Numerical simulations of the electron glass
(in and out of equilibrium)

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with
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Electron glass model (Efros)

quenched random potential

$$\mathcal{H} = \frac{e^2}{2\kappa}\sum_{i\neq j}(n_i - K)\frac{1}{r_{ij}}(n_j - K) + W\sum_i n_i\varphi_i \qquad \sum_{i=1}^{N} n_i = KN$$

- Inspired from "classical impurity band" for compensated semiconductors.
- Relevant for other materials? (amorphous semiconductors, granular metals)

Outline:

- Phase diagram and existence of an equilibrium glass phase
- Shape of the Coulomb gap in 3D
- Pair density of states and polaronic shift
- (Avalanches)

M. Goethe and MP, Phys. Rev. Lett. 103, 045702 (2009)
Ann. Phys. (Berlin) 18, 868 (2009)

Electron glass model (Efros)

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$$\mathcal{H} = \frac{e^2}{2\kappa} \sum_{i \neq j} (n_i - K) \frac{1}{r_{ij}} (n_j - K) + W \sum_i n_i \varphi_i \qquad \sum_{i=1}^{N} n_i = KN$$

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Simulation details:

- Cubic (3D) and square (2D) lattice
- $K = 1/2$
- Gaussian distributed φ_i
- Computational methods:
  1. Equilibrium Monte Carlo simulation (Parallel Tempering algorithm)
  2. Local relaxation (T=0 quench) with one particle hops
- Infinite periodic system. Ewald sum (with dipole surface term in 3D)

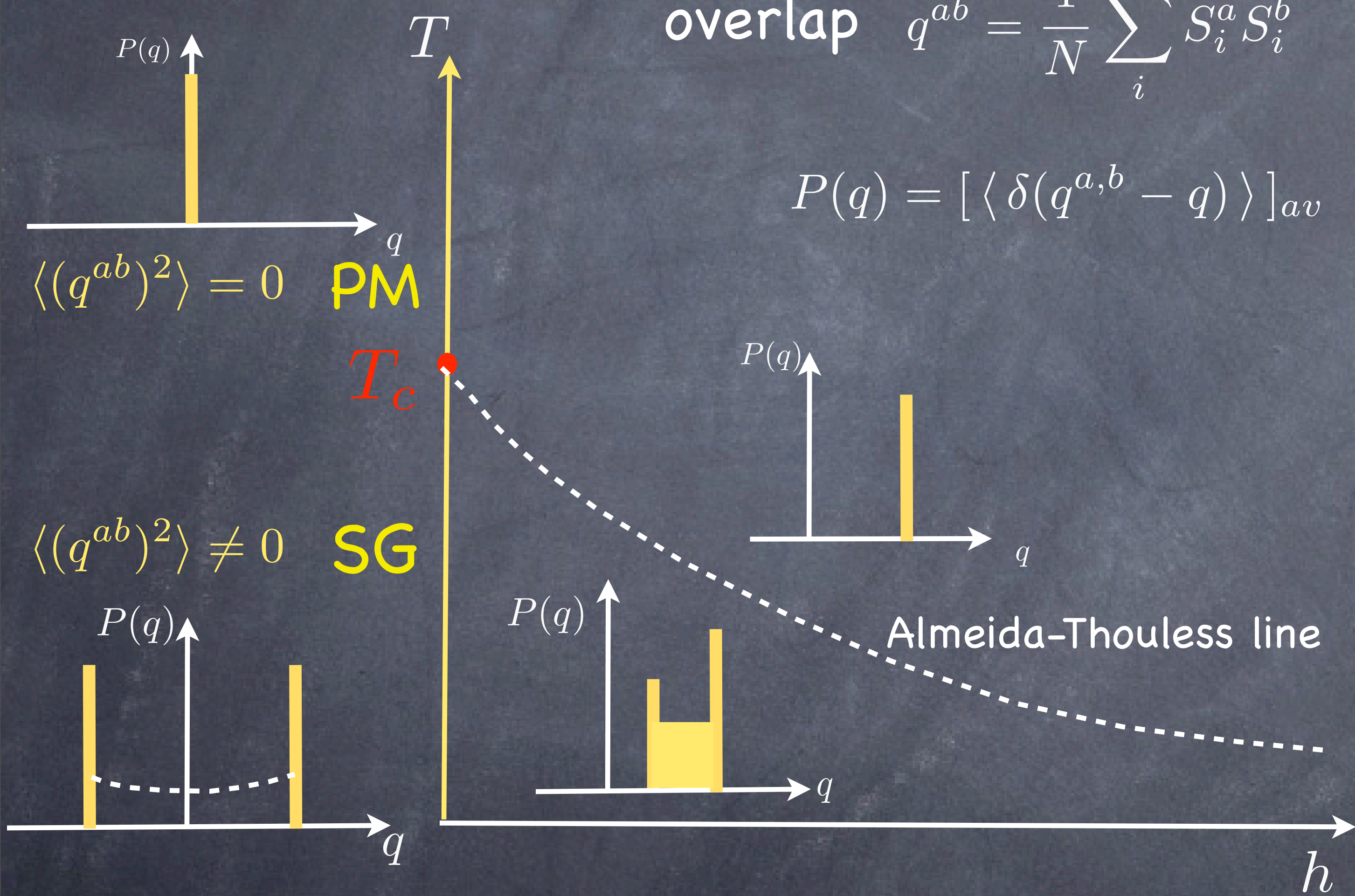
Is there an equilibrium glass phase?

Ising spin glass

$$\mathcal{H} = \sum_{(i,j)} J_{ij} S_i S_j - h \sum S_i \qquad [J_{ij}]_{av} = 0$$

overlap $q^{ab} = \frac{1}{N} \sum_i S_i^a S_i^b$

$$P(q) = [\,\langle\, \delta(q^{a,b} - q)\,\rangle\,]_{av}$$



Phase transition in 3D at h=0

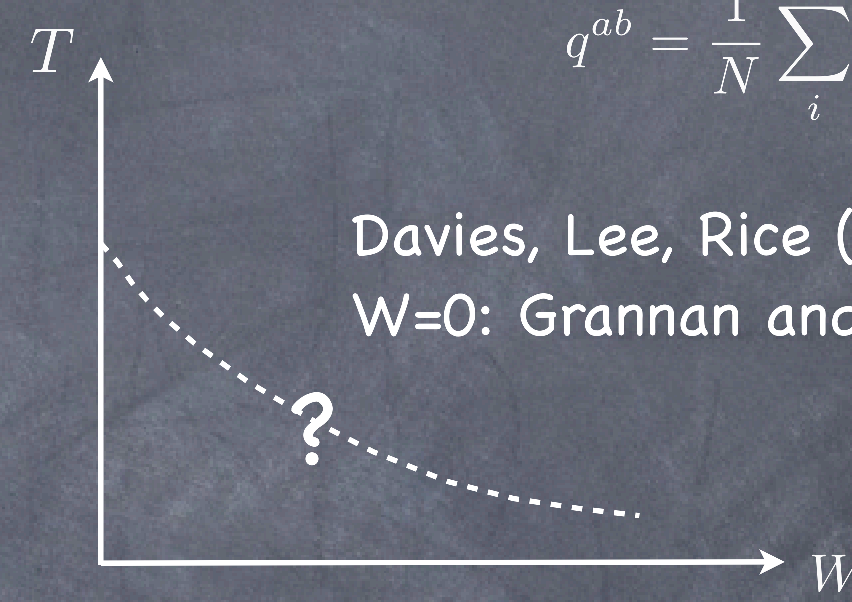
(Palassini and Caracciolo, PRL 1999, Ballesteros et al., PRB 2000)

Parisi solution of the infinite-range SK model: exp(N) thermodynamic states

Electron glass

$$\mathcal{H} = \sum_{i<j} \frac{1}{r_{ij}} n_i n_j + W \sum_i n_i \varphi_i$$

$$q^{ab} = \frac{1}{N} \sum_i n_i^a n_i^b$$

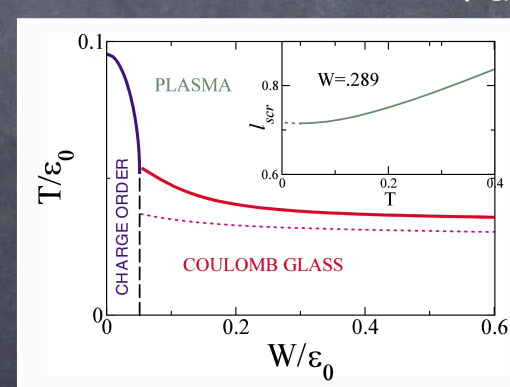


Davies, Lee, Rice ('82)

W=0: Grannan and Yu ('93)

Mean field theory (3D): $T < T_g \sim 1/\sqrt{W}$

Pankov and Dobrosavljevic, 2005
Müller and Ioffe, 2005
Müller and Pankov, 2007



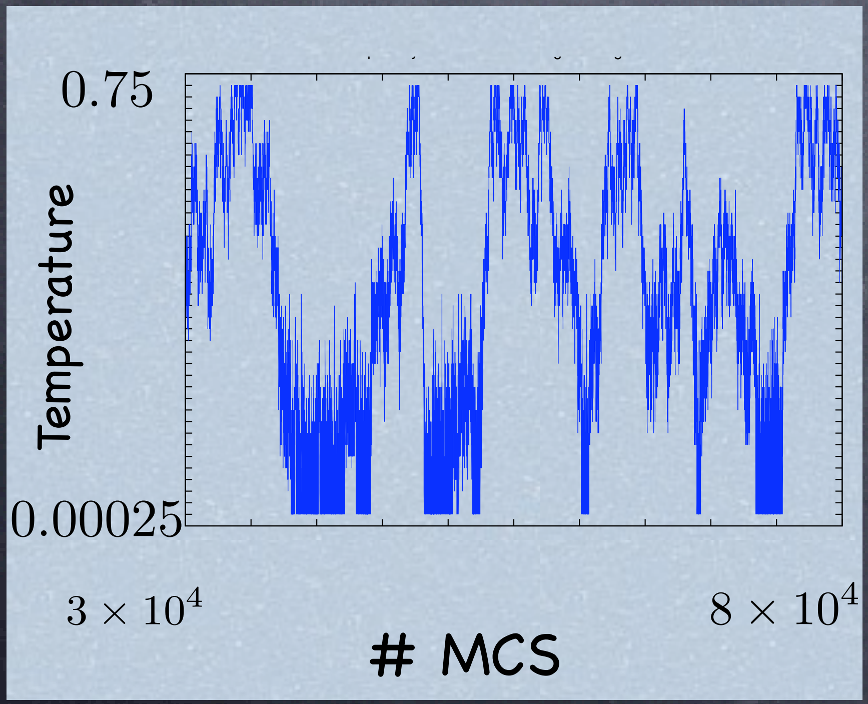
Experimental consequences:

- diverging nonlinear capacitance
- nonlinear screening (Baranovski et al. 1984)

Equilibrium Monte Carlo

- long range interaction
- sample averaging
- frustration
- low T -> very low acceptance
- critical slowing down
- supercritical slowing in the COP

