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Smeared phase transitions in binary $A_x B_{1-x}$ alloys

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Outline

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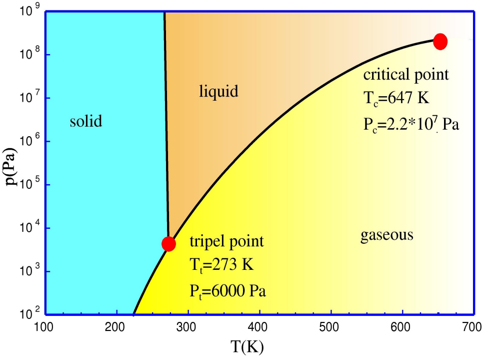
Outline

Introduction to phase transitions

Phase diagram for water



- Phase transitions− singularities in free energy, requires macroscopic system.
  They occur by changing control parameters

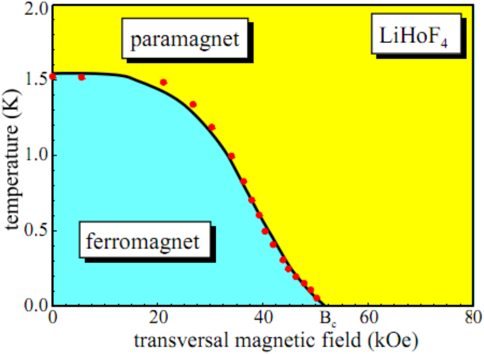
- 1st order phase transition: phase coexistence, latent heat, finite correlation length

- 2nd order phase transition: no phase coexistence, no latent heat
  correlation length diverges $\xi \sim |t|^{-\nu}$
  critical behavior of observables: $\Delta\rho \sim |t|^{\beta}$, $\kappa \sim |t|^{-\gamma}$

Universal critical exponents

Quantum phase transitions

- QPTs occur at absolute zero temperature by changing external parameter such as pressure, magnetic field and chemical composition
- They are driven by quantum rather then thermal fluctuations



Bitko and Rosenbaum (1996)

Transverse-field Ising model

$$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$

- transverse magnetic field induces spin flip via $\sigma^x = \sigma^+ + \sigma^-$
- transverse field destroys magnetic order

Quantum to classical mapping

Classical partition function: statics and dynamics decouple

$$Z = \int dp e^{-\beta H_{\rm kin}} \int dq e^{-\beta H_{\rm pot}} = Z_{\rm kin} Z_{\rm pot}$$

Quantum partition function: statics and dynamics coupled
(Trotter decomposition)

$$Z = Tr\ e^{-\beta \hat{H}} = Tr \lim_{N\to\infty} (e^{-\beta\hat{T}/N} e^{-\beta\hat{U}/N})^N = \int D[q(\tau)] e^{S[q(\tau)]}$$

imaginary time τ acts as additional dimension

At $T = 0$, the extension in this direction becomes infinite

quantum phase transition in d space dimensions is related to a classical transition in $d+1$ space dimensions

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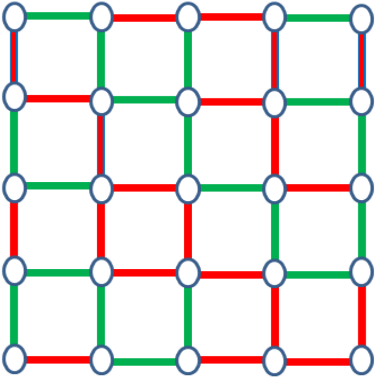
Disorder and phase transitions

Many materials often feature considerable amounts of quenched disorder

- weak disorder: bulk phases are not changed qualitatively in the presence of disorder
- disorder: spatial variation of coupling constant



Will phase transition remain sharp?

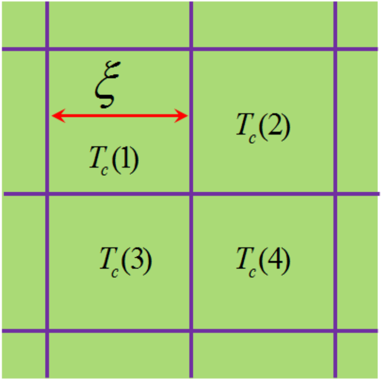
Will order of transition change?

Will critical behavior change?

Harris criterion for stability of clean critical point

Harris criterion:
fluctuations δT_c between regions must be smaller than global distance $t = T - T_c$ from criticality, $\delta T_c < t$

- fluctuations: $\delta T_c \sim \xi^{-d/2}$
- global distance: $t \sim \xi^{-1/\nu}$



