Critical behaviour of the Coulomb-glass model in the zero-disorder limit: Ising universality in a system with long-range interaction

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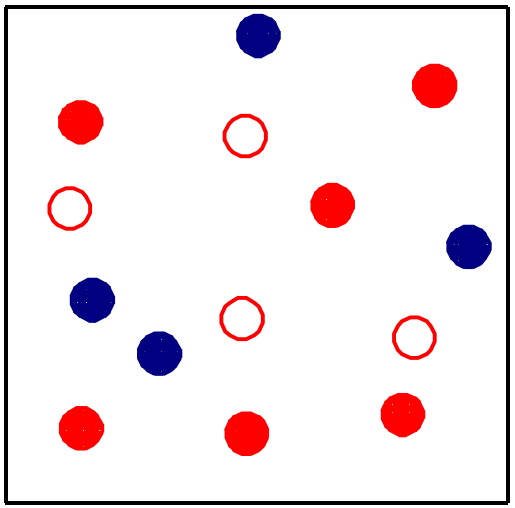
CompPhys09, Universität Leipzig, 27.11.2009

1. Motivation / introduction

Coulomb glass model = semiclassical model of diluted impurity band in amorphous or crystalline semiconductor, invented by Pollak, 1970, and Efros and Shklovskii, 1975



- occupied donor
- empty donor
- occupied acceptor

$$H = -\sum_{i,n} \frac{1-n_i}{|\vec{x}_i - \vec{x}_n|} + \sum_{i<j} \frac{(1-n_i)(1-n_j)}{|\vec{x}_i - \vec{x}_j|}$$

↑ acceptor potential

↑ donor-donor interaction

Characteristic energy for Si:P with $n = 10^{18}$ cm^{-3} :

interaction energy of nearest neighbours ~ 12 meV

Presumptions of Coulomb glass model:

- Temperature so low, that excitations to the conduction band / from the valence band negligible
- Concentration so low, that quantum interference of the states at neighbouring sites irrelevant

Further simplifications:

Sites at lattice, acceptors emulated by background charge, disorder by on-site potential:

$$H = \sum_i \varphi_i n_i + \frac{1}{2} \sum_{i \neq j} \frac{(n_i - K)(n_j - K)}{|\vec{x}_i - \vec{x}_j|}$$ and single-particle energy $$E_i = \varphi_i + \sum_{j \neq i} \frac{(n_j - K)}{|\vec{x}_i - \vec{x}_j|}$$

mostly φ_i uniformly distributed in $[-B/2, B/2]$.

Advantage: Interaction matrix can be stored for larger systems.

Danger: Modification of interaction spectrum, correlation of static potential lost.

Experimental evidence for predictions by Efros & Shklovskii, 1975

Coulomb gap in single-particle density of states $g(E) \propto |E - \mu|^{d-1}$ for $T = 0$:

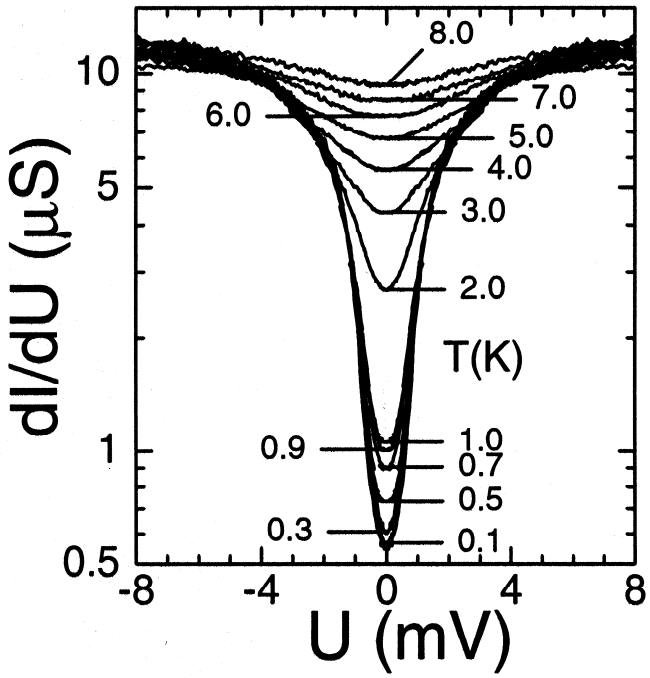
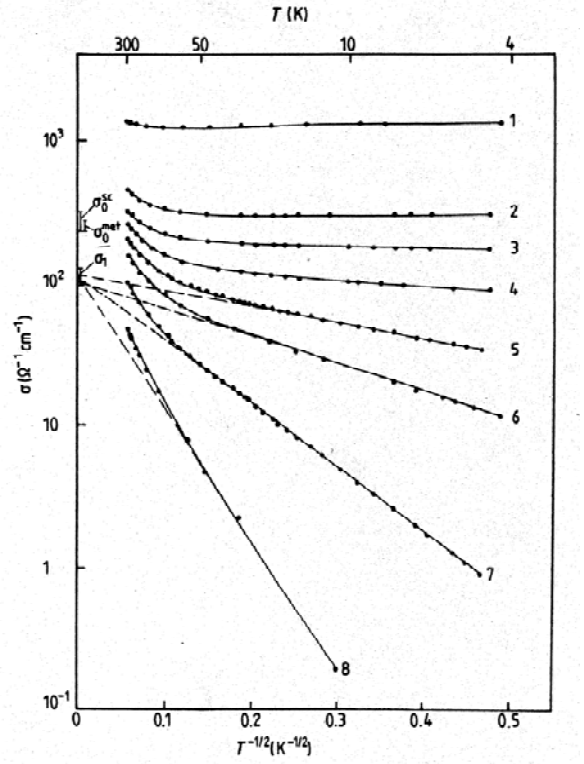


FIG. 1. dI/dU vs U spectra of the Ge sample with $N_d = 1.26 \times 10^{17}$ cm^{-3} at the indicated temperatures.