Parallel Tempering algorithm

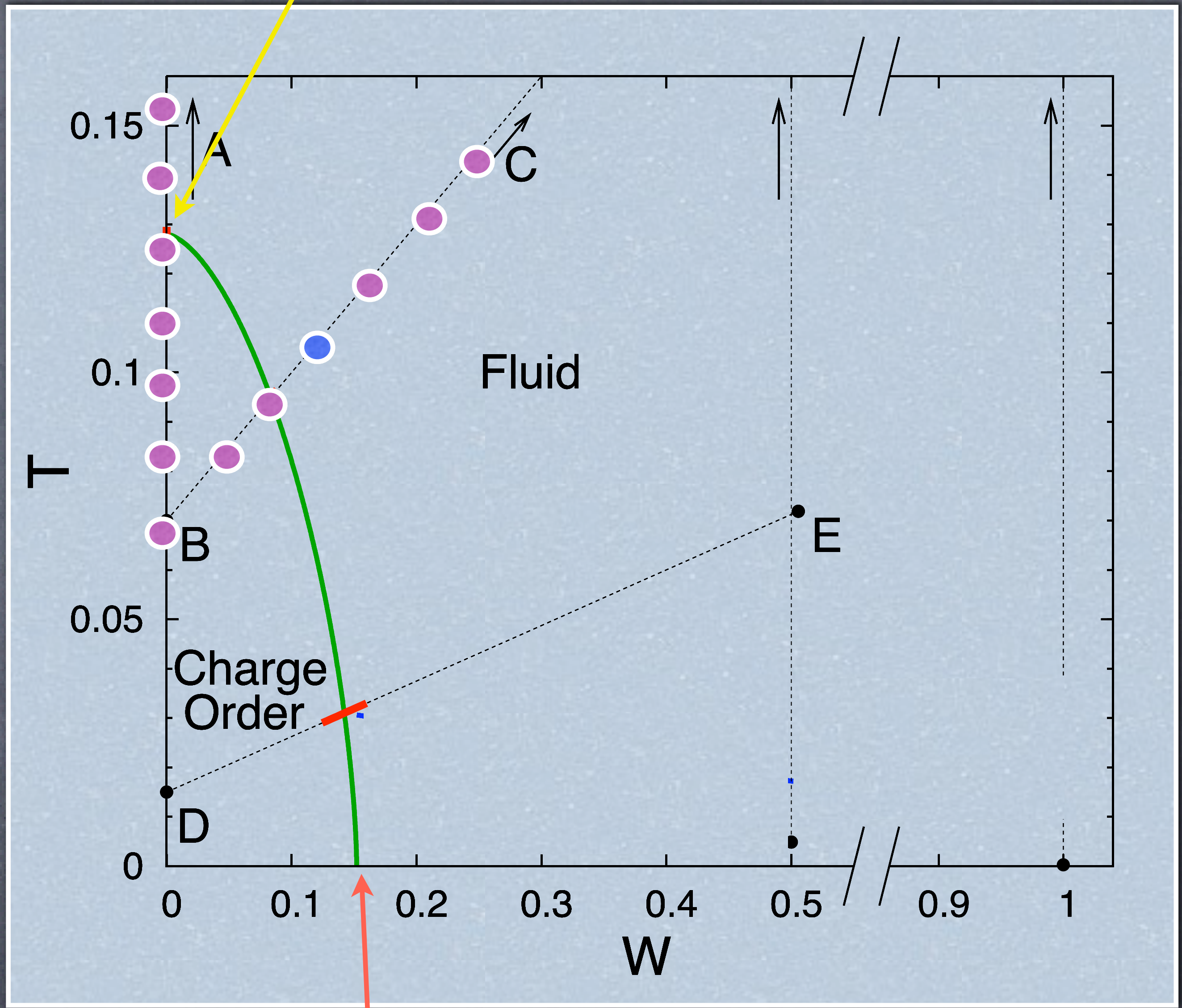


30 years CPU time, L<=12

$T_c = 0.1287 \pm 0.004$

$W = 0$

(Möbius and Rössler 2003)



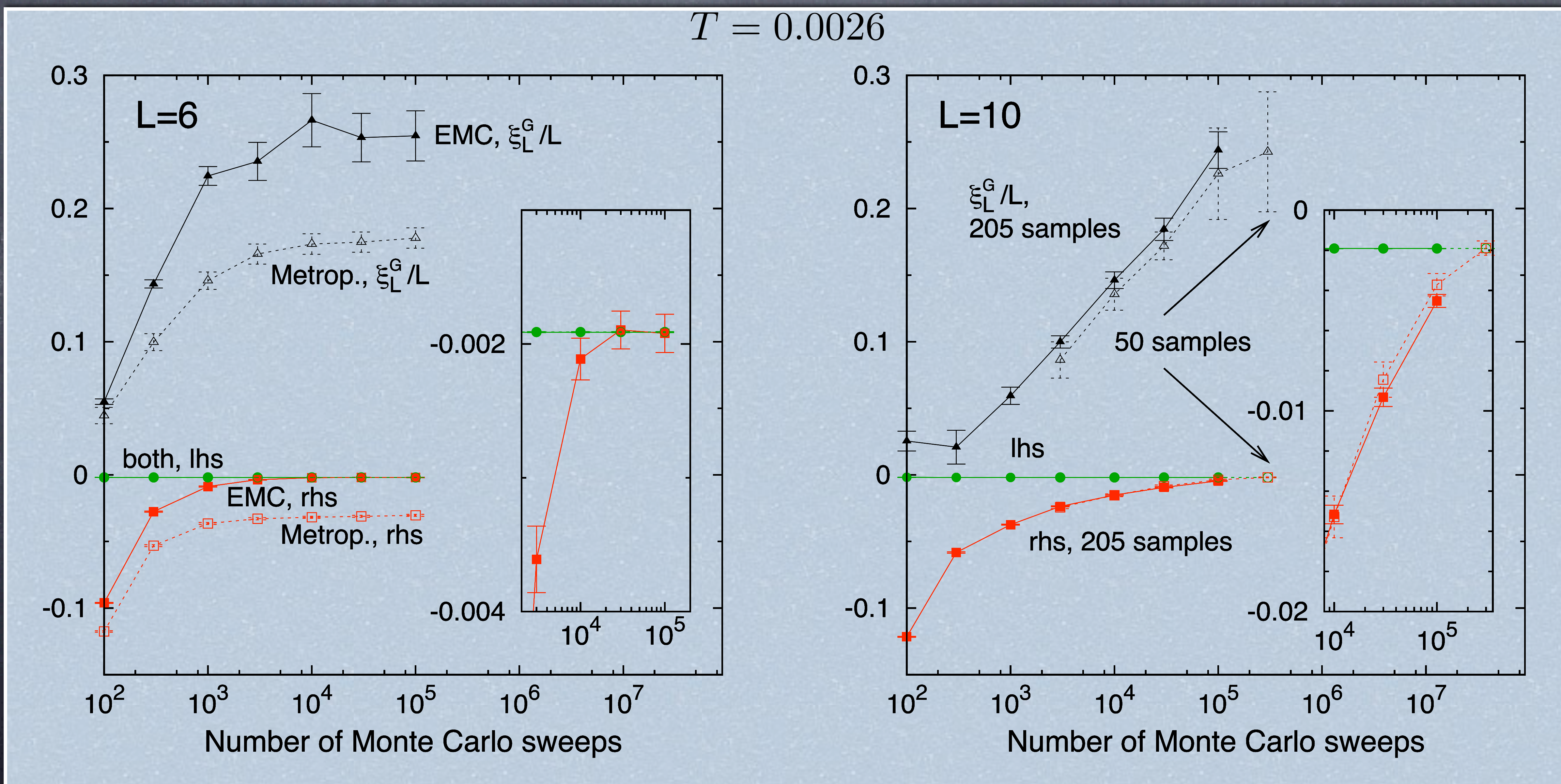
$W_c > 0$ at $T = 0$ (Möbius)

Equilibration

1. Thermal averages not changing when tripling the # of MCS

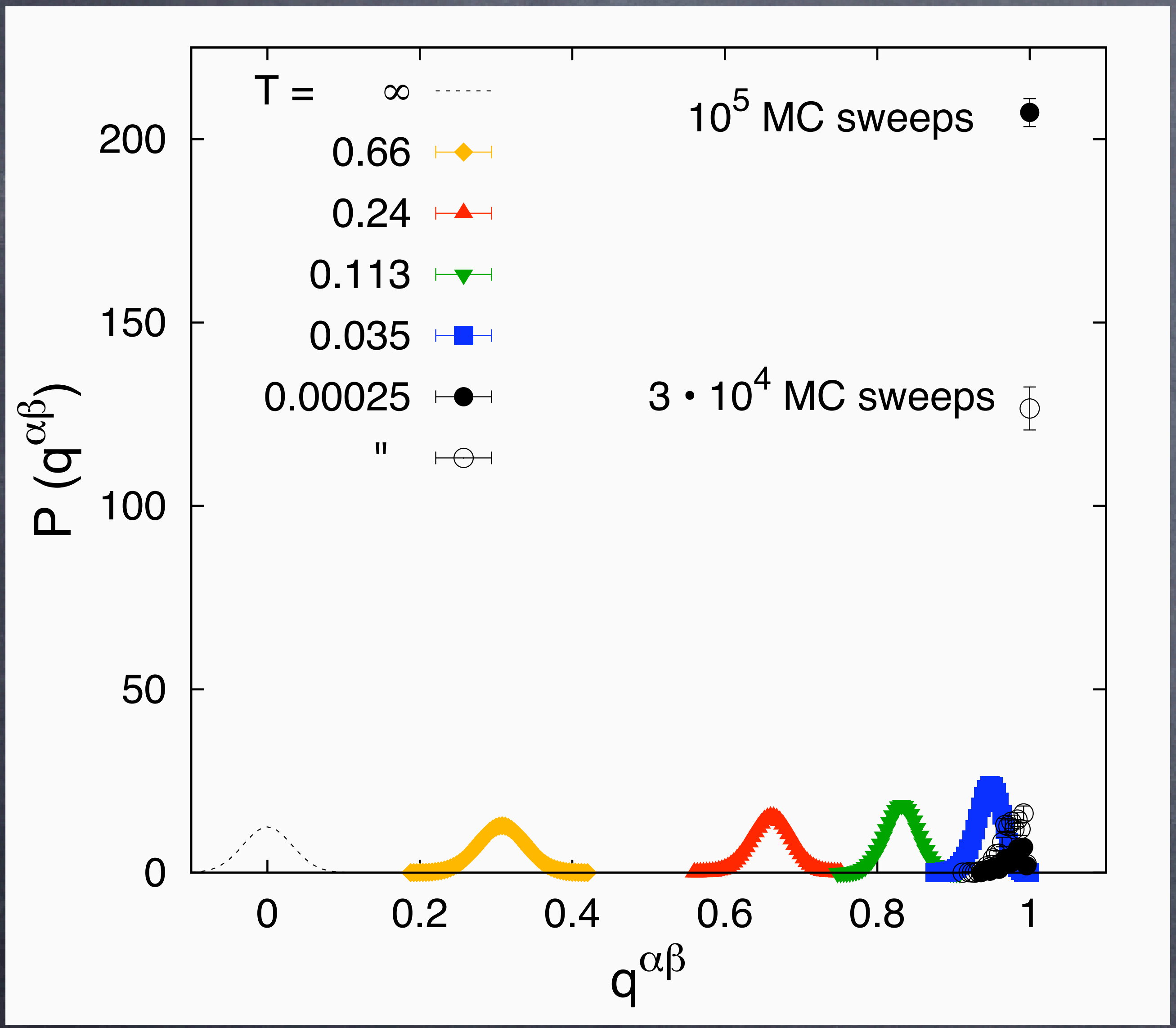
2. Necessary condition

$$2TN^{-1}[\langle \sum_i n_i \varphi_i \rangle]_{av} = W(2N^{-1}\sum_{i=1}^{N}[\langle n_i^{(a)} n_i^{(b)} \rangle]_{av} - 1)$$