Harris criterion:

$$\delta T_c < t \Longrightarrow d\nu > 2$$

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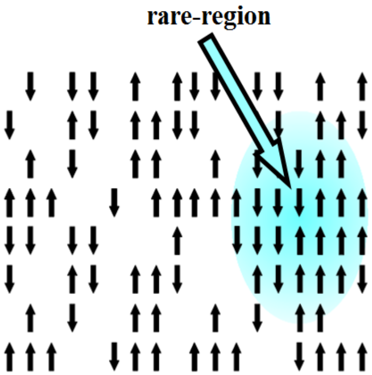
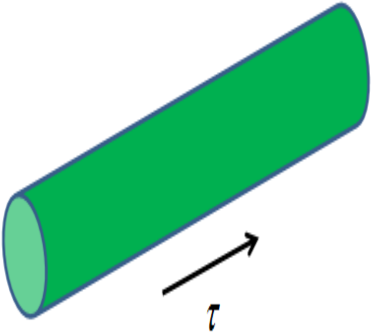
Rare regions

- dilution reduces critical temperature T_c form clean value T_c^0
- Griffiths: rare regions leads to singularities in free energy in $T_c < T < T_c^0$ range which is known as Griffiths phase
- at classical phase transitions rare regions are finite object



Rare regions at quantum phase transitions ($T = 0$)

- imaginary time acts as an additional dimension
- rare regions at QPT are finite in space but infinite in imaginary time



$\Longrightarrow$ Rare regions effects are enhanced at quantum phase transitions

- if interaction in time direction is short-ranged, rare regions do not develop static order, but fluctuate very slowly

transition is still sharp

Outline

Smeared phase transitions

Magnetic fluctuations are damped due to coupling to electrons

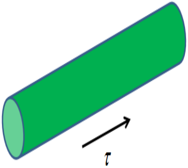
Example:

antiferromagnetic quantum phase transitions of itinerant electrons

Landau-Ginzburg-Wilson free energy functional

$$S = T \sum_{q,\omega_n} \phi(q,\omega_n)[r_0 + q^2 + |\omega_n|]\phi(-q,-\omega_n) + u \int d^d x d\tau \phi^4(x,\tau)$$

- in imaginary time: long-range power-law interaction $\sim 1/(\tau - \tau')^2$
- one-dimensional Ising model with $1/r^2$ interaction is known to have an ordered phase

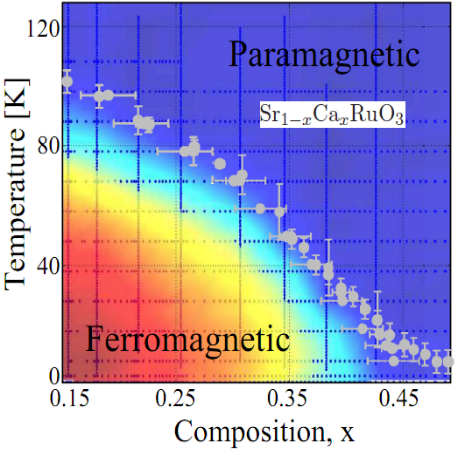


$\Longrightarrow$ in a system with overdamped dynamics and Ising symmetry, an isolated rare region can develop a static magnetization

quantum phase transition is smeared by disorder

Smeared phase transition in binary alloy

Example: smeared phase transition in $Sr_{1-x}Ca_xRuO_3$



$A_{1-x}B_x$ Binary alloy
consisting of two substances

- A magnetic atoms
  $r_A < 0$
- B non-magnetic atoms
  $r_B > 0$

Demkó et al., Phys. Rev. Lett. **108**, 185701 (2012)

Optimal fluctuation theory

$$r_{\rm av} = x r_{\rm B} + (1-x) r_{\rm A}$$

- Mean-field critical concentration for a binary alloy $x_c^0 \sim -r_A/(r_B - r_A)$

- Critical concentration for rare-region $x_c(L_{RR}) \sim x_c^0 - D L_{RR}^{-2}$

- Minimum size of rare-region $L_{\rm min} = (D/x_c^0)^{1/2}$

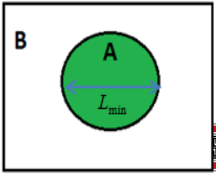
rare region of A atoms with size larger than $L_{\rm min}$ shows static magnetization

The probability of finding $N_{\rm B} = N x_{\rm loc}$ occupied by B atoms in region with total of $N \sim L_{\rm RR}^d$ sites (binomial distribution)

$$P(N, x_{\rm loc}) = \binom{N}{N_B} (1-x)^{N-N_B} x^{N_B}$$

Total ordered parameter

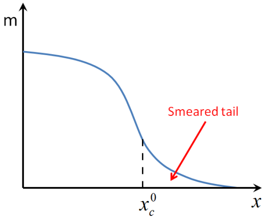
$$M \propto \int_{L_{\rm min}}^{\infty} dL_{RR} \int_0^{x_c(L_{RR})} dx_{loc} m(N, x_{\rm loc}) P(N, x_{\rm loc})$$



Observables in tail of smeared transition

- regime where $x \geq x_c^0$

$$M \propto \exp\left[-C\frac{(x-x_c^o)^{2-d/2}}{x(1-x)}\right]$$ Exponential decay



- the far tail of transition at $x \to 1$

$$M \propto (1-x)^{L^d_{\min}}$$ Power-law

$\Longrightarrow$ ordered phase is extended over the entire composition range $x < 1$