Sandow et al., PRL, 2001

Temperature dependence of conductivity for variable range hopping with interaction, $\sigma \propto \exp\{-(T_0/T)^{1/2}\}$, here a-$Si_{1-x}Cr_x$:



see AM et al., JPC, 1985

Current research in this field: Glass transition

Huge number of local minima concerning single-particle hops

$\Rightarrow$ broad scale of relaxation times, see Schreiber et al. 1996, Pérez-Garrido et al. 1999

$\Rightarrow$ non-ergodicity causes e.g. measuring time dependence of specific heat

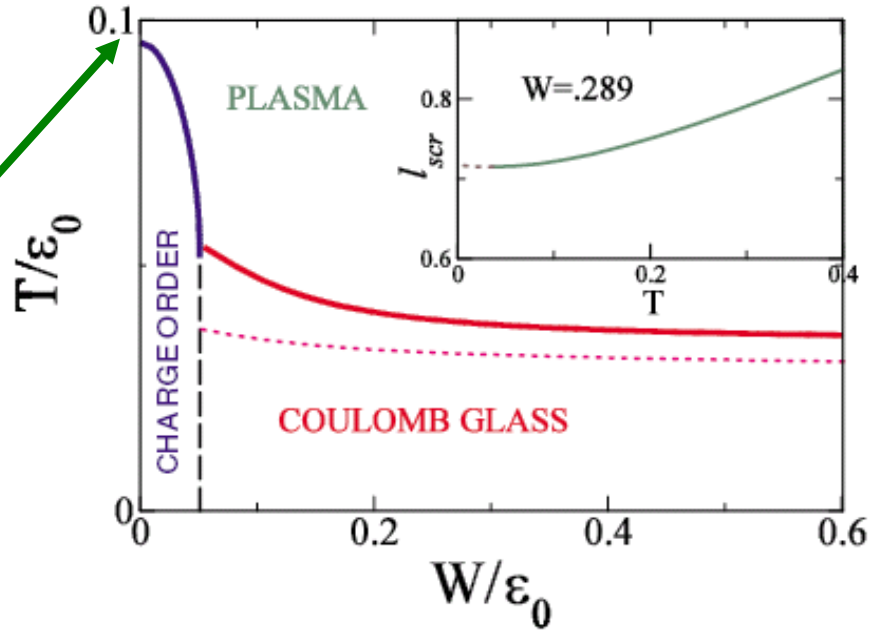
But what about the glass transition?

Purely dynamic feature or
thermodynamic phase transition behind?

Under which conditions does phase
transition exist?

No glass transition found by
Surer et al. PRL 2009,
Goethe and Palassini, PRL 2009.

Our aim in this work: precise study of nature of order-disorder transition for $K = 0.5$



Phase diagram of 3d Coulomb glass by
Pankov & Dobrovsavljević, PRL, 2005

2. Simulation method

As ususal: substitution of time averaging for ensemble averaging

Problem: Cluster algorithm seems not to be available for the antiferromagnetic Coulomb interaction because of frustration (Swendsen, priv. com.)

Our approach: introducing by hand set of system modifications of various complexity:

one-particle exchange with surroundings (single-spin flip),

one-electron-hop over distance below certain bound (two-spin flip),

two-electron hops changing n_i for four neighbouring sites (four-spin flip)

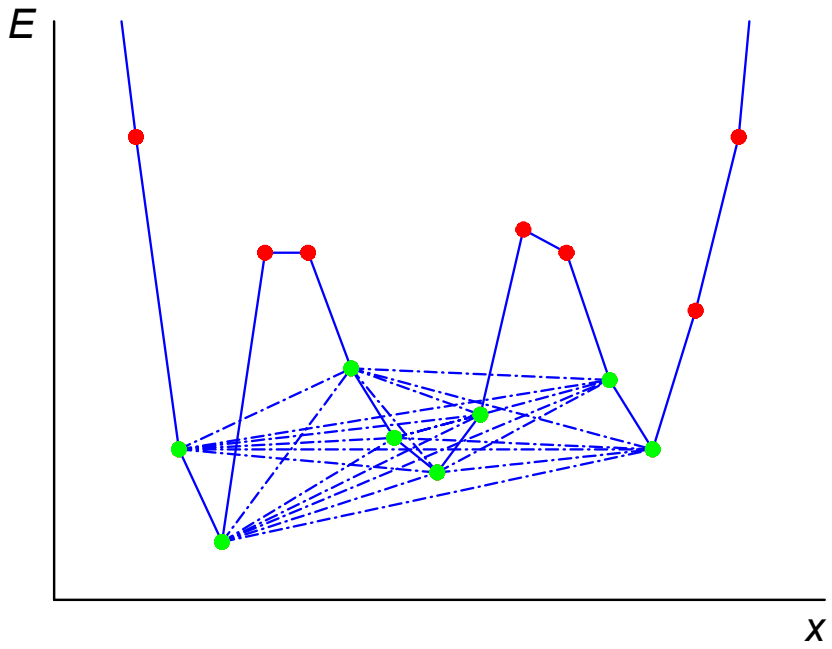
Efficient error control: decomposition of simulation in 100 intervals of simulation time τ with random start and equilibration during $\tau/3$ before starting integration

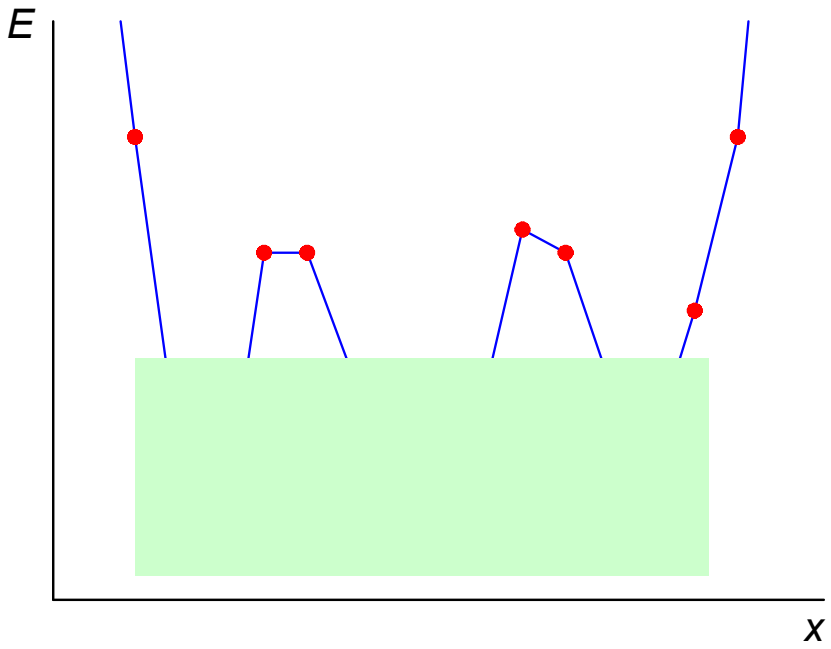
$\Rightarrow$ Estimation of mean values and errors, and restart with increased τ if needed.