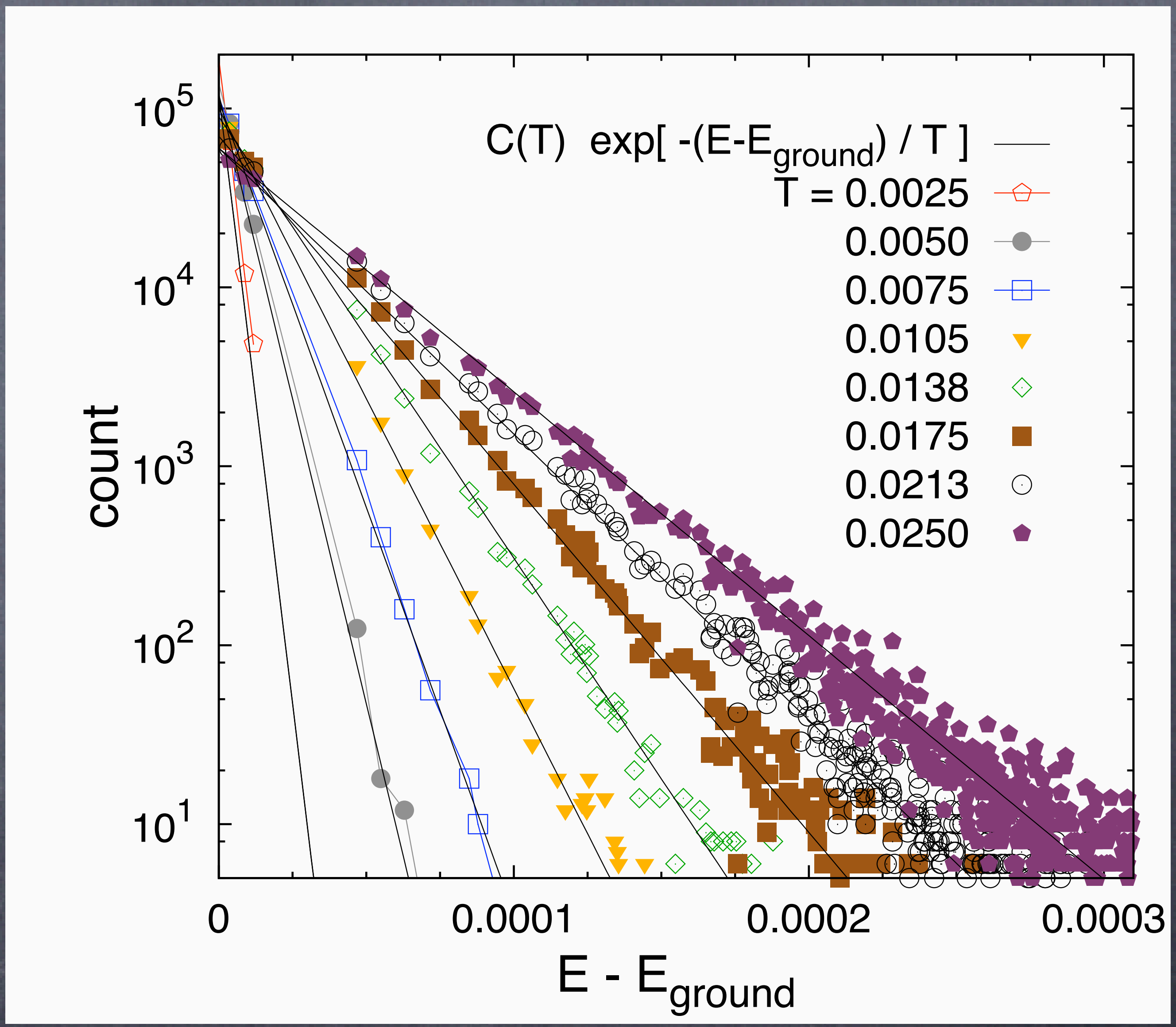


Equilibration

3. Ground state reached with high frequency



4. Low energy states are Boltzmann-distributed



Numerical probes of the glass phase

$$T > T_g \qquad \langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle \sim \exp -r/\xi$$

$$T < T_g \qquad \langle n_i n_j \rangle_\alpha - \langle n_i \rangle_\alpha \langle n_j \rangle_\alpha \sim r_{ij}^{-\lambda} \to 0$$

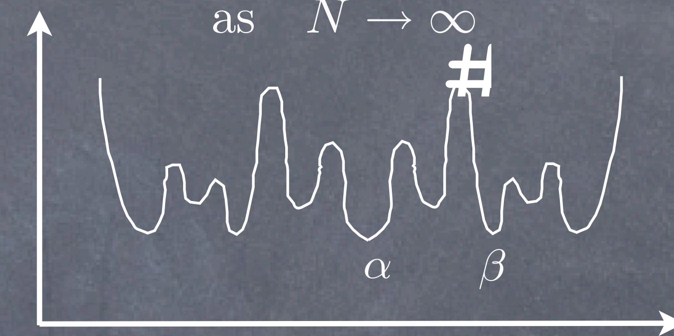
$$(\langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle)^2 \to const. \quad r_{ij} \to \infty$$

$$\langle \cdot \rangle = \sum_{states\ \alpha} w_\alpha \langle \cdot \rangle_\alpha$$

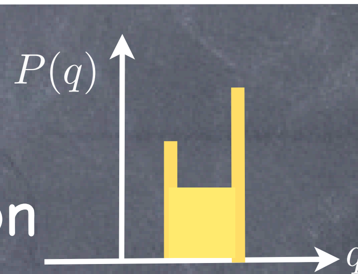
$$F_\# - F_\alpha \to \infty$$

$$F_\alpha - F_\beta = O(1)$$

$$\text{as} \quad N \to \infty$$



Overlap distribution



Finite-size correlation length

F. Cooper, B. Freedman, and D. Preston, Nucl. Phys. B 210, 210 (1982)
M. Palassini and S. Caracciolo, Phys. Rev. Lett. 82, 5128 (1999)

$$\xi_L^G = \frac{1}{2\sin(|\mathbf{k}_{min}|/2)} \left(\frac{\chi_L^G(0)}{\chi_L^G(\mathbf{k}_{min})} - 1 \right)^{\frac{1}{2}}$$

$$\chi_L^G(\mathbf{k}) = \frac{1}{L^d} \sum_{i,j} [(\langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle)^2]_{av} e^{i\mathbf{k}\cdot\mathbf{r}_{ij}}$$

$$\mathbf{k}_{min} = (2\pi/L, 0, 0)$$

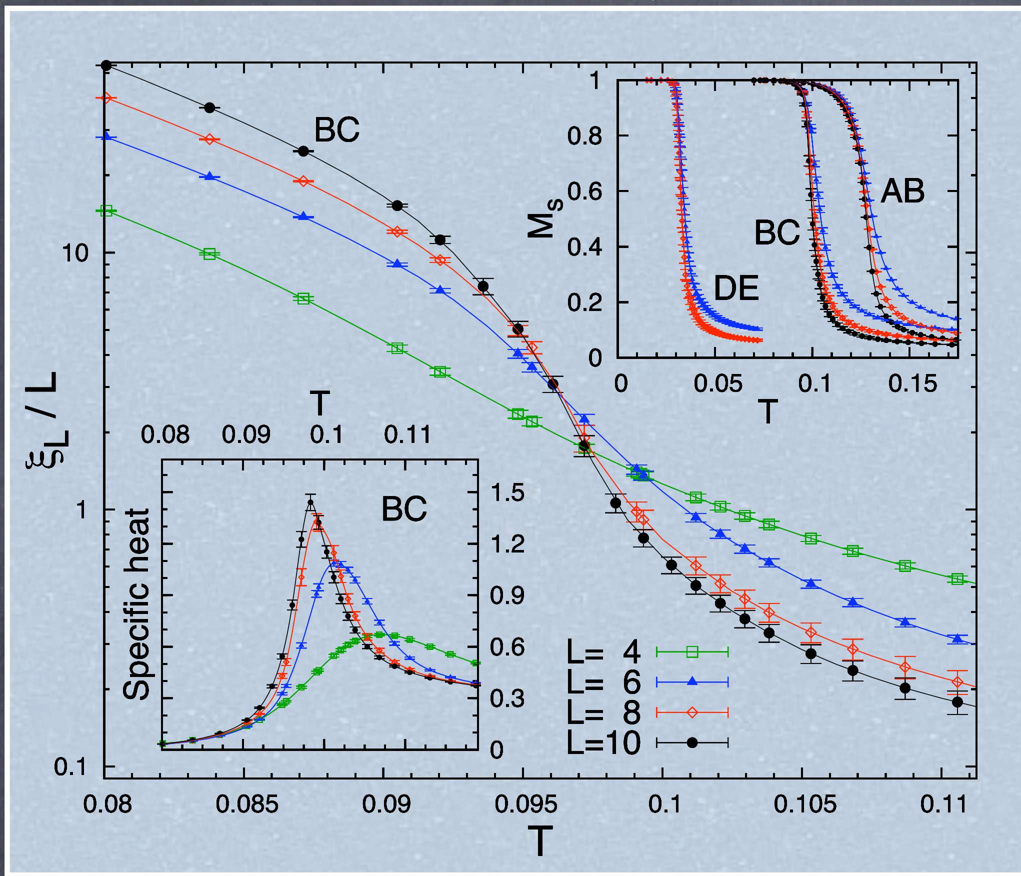
$$T > T_g \qquad \frac{\xi_L^G}{L} \sim \frac{\xi}{L} \to 0 \qquad \text{as } L \to \infty$$

$$T < T_g \qquad \frac{\xi_L^G}{L} \sim L^{d/2} \to \infty$$

$$T = T_g \qquad \frac{\xi_L^G}{L} \to \text{const.}$$

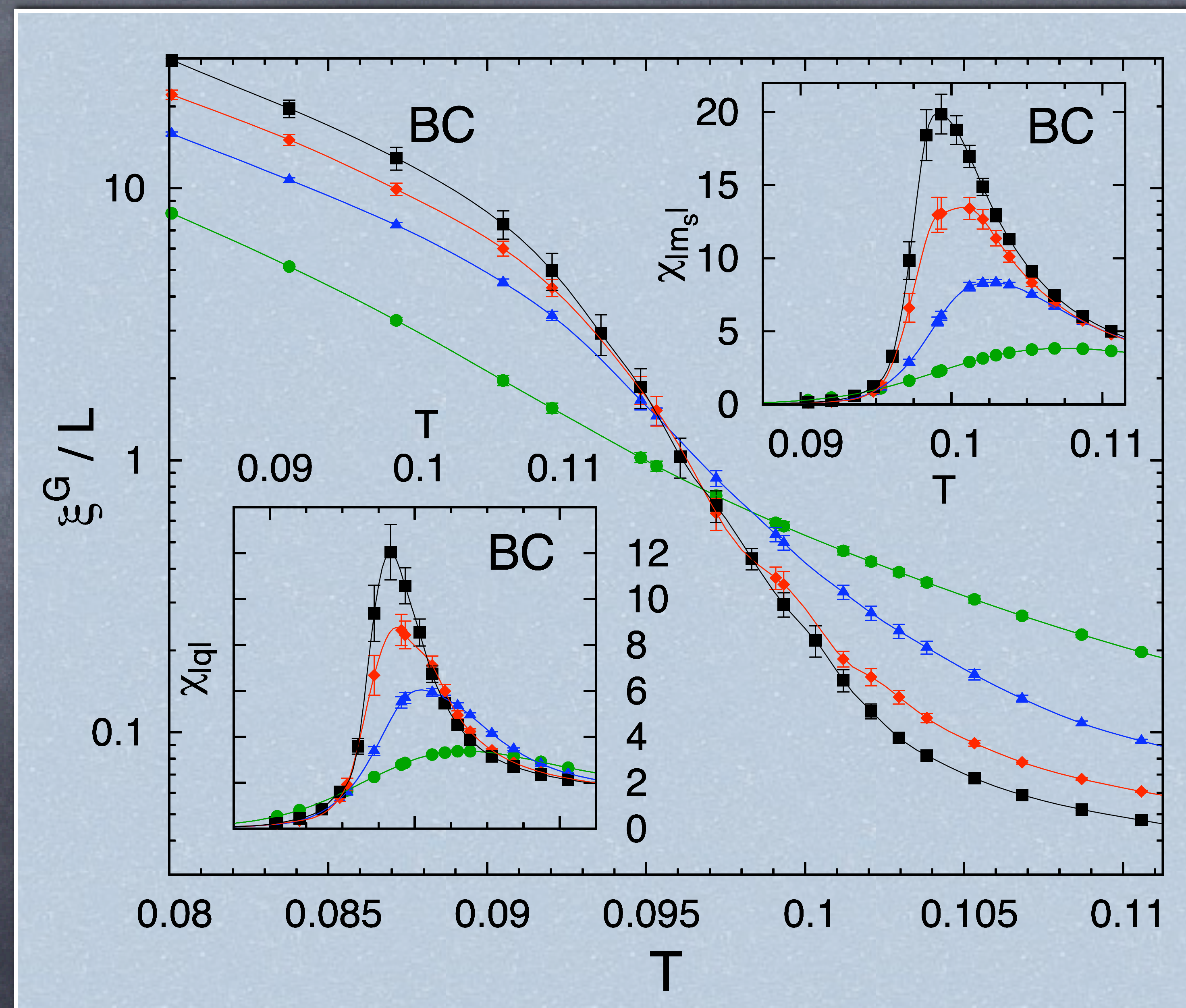
$$\frac{\xi_L^G}{L} = f((T - T_g)L^{1/\nu})$$

