomena in **realistic conditions** can be described by FSS and TSS.
- FSS and TSS can be applied to quantum transitions.
- ...and in particular to quantum first order transitions.

Future developments

- The low energy spectrum of the quantum Potts model may deserve a closer look.
- Bosonic mixtures present a rich phase diagrams for further tests of FSS and TSS.

Thanks.

Q&A?

Slides will be made available on `www.pi.infn.it/~jnespolo/physics`

FSS - Corrections from irrelevant perturbations

- Irrelevant operators cause corrections to FSS.
- Let $\omega = -y_3 =$ scaling dimension of first irrelevant perturbation.

At the transition ($u_1 = 0$),

$$\mathcal{F}_{\text{sing}}(u_2) = L^{-d/y_1}\left[f(u_2 L^{-y_2/y_1}) + L^{-\omega} f_\omega(u_2 L^{-y_2/y_1})\right] + \text{corr.}$$

Universality

- f is a **universal** function; one for each RG invariant observable.

$$\mathcal{O} = L^{y_\mathcal{O}/y_1} f_\mathcal{O}(u_2, L).$$

FSS at first order transitions

Ferromagnetic Ising chain in transverse field ($g < 1$).

$$H_{\rm Ising} = -\sum_i \sigma_i^x \sigma_{i+1}^x - h \sum_i \sigma_i^z - g \sum_i \sigma_i^x.$$

First order quantum transition (FOQT) at $g_c = 0$ for any $h < 1$.
$m(i) = \langle \sigma_i^x \rangle$ jumps from $+m_0$ to $-m_0$ across the transition.

$\Delta \sim h^L$ with open boundaries;
$\Delta \sim L^{-2}$ with fixed-opposite (kink) boundaries.

Scaling ansätze

$$\begin{cases} \Delta(L, g) = \Delta(L, g_c) f_\Delta(\kappa), \\ m(L, g) = m_0 f_m(\kappa), \end{cases} \qquad \kappa = \frac{gL}{\Delta(L, g = 0)}.$$

[M.Campostrini, JN, A.Pelissetto and E.Vicari, Phys. Rev. Lett. **113**, 070402 (2014)]

TSS: The exponent θ at continuous transitions

Suppose that $U(x) = v^p|\mathbf{x}|^p$
couples to $\Phi(\mathbf{x})$, of scaling dimension y_Φ.

$$P_U = \int d^dx \; v^p|\mathbf{x}|^p\Phi(\mathbf{x}) \quad \Rightarrow \quad p(y_v - 1) + y_\Phi = d$$

$$\theta \equiv y_v^{-1} = \frac{p}{d - y_\Phi + p}$$

Scaling ansatz

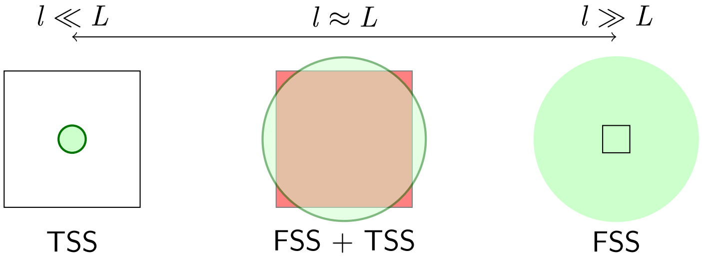
$$\mathcal{F}_{\rm sing}(u_1, u_2, u_v, \mathbf{x}) = b^{-d}\mathcal{F}_{\rm sing}(b^{y_1}u_1, b^{y_2}u_2, b^{y_v}u_v, \mathbf{x}/b)$$

Fixing $u_v b^{y_v} = 1$,

$$\mathcal{F}_{\rm sing}(u_1, u_2, \mathbf{x}) = \ell^{-d\theta}\mathcal{F}_{\rm sing}(\ell^{y_1\theta}u_1, \ell^{y_2\theta}u_2, r\ell^{-\theta})$$

[Campostrini, Vicari, Phys.Rev.Lett. **102**, 240601 (2009)]

TSS: What about traps in a finite box?



FSS + TSS

- Need to take both l and L into account.

$$\mathcal{F}_{\text{sing}}(u_1, u_2, u_v, L, r) = L^{-d}\mathcal{F}_{\text{sing}}(L^{y_1\theta}u_1, L^{y_2\theta}u_2, Ll^{-\theta}, rl^{-\theta}).$$

- Trap simulations always include a hard wall boundary.
- Often $l \ll L$ limit not accessible.

[de Queiroz, dos Santos, Stinchcombe, Phys.Rev.E **81**, 051122 (2010)]

Concluding remarks

- **No kitten** was used to make this presentation.
- This presentation **does not use** *Comic Sans MS*.