Method is advantageous also due to **better sampling of configuration space.**

At low *T*, acceleration by modifying dynamics

*AM and P. Thomas, Phys. Rev. B **55** (1997) 7460*





A) 'Drive tunnels' between states of low-energy subset $S^{(l)}$ (tabulated)

B) Increase rates of auxiliary transition

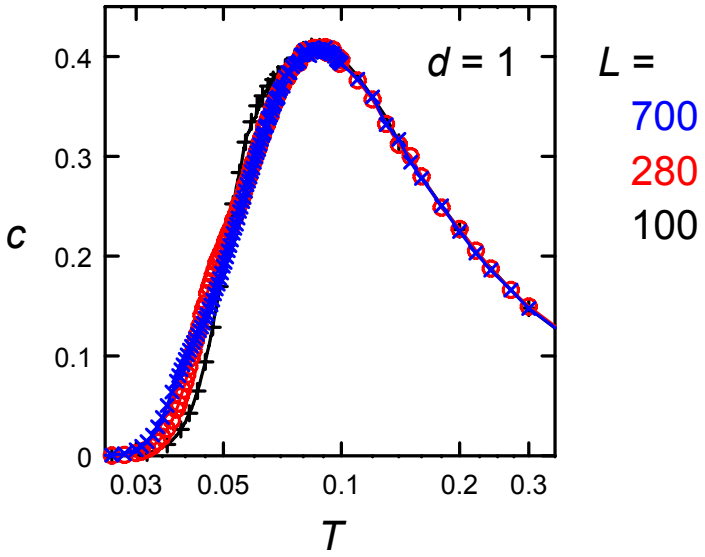
$\rightarrow$ treat low-energy subset analytically

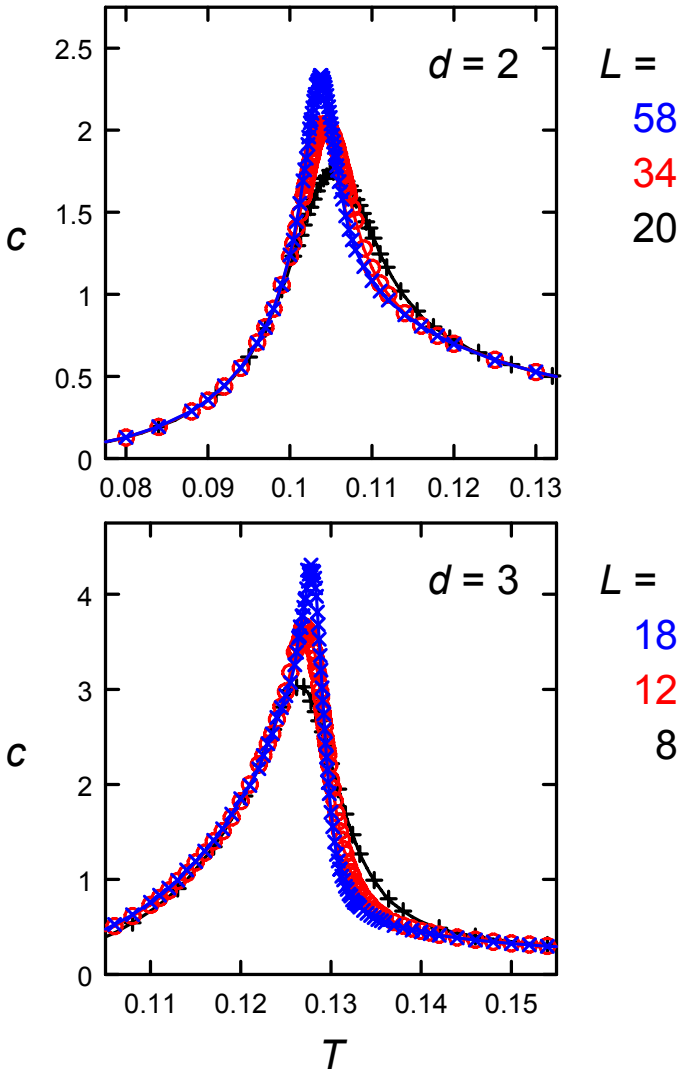
3. Raw data

a) Specific heat

$$c = \left(\left\langle H^2 \right\rangle - \left\langle H \right\rangle^2\right) \Big/ \left(T^2 L^d\right)$$

indicates phase transition at finite T for d = 2 and 3, but not for d =1.





b) Staggered occupation

characterises degree of order analogously to antiferromagnet,

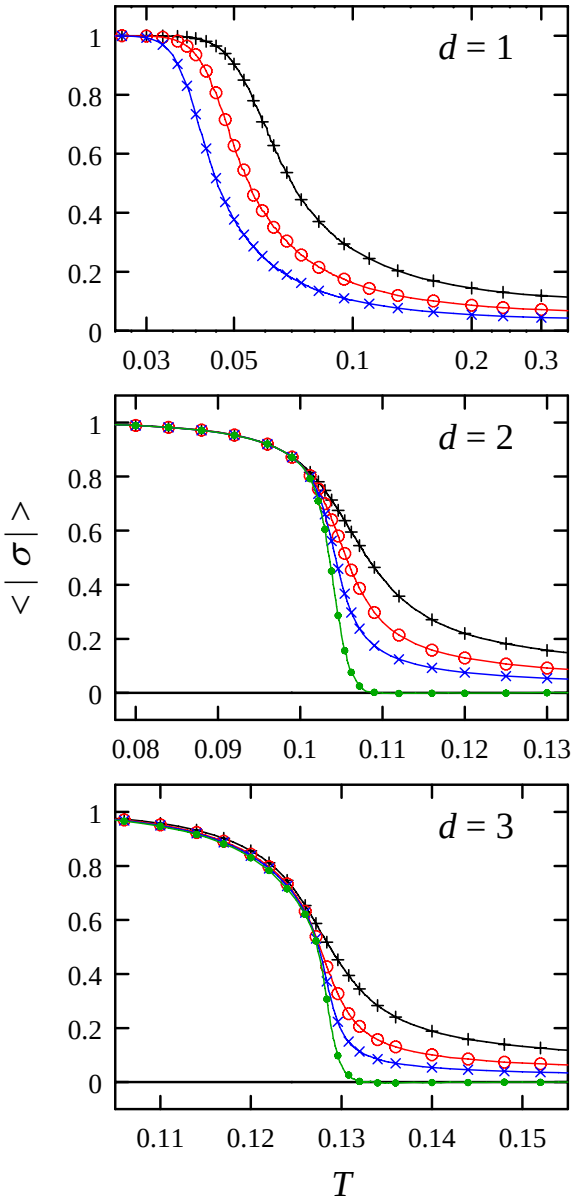
$$\sigma_i = (2n_i - 1) \cdot (-1)^{x_i + y_i + z_i}$$