Location of the transition to the charge-ordered phase and critical behavior



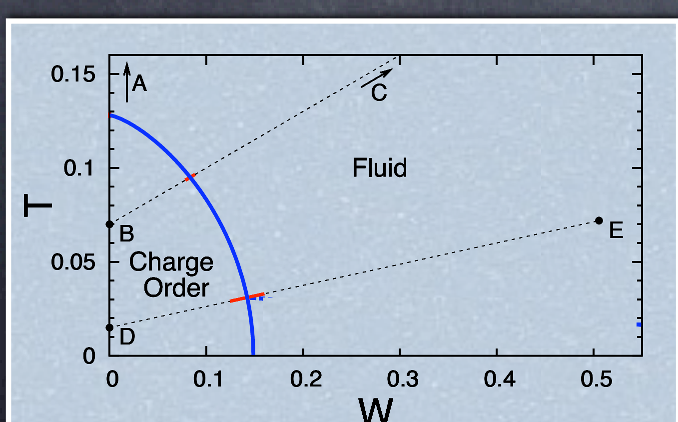
$$\chi_{|m_s|} = N[\langle m_s^2 \rangle - \langle |m_s| \rangle^2]_{av} \qquad m_s = \frac{1}{N} \sum_i \sigma_i$$

$$M_s = [\langle |m_s| \rangle]_{av} \qquad \sigma_i = (2n_i - 1)(-1)^{x_i + y_i + z_i}$$



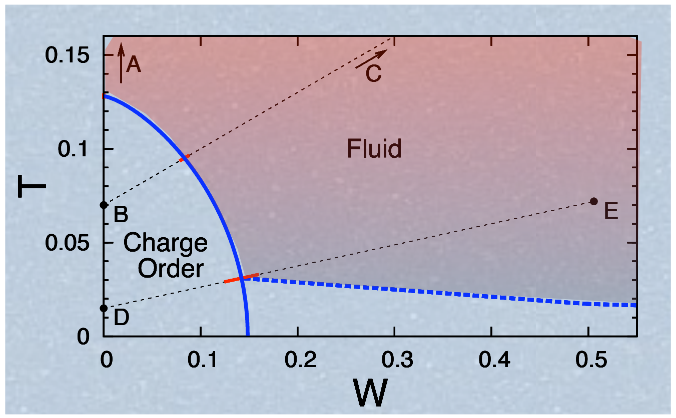
$$\xi_L^G \quad : \quad \xi_L$$

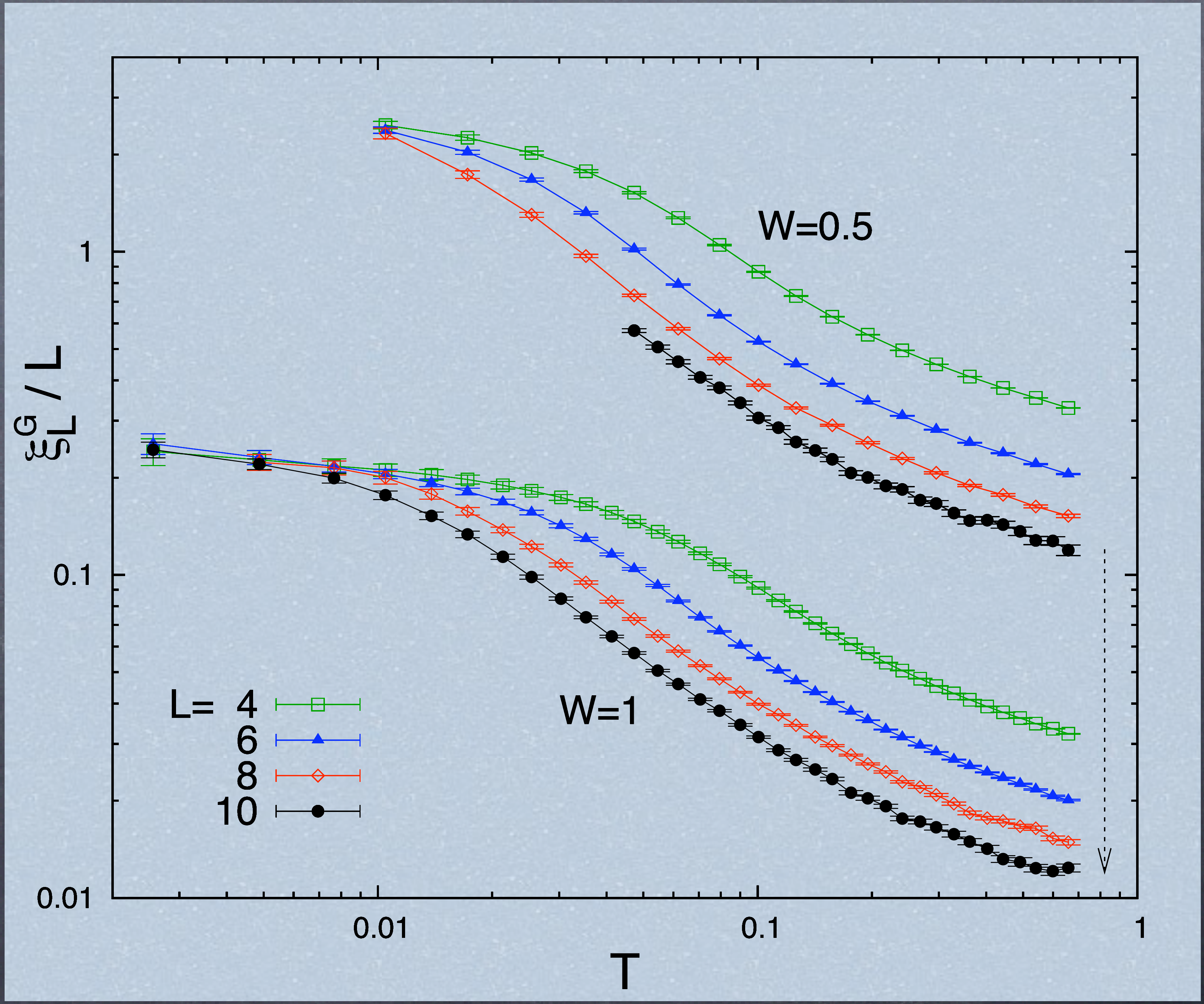
$$(\langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle)^2 \quad : \quad \langle \sigma_i \sigma_j \rangle$$



The correlation length shows no sign of a glass phase down to extremely low temperatures

Similar results:
Surer, Katzgraber, Zimanyi, Allgood, Blatter, PRL 102, 067205 (2009)

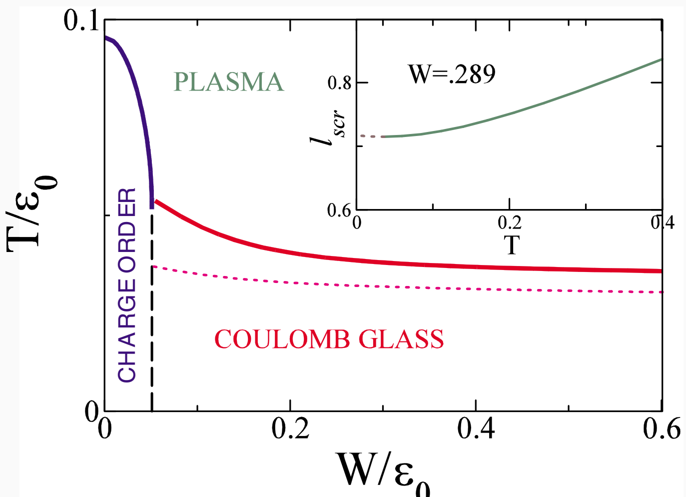


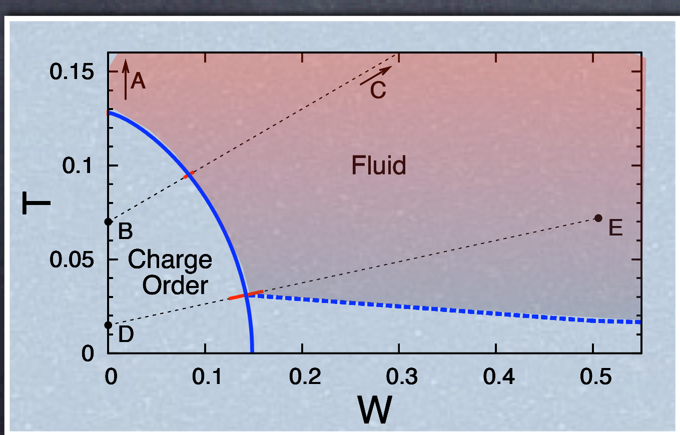


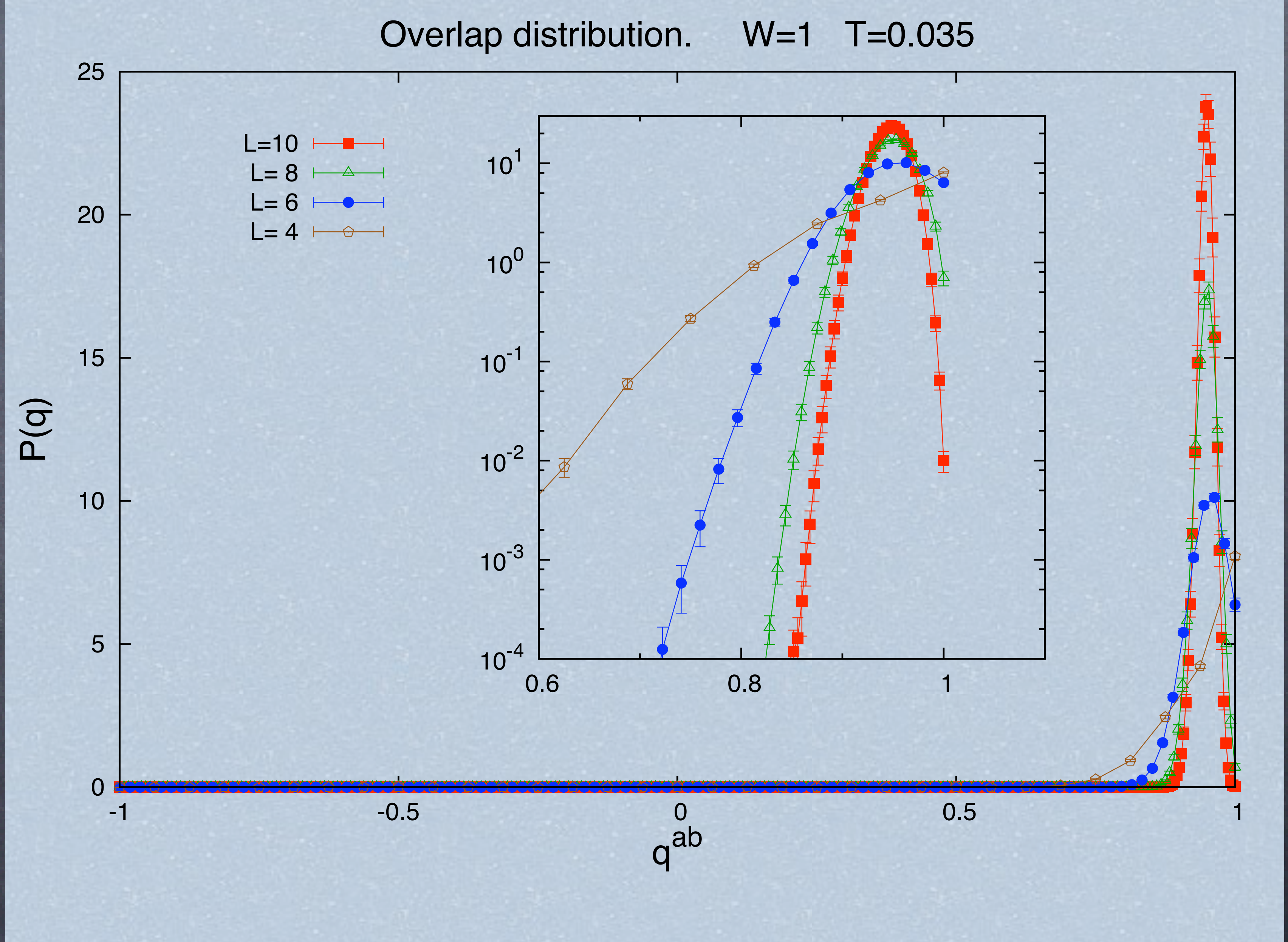
The overlap distribution also shows no sign of a glass phase