Transition is smeared

The composition dependence of the critical temperature

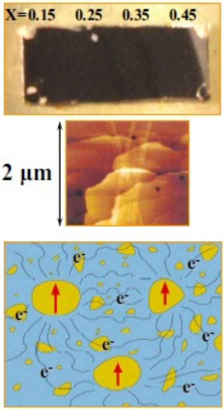
$$T_c \sim \exp\left[-C\frac{(x-x_c^0)^{2-d/\phi}}{x(1-x)}\right]$$

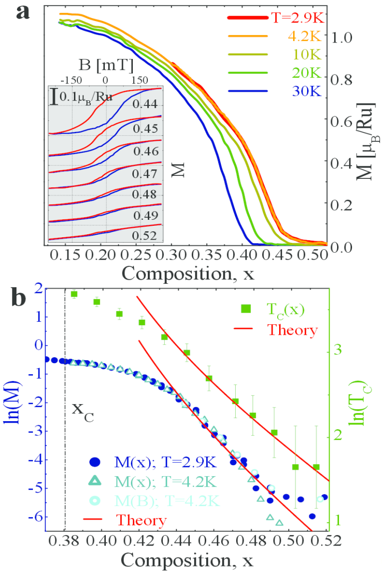
for compositions somewhat above x_c^0 and

$$T_c \sim (1-x)^{L^d_{\min}}$$

in the far tail of the smeared transition, $x \to 1$.

Rounding of the quantum phase transition in $Sr_{1-x}Ca_xRuO_3$





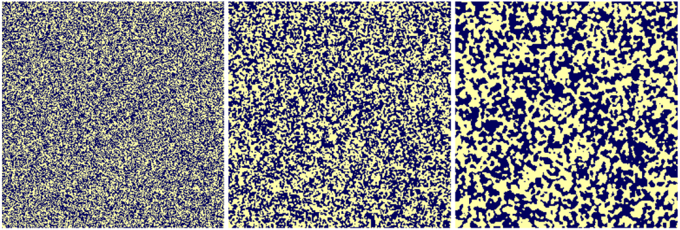
Effect of spatial disorder correlations on phase transitions

For positive disorder correlations, like atoms tend to cluster

Critical point

uncorrelated disorder and short-range correlated disorder, as long as correlations decay faster than r^{-d} have same effect on stability of a critical point (Harris Criterion)

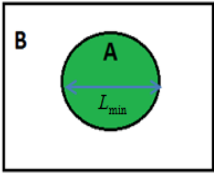
$\Longrightarrow$ short-range correlations are irrelevant



What is the influence of disorder correlations on smeared phase transitions?

Observables in tail of smeared transition

rare region of A atoms with size larger than $L_{\min}$ shows static magnetization



1. regime where $x > x_c^0$

   $$M \propto \exp\left[-\frac{C}{1+a\xi_{\mathrm{dis}}^d}\frac{(x-x_c^0)^{2-d/2}}{x(1-x)}\right]$$

2. the far tail of transition at $x \to 1$

   $$M \propto (1-x)^{\beta} \qquad \beta = (aL_{\min}^d + a\xi_{\mathrm{dis}}^d)/(1+a\xi_{\mathrm{dis}}^d)$$

$\Longrightarrow$ exponent β depends on ξ_{dis}

- for small disorder correlation length $\xi_{\mathrm{dis}} \ll L_{\min}$

  $$\beta \approx L_{\min}^d$$

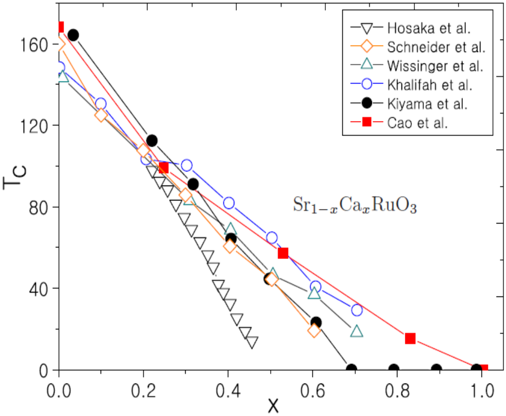
- for large disorder correlation length $\xi_{\mathrm{dis}} \geq L_{\min}$

  $$\beta \approx 1$$

Disorder correlations qualitatively modify smeared phase transitions

Smeared phase transitions

unusually large variations in magnetization curves in $Sr_{1-x}Ca_xRuO_3$ compounds



Outline

Conclusions

- disorder can destroy a sharp phase transition by smearing if static order forms on rare spatial regions
- ordered phase in the alloy $A_{1-x}B_x$ extends over the entire composition range $x < 1$, in the tail, magnetization vanishes as $(1-x)^\beta$
- experimentally observed in $Sr_{1-x}Ca_xRuO_3$
- short-range disorder correlations qualitatively modify behavior of smeared phase transitions
- positive correlations enhance tail of smeared phase transitions
- negatively correlations suppress smeared phase transitions

Thank you