Sample average: $\sigma = \Sigma \sigma_i / L^d$

Thus: $\langle |\sigma| \rangle =$ order parameter, introduced by Vojta 1993

Behaviour of $\langle |\sigma| \rangle (T, L) \Rightarrow$ phase transition at finite T for d = 2 and 3, but presumably not for d = 1.

Confirmed by extrapolation $L \to \infty$ based on high-temperature relation $\langle |\sigma| \rangle \propto L^{-d/2}$



c) Generalised susceptibility

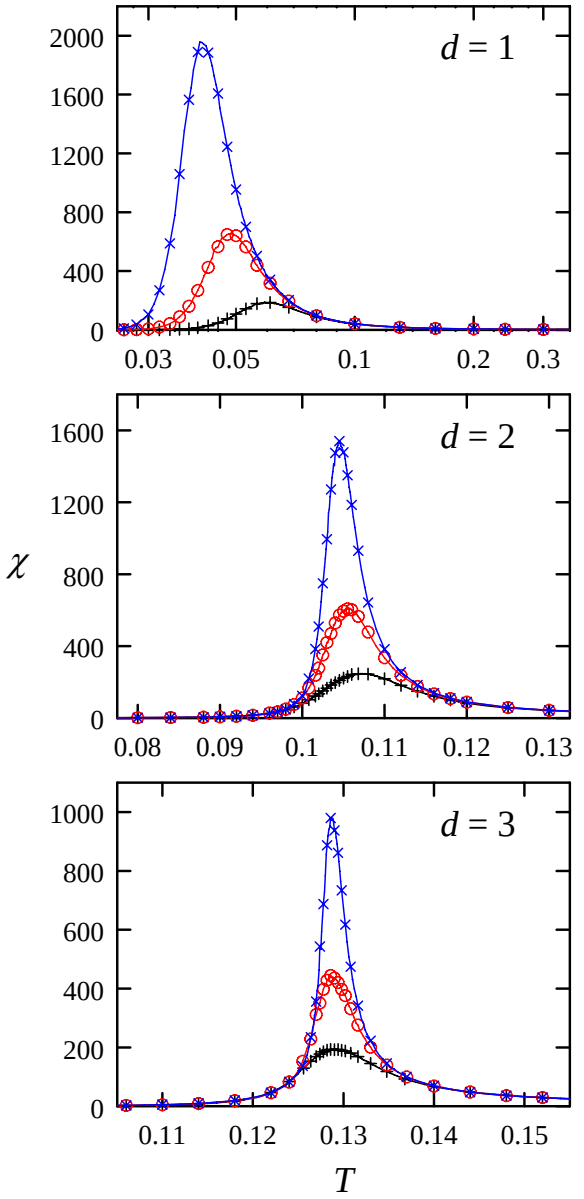
related to $\langle|\sigma|\rangle$:

$$\chi = L^d(\langle\sigma^2\rangle - \langle|\sigma|\rangle^2)/T$$

Peaks evolve with increasing L,

broad on logarithmic scale for $d = 1$,

sharp for $d = 2$ and 3



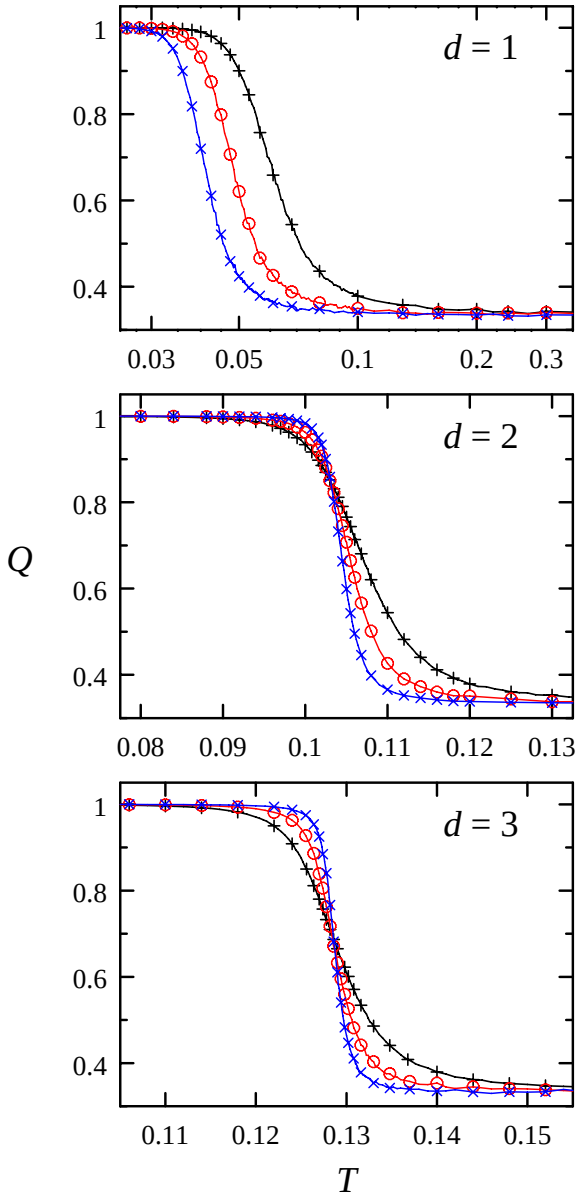
d) Binder parameter = fourth moment ratio

In sense of Binder-cumulant analysis,
at transition from ordered to disordered phase,
ratio

$$Q = \langle \sigma^2 \rangle^2 / \langle \sigma^4 \rangle$$

changes from 1 to 1/3.