Overlap $q^{ab} = \frac{1}{N}\sum_i (2n_i^a - 1)(2n_i^b - 1)$ $P(q) = [\langle\, \delta(q^{a,b} - q)\,\rangle]_{av}$

Pankov & Dobrosavljevic

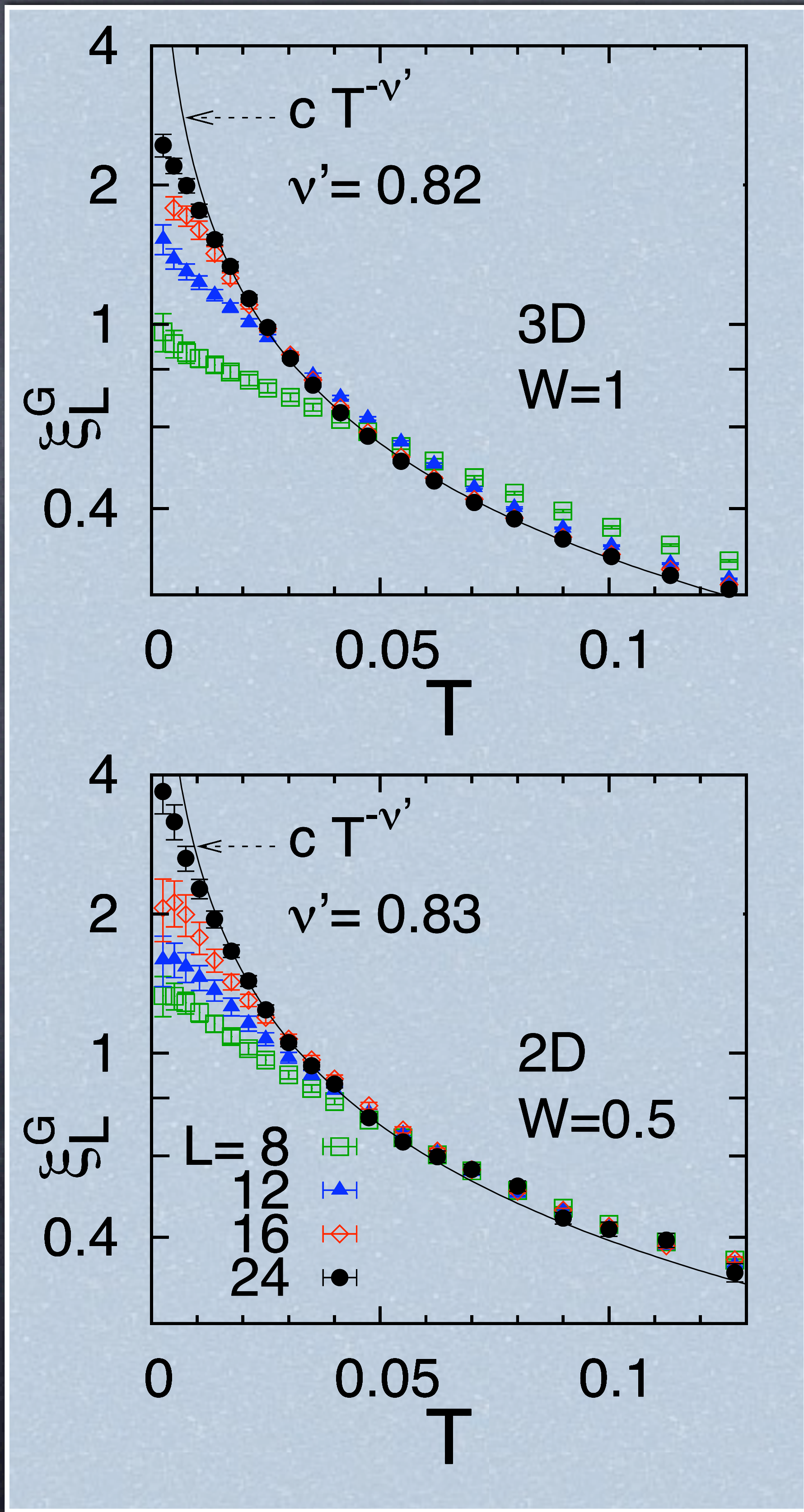


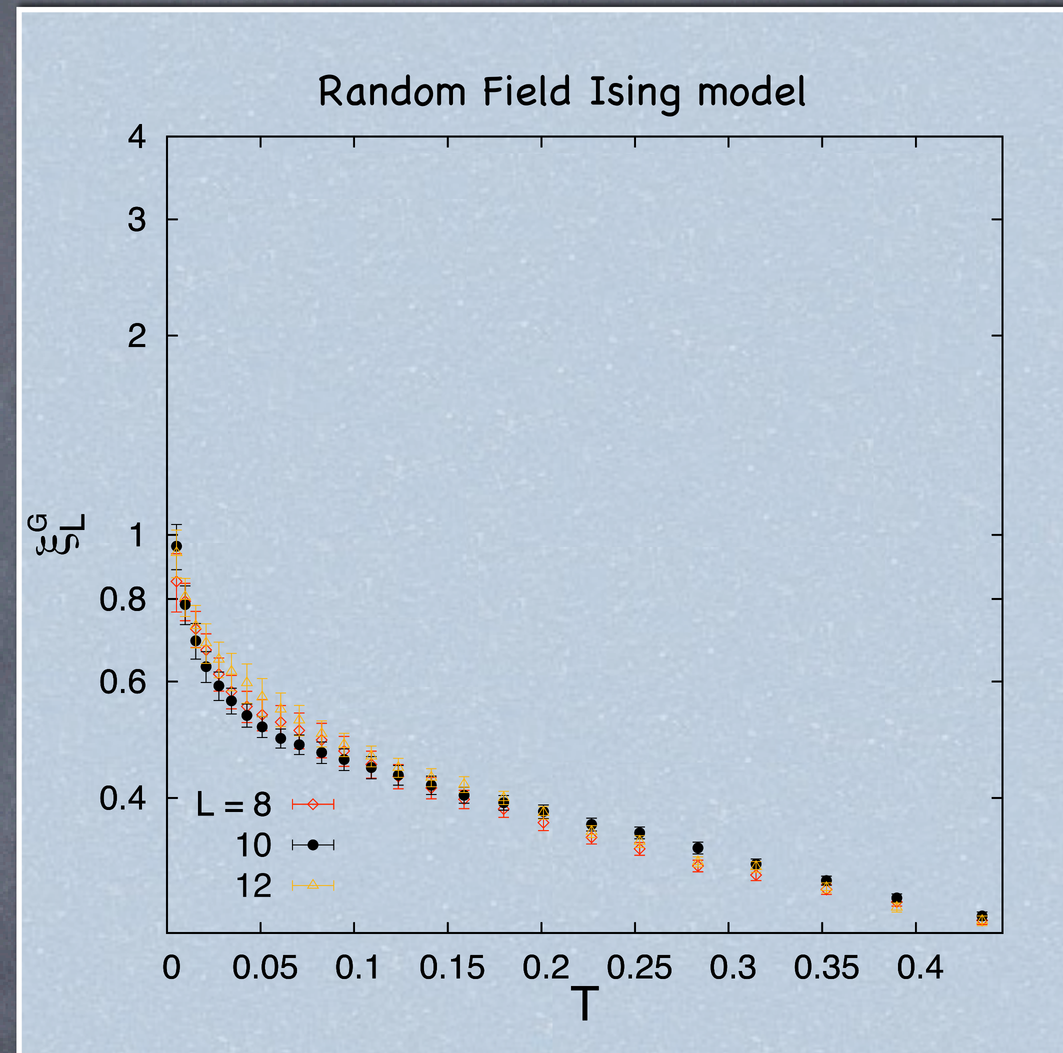




M.Goethe and MP, unpublished

The correlation length behaves similarly in 2D, 3D, and in the 3D RFIM



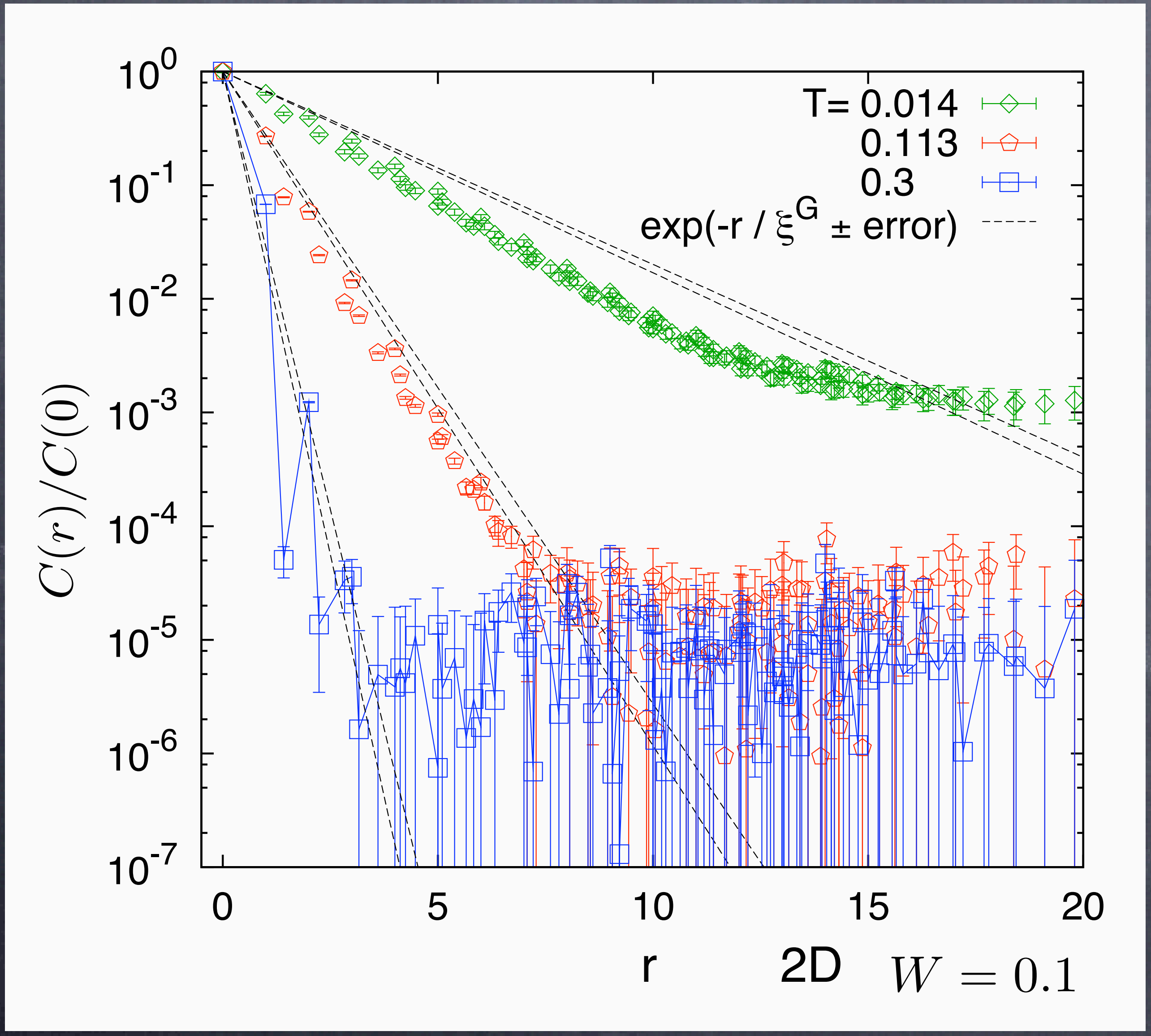


Proposal of a glass phase in the RFIM:

Mezard, Parisi, J. Phys. A23, L1229 (1990)
Mezard, Young, Europhys. Lett. 18, 653(1992).
Mezard, Monasson, Phys.Rev. B50, 7199(1994)
Brezin, DeDominicis, Europhys. Lett. 44, 13(1998);
Parisi, V.S.. Dotsenko, J. Phys. A25, 3143(1992)

Measurement of the correlation function in 2D

$$C(\mathbf{r}_{ij}) = [(\langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle)^2\,]_{av}$$



The Coulomb gap

- Pollak (1970), Srinivasan (1971): the long-range Coulomb interaction depletes the single-particle density of states at the Fermi level

- Efros-Shklovskii (1975): $$g(\epsilon) = \frac{1}{V}\sum_{i=1}^{N}[\langle\delta(\epsilon-\epsilon_i)\rangle]_{av} \leq \; c_d\,|\epsilon-\mu|^{d-1}$$

$$\epsilon_i = \sum_{j\neq i}\frac{n_j - K}{r_{ij}} + \varphi_i$$

$$|\epsilon-\mu| \ll \Delta \sim W^{-1/2}$$

- Variable-range hopping conductivity (assuming saturated bound d-1):

Mott law

$$\sigma = \sigma_0 \exp - \left(\frac{T_M}{T}\right)^{1/4}$$

$\longrightarrow$

Efros-Shklovskii law

$$\sigma = \sigma_0 \exp - \left(\frac{T_{ES}}{T}\right)^{1/2}$$

- Self consistent methods: $c_3 = 3/\pi, c_2 = 2/\pi$

  (Efros 1976, Baranovskii et al. 1978, Mogilyanskii and Raikh 1989)

- Mean-field theory: - saturated ES bound

  (Müller and Pankov, 2007) - gap width $\Delta \sim T_g$

- Thermal filling of the gap: $g(\epsilon, T) \sim T^{d-1}\;\tilde{g}(|\epsilon|/T) \underset{\epsilon/T \ll 1}{\sim} T^{d-1}$

Experimental observation of the Coulomb gap

Massey and Lee, PRL 1995 (Si:B)

Conductivity

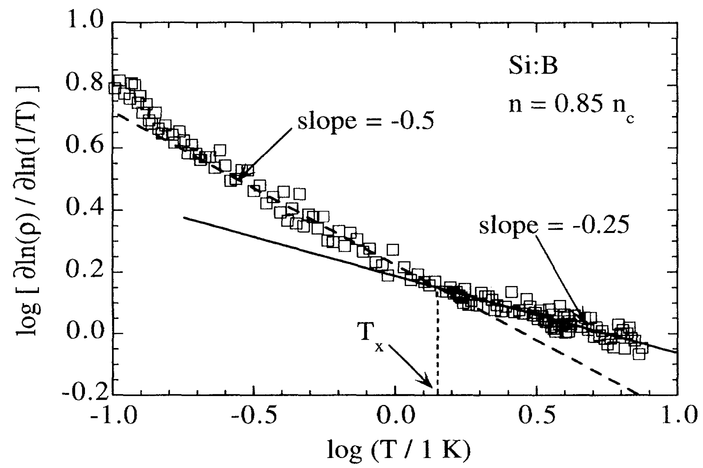
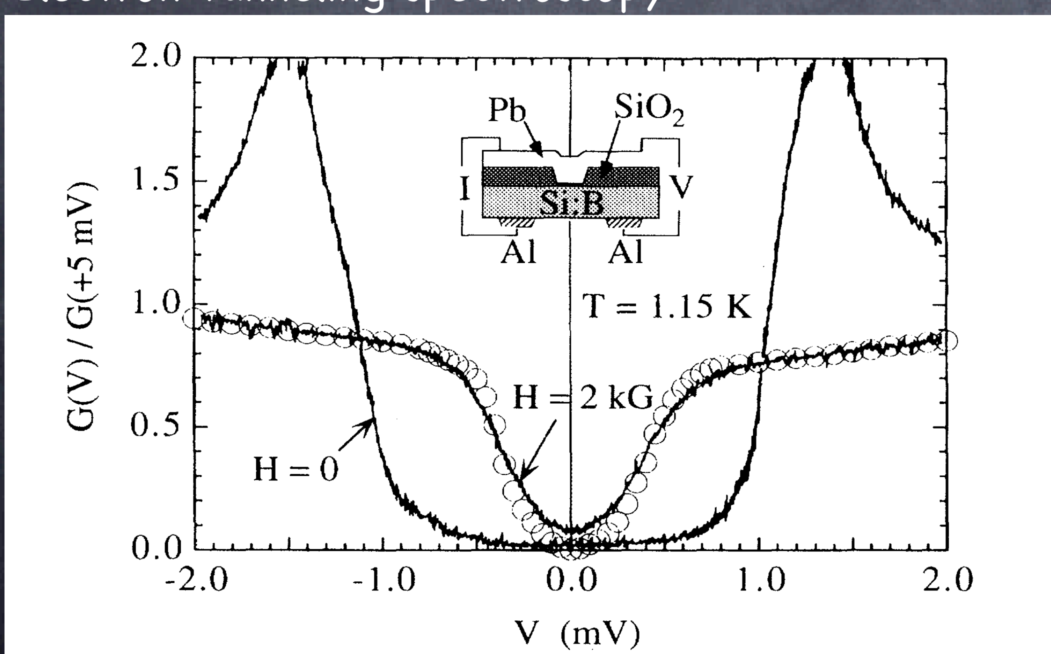


FIG. 3. Plot of $\log[\partial\ln(\rho)/\partial(1/T)]$ vs $\log[T]$. The slope of the data gives the negative of the hopping exponent. The solid line is a linear fit to the range $1.5 < T < 10$ K. The dashed line is a linear fit in the range $0.3 < T < 0.8$ K. These lines intersect at 1.4 K.

Electron tunneling spectroscopy



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Electronic Correlation Effects and the Coulomb Gap at Finite Temperature

B. Sandow,[1] K. Gloos,[2,3] R. Rentzsch,[1] A. N. Ionov,[4] and W. Schirmacher[5]

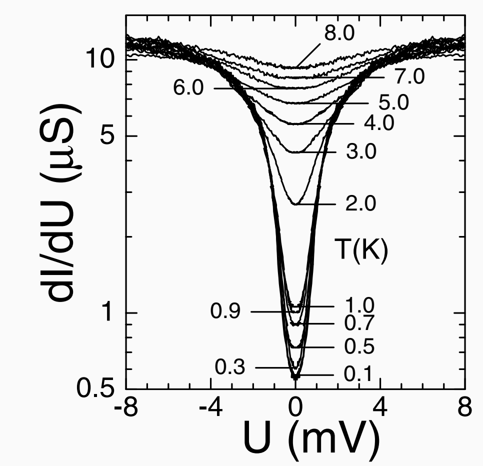


FIG. 1. dI/dU vs U spectra of the Ge sample with $N_d = 1.26 \times 10^{17}$ cm^{-3} at the indicated temperatures.

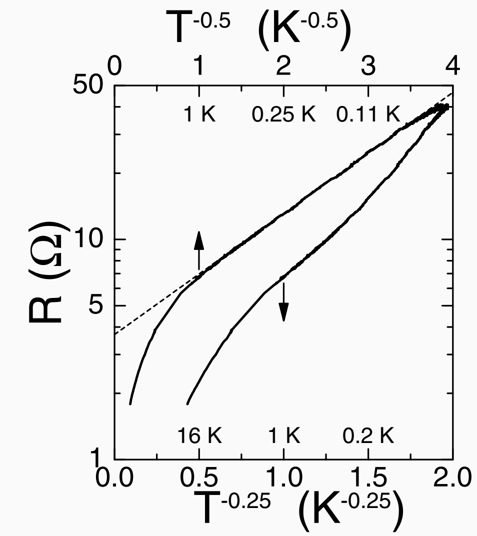


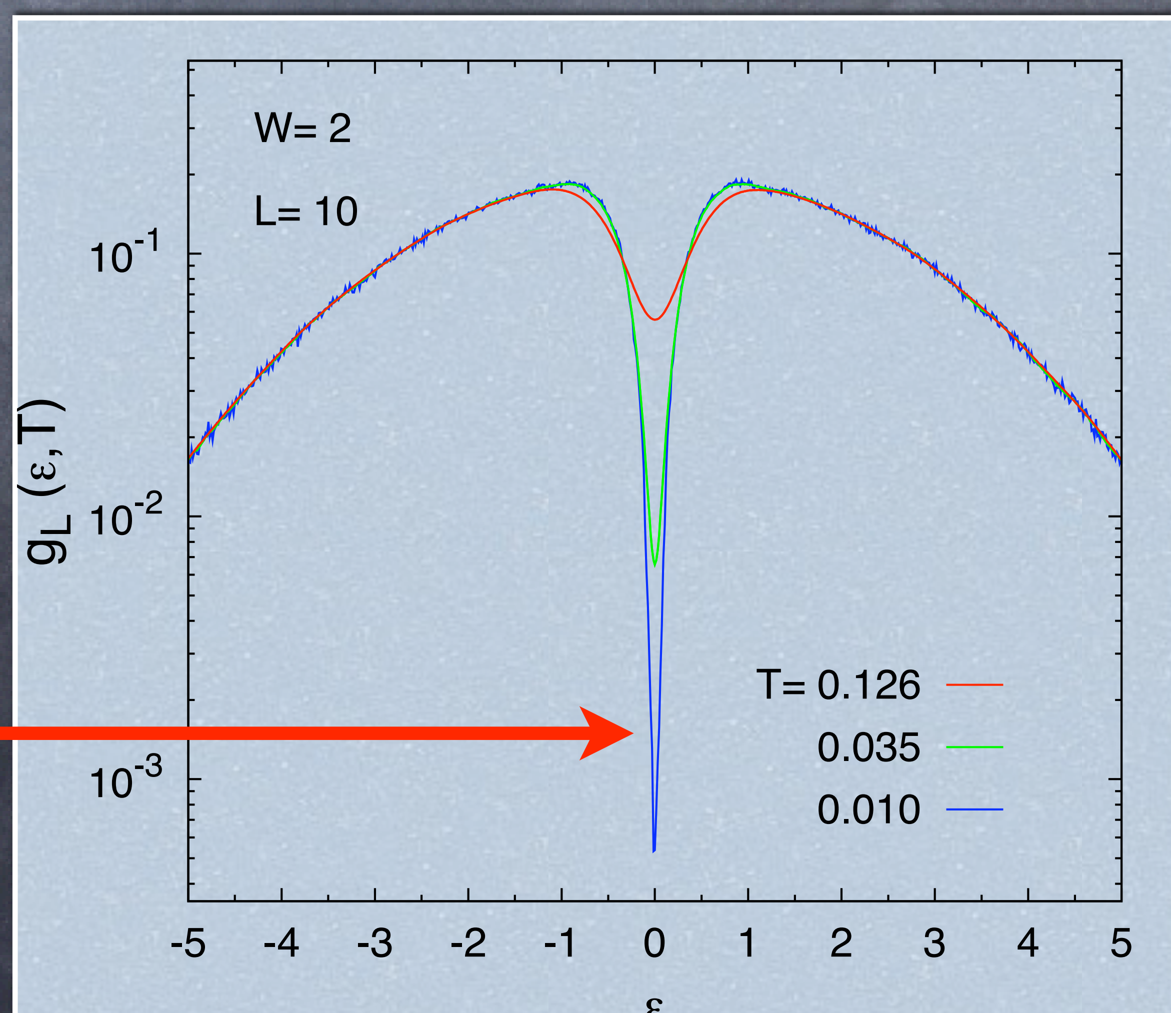
FIG. 2. Electrical resistance of the bulk Ge sample R vs $T^{1/4}$ and $T^{1/2}$, respectively. The dashed line is a fit to the ES law with $T_{ES} = 0.40$ K. $N_d = 1.26 \times 10^{17}$ cm^{-3}.