Scaling in this T region $\Rightarrow$ critical exponents



4. Data evaluation

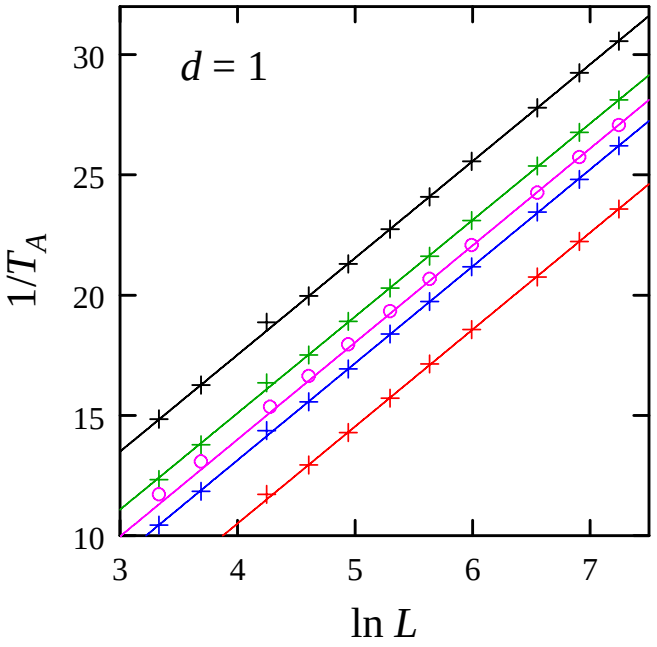
a) $d = 1$: There seems to be no phase transition in this case.

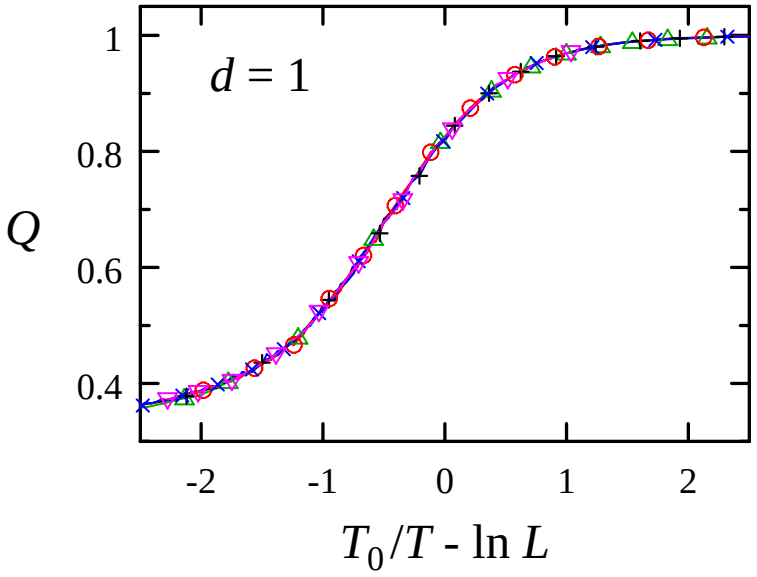
Solution of $Q(T_A,L) = A$

for A = 0.90, 0.75, 0.60, and 0.45 yields

exponential vanishing of T_A with rising L.

Similar behavior of susceptibility maximum. $\Rightarrow$ Scaling $Q(T,L) = Q(T_0/T - \ln L)$, here for L = 40, 100, 280, 700, and 1400.





b) $d = 2$ and $d = 3$

Numerical procedure in analysing Binder ratio:

To **reduce curvature** we consider

$$q_2 = -\ln(1-q)$$

and

$$q_3 = \tan((3q/2-1)\pi)$$

Deviations from scaling described by

L dependence of $T_{c,d}$ (Hasenbusch 2001)

Ansatz

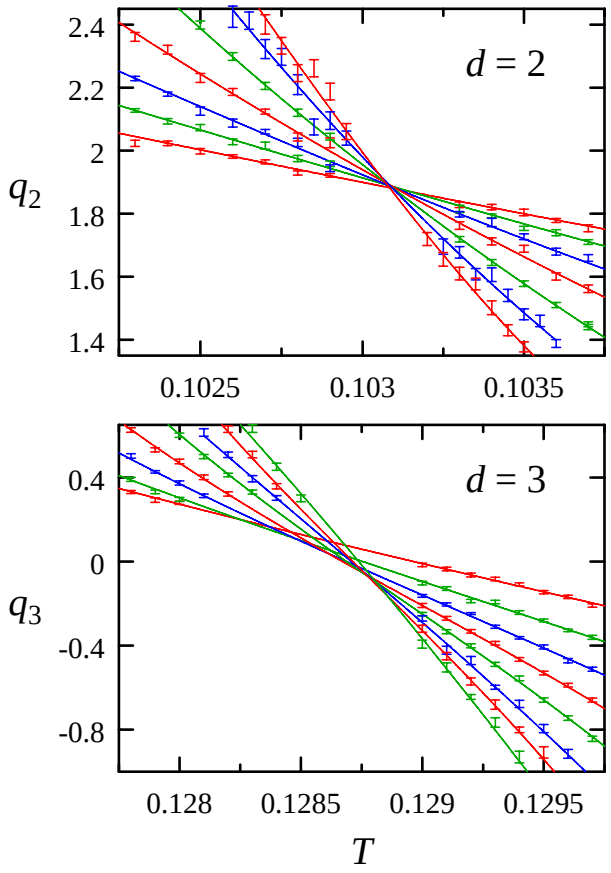
$$q_d(T,L) = q_{d,0} + t + b_d t^2 + c_d t^3$$