Numerical studies of the Coulomb gap

$$g(\epsilon) = c_d|\epsilon - \mu|^\delta$$

Baranovskii, Efros, Gelmont, Shklovskii, J. Phys. C (1979)
Davies, Lee, Rice, PRB (1984)
Li, Phillips, PRB (1994). $\delta = 2.38 \ \ (3\mathrm{D})$
Moebius, Richter, Drittler, PRB (1992) $\delta = 2.6 \pm 0.2 \ \ (3\mathrm{D}); 1.2 \pm 0.1 \ \ (2\mathrm{D})$
Sarvestani, Schreiber, Vojta, PRB (1995). $\delta = 2.7 \ \ (3\mathrm{D}); 1.75 \ \ (2\mathrm{D})$
Overlin, Wong, Yu, PRB (2004). $2.1 \leq \delta \leq 2.6 \ \ (3\mathrm{D})$

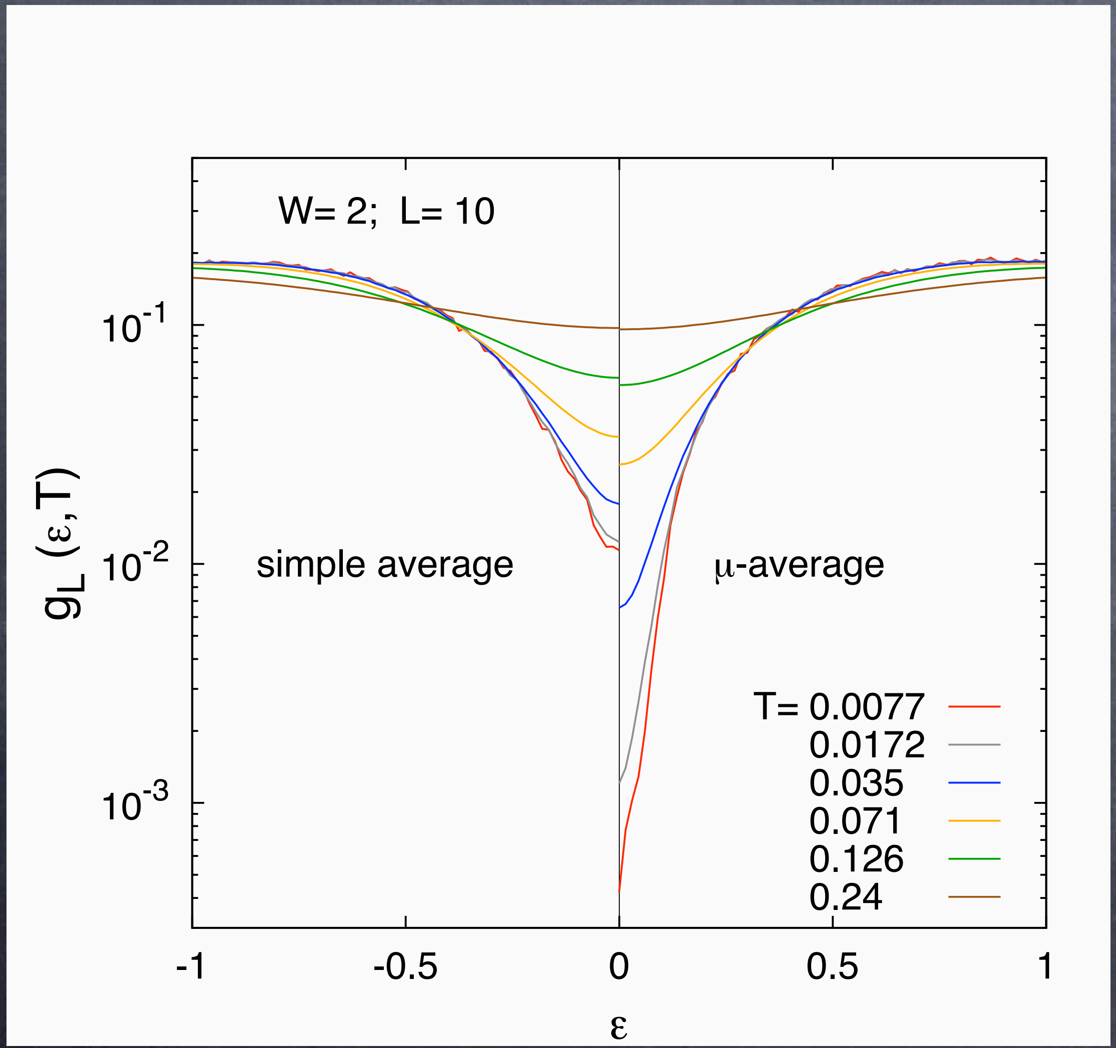
M.Goethe and MP



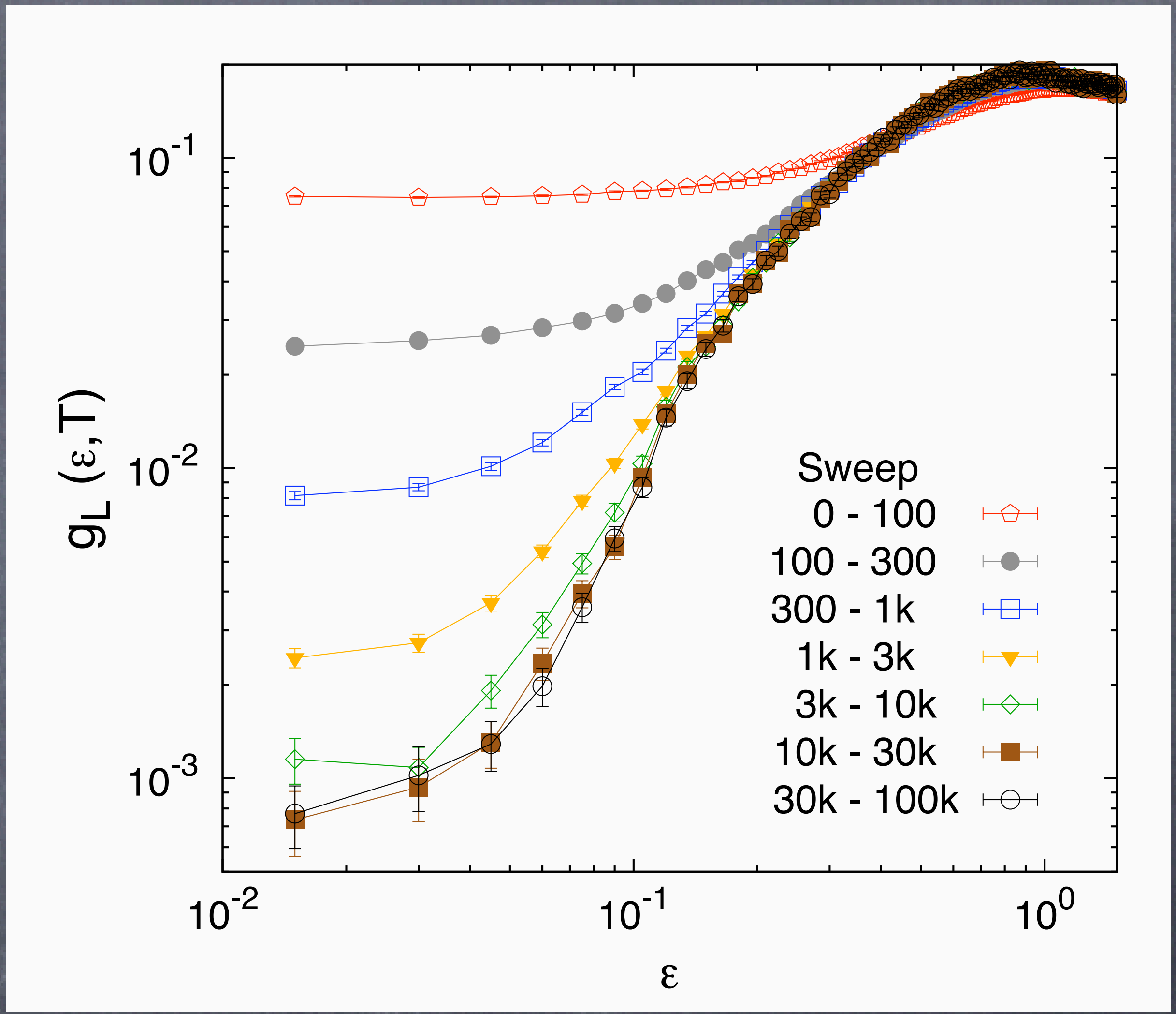
Determining the single particle DOS at finite T