with

$$t = a_d(L)(T - T_{c,d}(L))$$

and universal $q_{d,0}$, b_d, c_d enables

high accuracy of $a_d(L)$



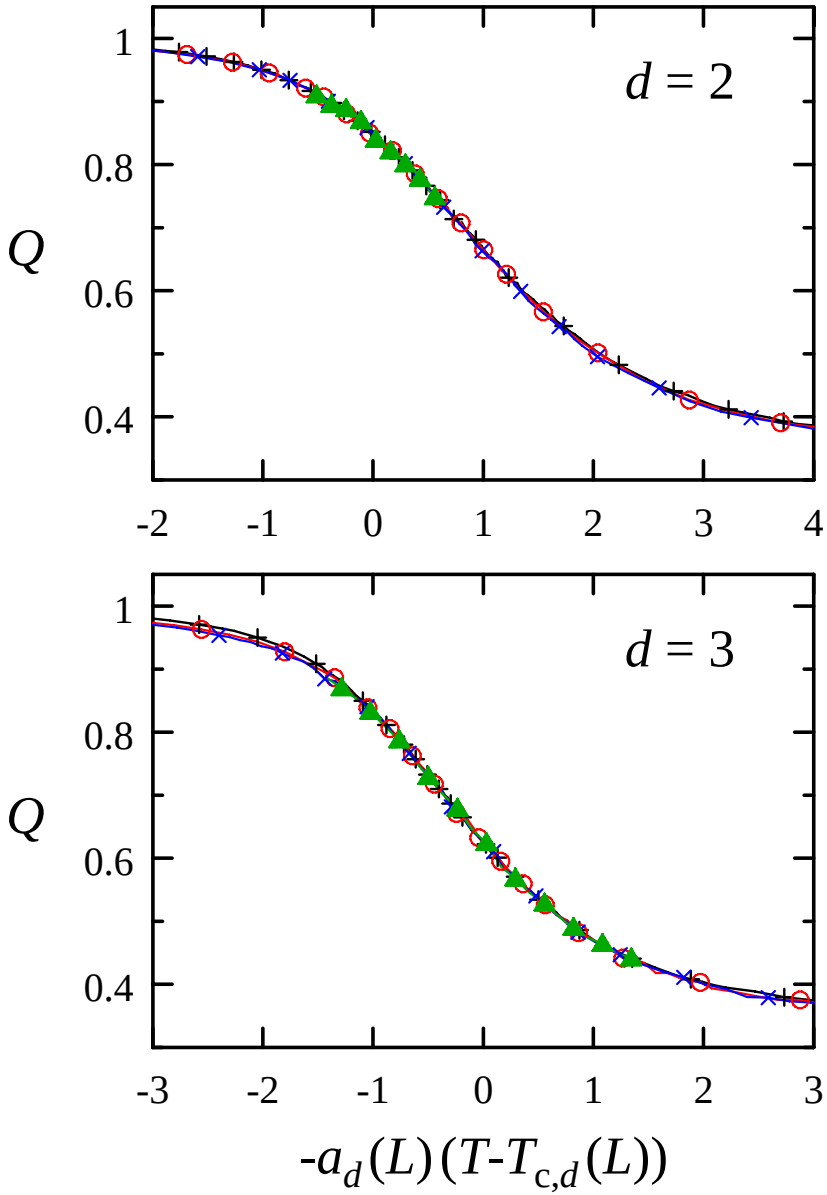
L = 16, 24, 34, 48, 68, 88, and 112 for d = 2, and

L = 8, 10, 12, 14, 16, 18, 20, 22 for d = 3

Prerequisite:

high quality of

modified scaling of *Q*(T,L)



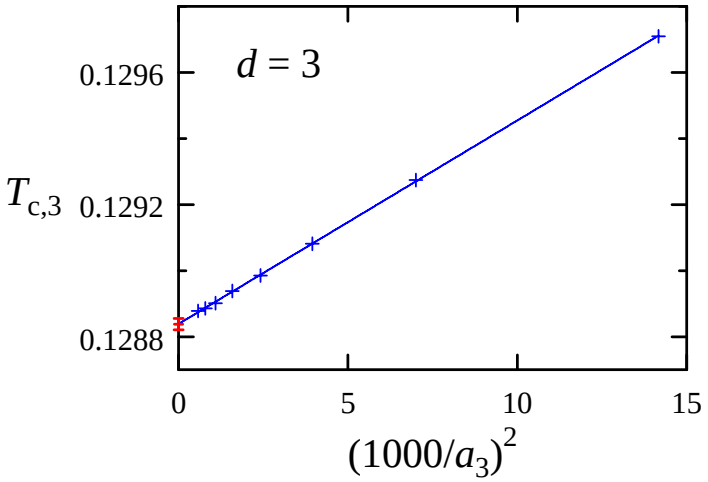
Problem: Adjustable $q_{d,0}$ $\Rightarrow$

linear contribution $\propto 1/a_d(L)$ to $T_{c,d}(L)$,

suppressed by

$Q_{2,0} = 0.8492(12)$,

$Q_{3,0} = 0.625(4)$

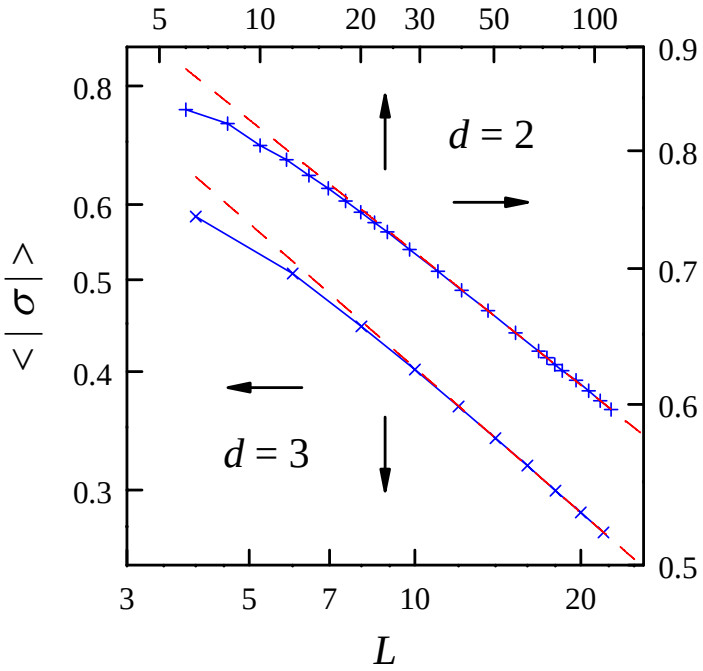


Extrapolation of quadratic relation

$\Rightarrow$ critical temperatures

$T_{c,2}(\infty) = 0.103082(9)$

$T_{c,3}(\infty) = 0.128838(17)$



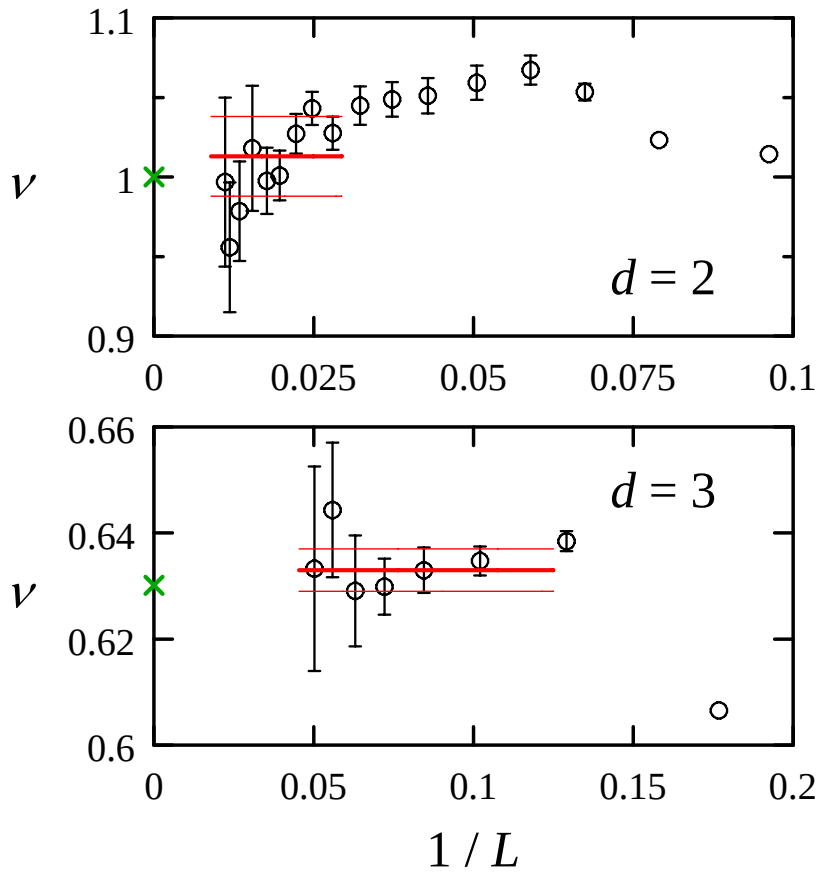
Calculate $c(T_c(L),L)$, $\langle|\sigma|\rangle(T_c,L)$, and $\chi(T_c,L)$

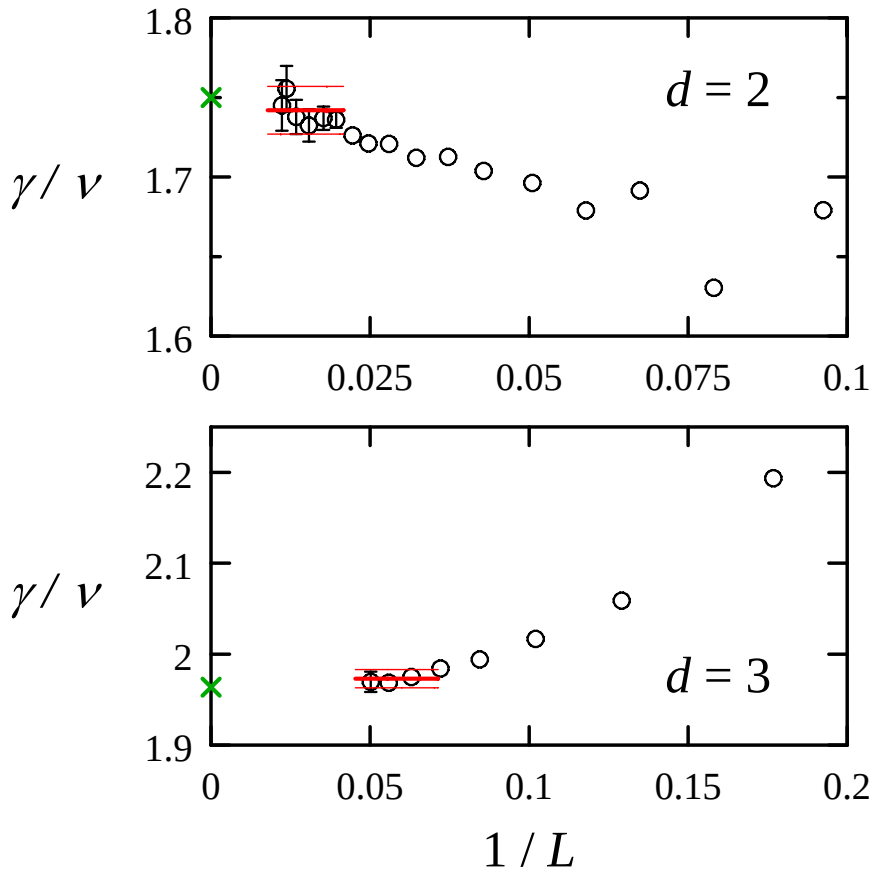
analogously to $q_d(T,L)$ analysis:

logarithms approx. by polynomials of 3rd order in t,

partly utilising parameter universalities

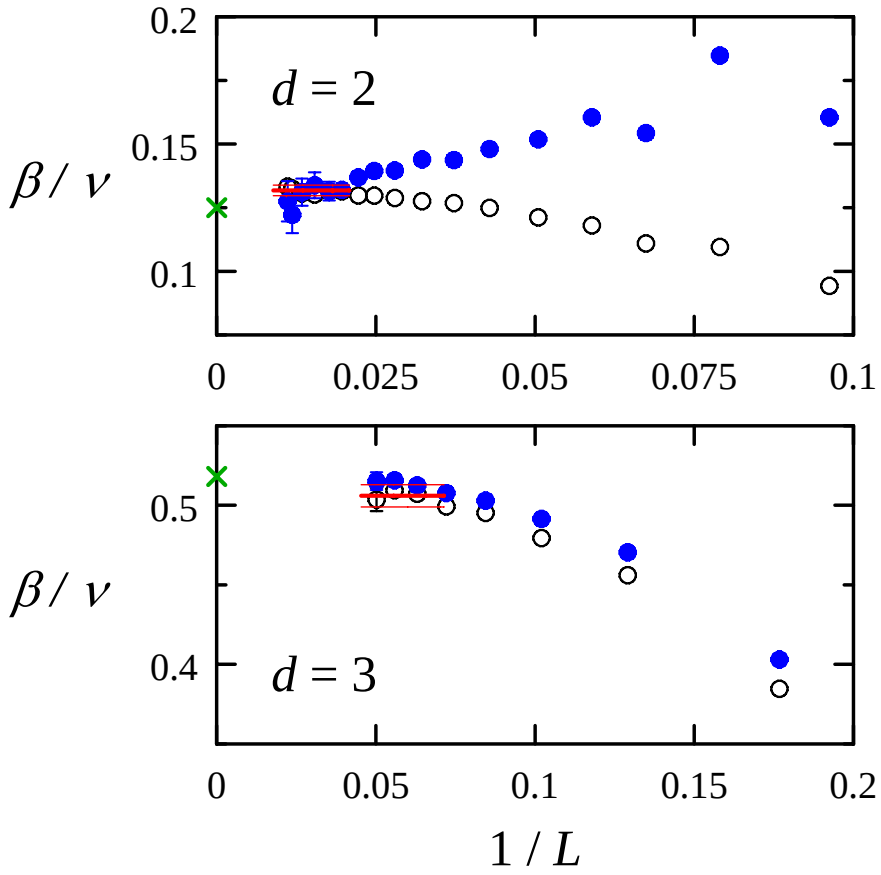
Critical exponents from differentiation as well as from power law fits for various L regions

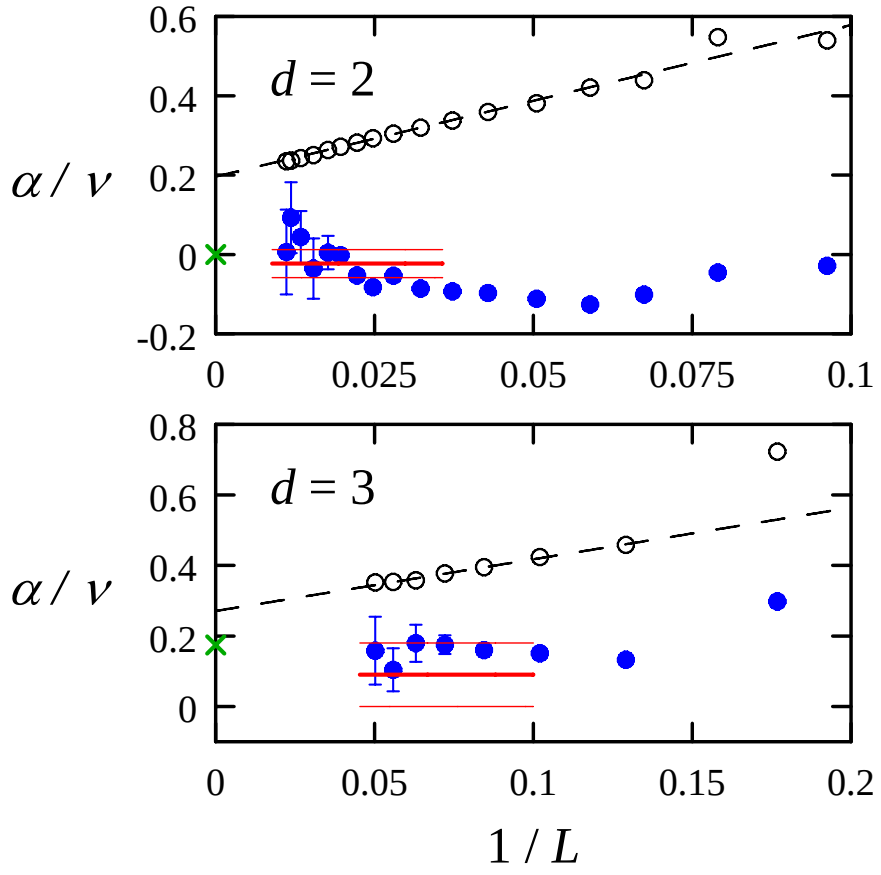




For order parameter and specific heat, alternatively by Widom and hyperscaling relations

Special for specific heat: approx. $c(L)$ by $a + b\,(L^p\text{-}1)/p$ instead of by $a + b\,L^p$





5. Summary of exponent values

quantity	*d*	*L* region	Coulomb	short-range Ising model	Agreement
α/ν	2	24 – 96	-0.02(4)	0 (ln)	+
β/ν	2	48 – 96	0.1318(21)	1/8	+/-
γ/ν	2	48 – 96	1.742(15)	7/4	++
ν	2	34 – 96	1.013(25)	1	++
α/ν	3	6 – 18	0.09(9)	0.1740[8]	+/-
β/ν	3	12 – 18	0.506(7)	0.51820[8]	+/-
γ/ν	3	14 – 18	1.973(10)	1.96361[15]	++
ν	3	10 – 18	0.633(4)	0.63012[16]	++

Widom relation: $\alpha + 2\,\beta + \gamma = 2$ ✓

Hyperscaling relation: $2 - \alpha = d\,\nu$ ✓

6. Conclusion

Studied: System of localised charges on half-filled lattice without static disorder

Result: **Critical exponents consistent with short-range Ising universality**,
in agreement with previous, less precise numerical data by Overlin et al., 2004.
Now, **all other known universality classes excluded**,
supporting analytical studies by Brognara et al., 2002, and Ciach, 2004.

⇒ **Screening is** so **efficient** that, in spite of long-range interaction, model belongs to same universality class as short-range Ising model.

Thus Coulomb glass resembles a chameleon:
Coulomb gap is long-range effect, while, for samples without static disorder, thermal order-disorder transition is short-range feature.

⇒ Challenge: Influence of static disorder

Details: *Phys. Rev. B 79, 174206 (2009)*

en.wikipedia.org/wiki/File:Caméléon_Madagascar_02.jpg