1. Parallel tempering MC

2. Shift the chemical potential to reduce finite-size effects



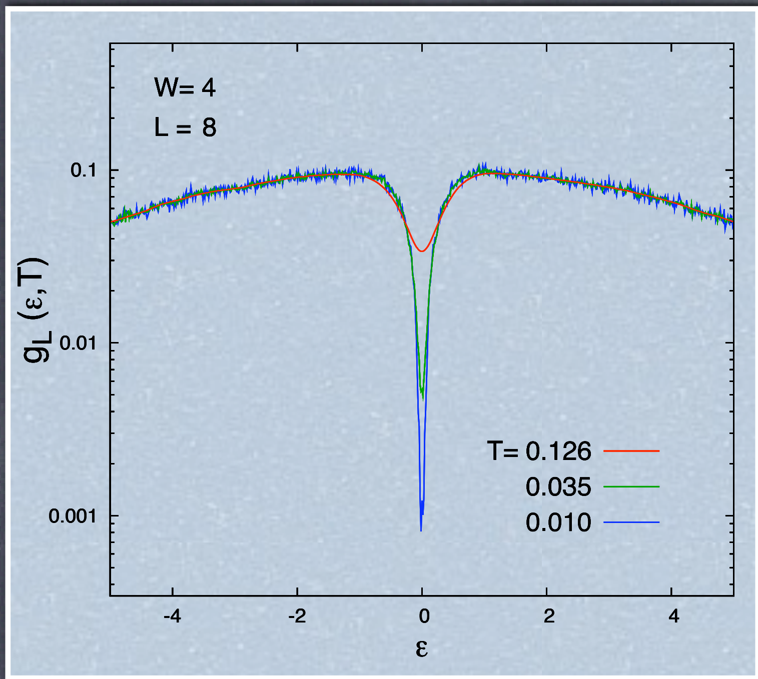
3. Check relaxation to equilibrium

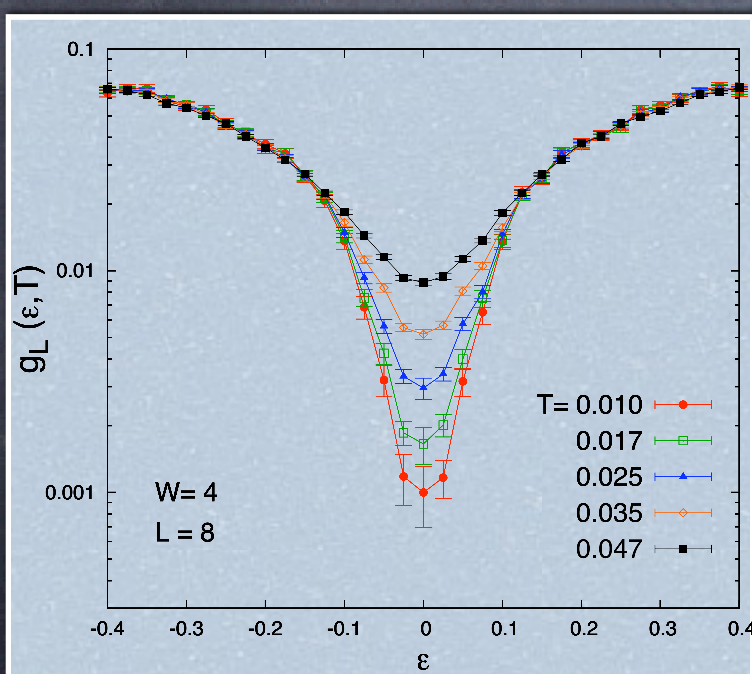


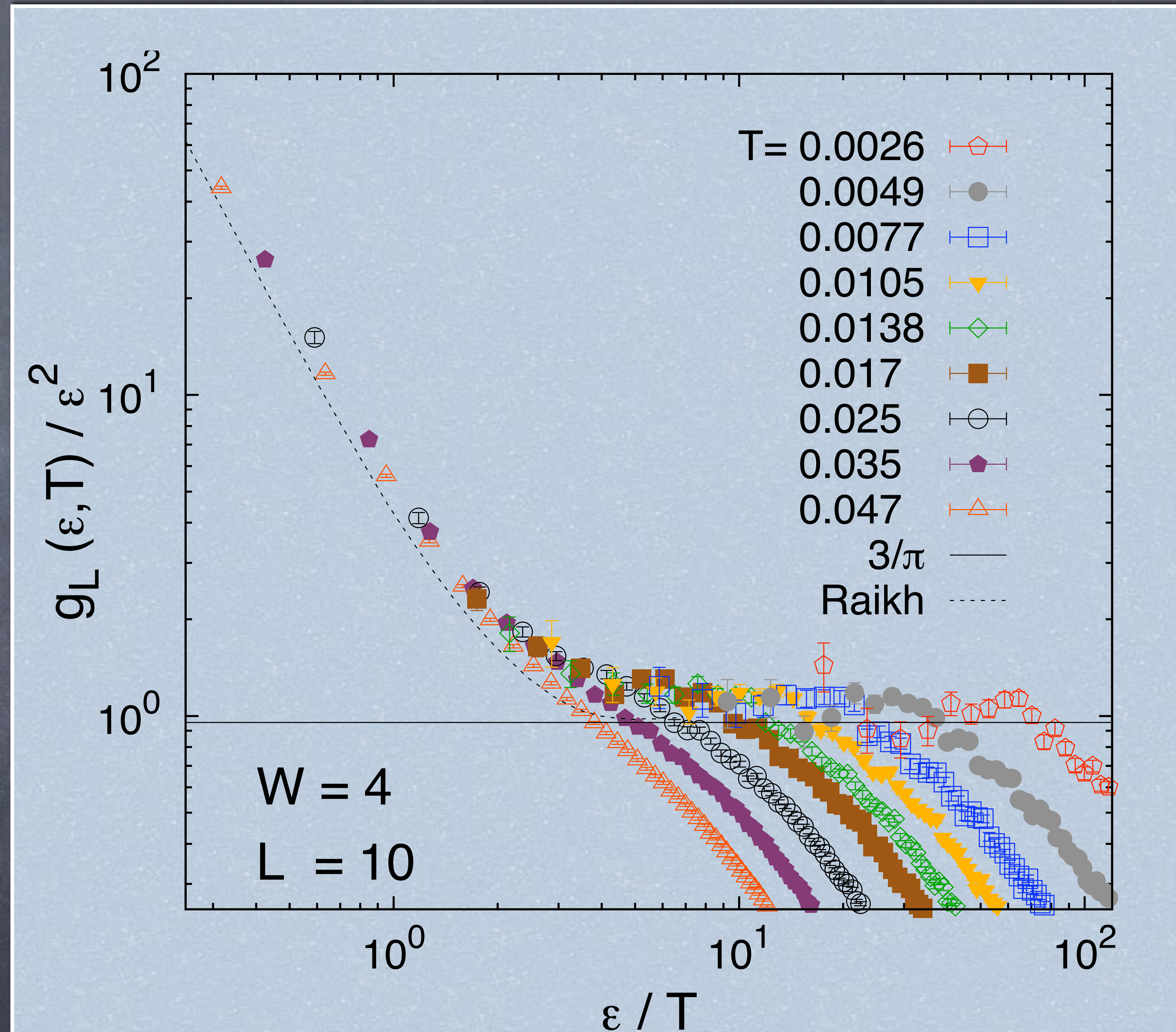
4. Use large disorder

5. Size and temperature scaling

Results at large disorder agree with saturated ES bound $\delta = 2$. Crossover to a hard gap at low disorder.







$$g(\epsilon, T) \sim T^{\delta} f(\epsilon/T)$$

Mogilyanskii and Raikh (1989)

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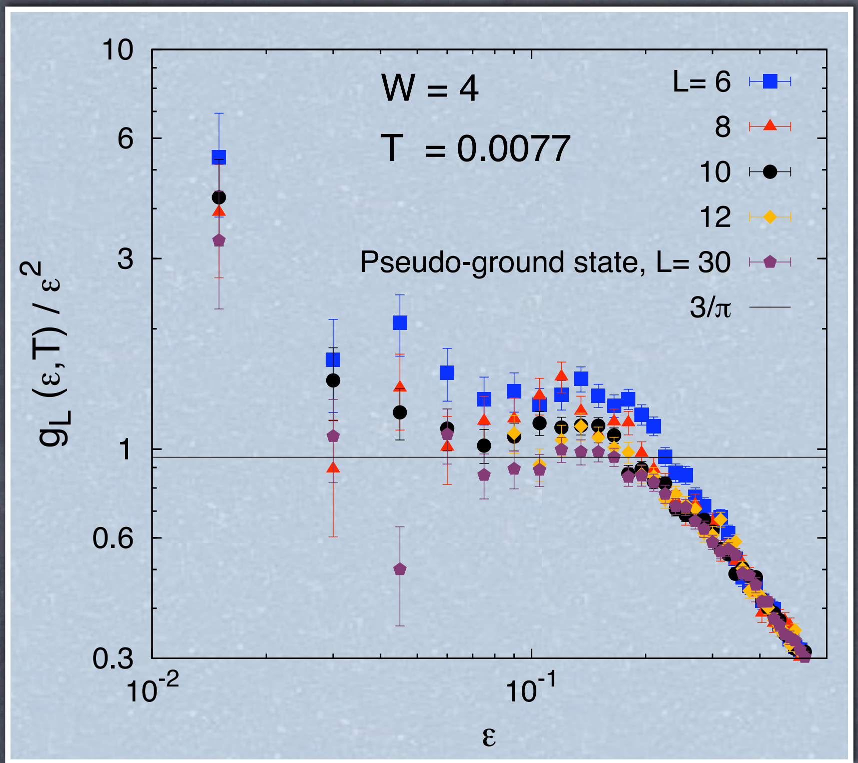

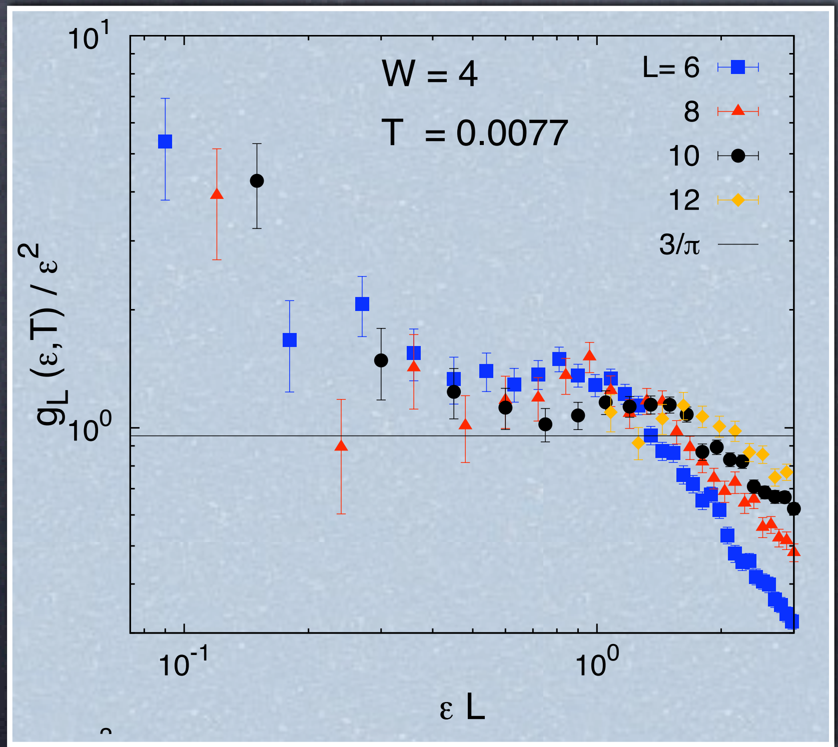

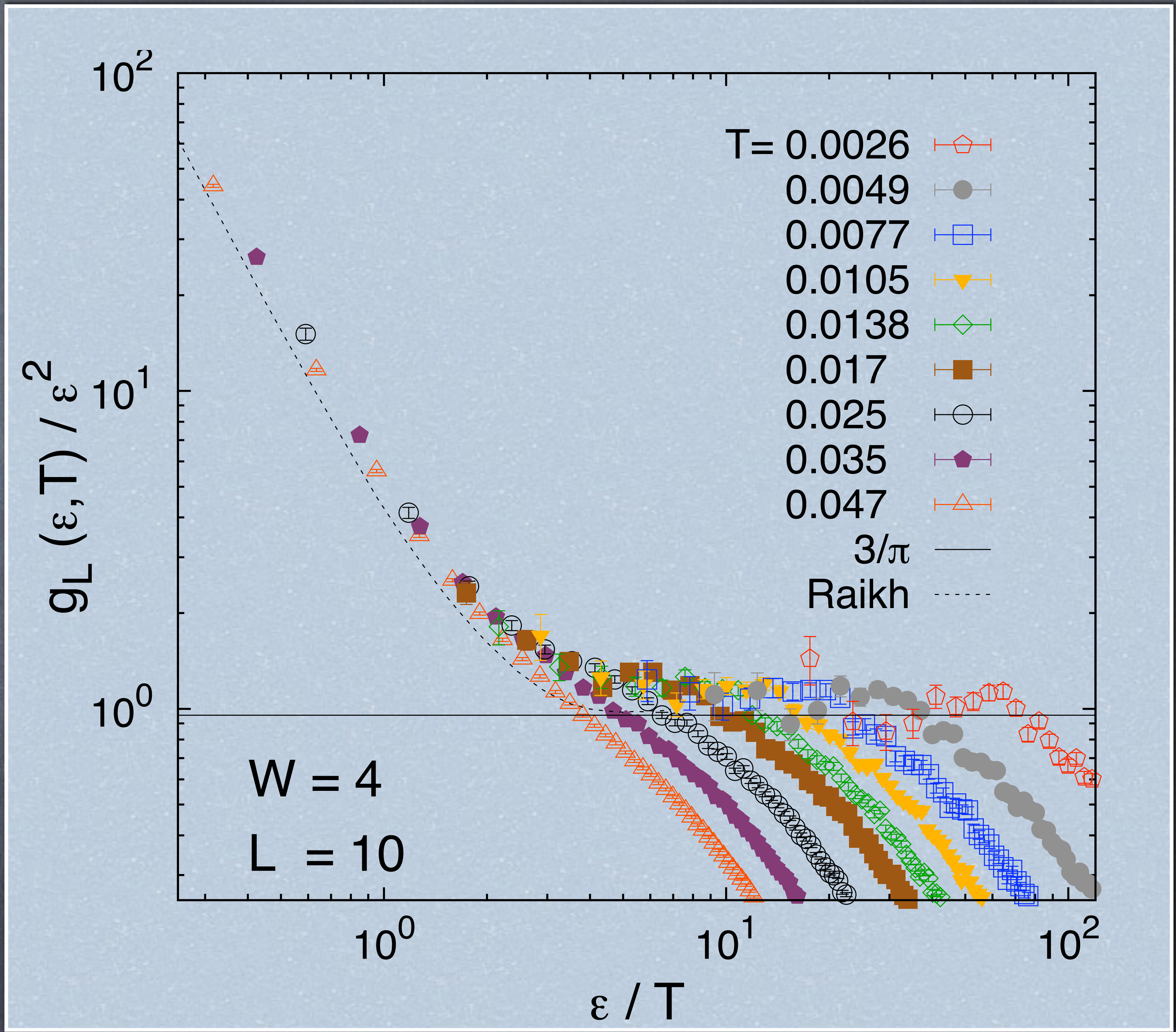

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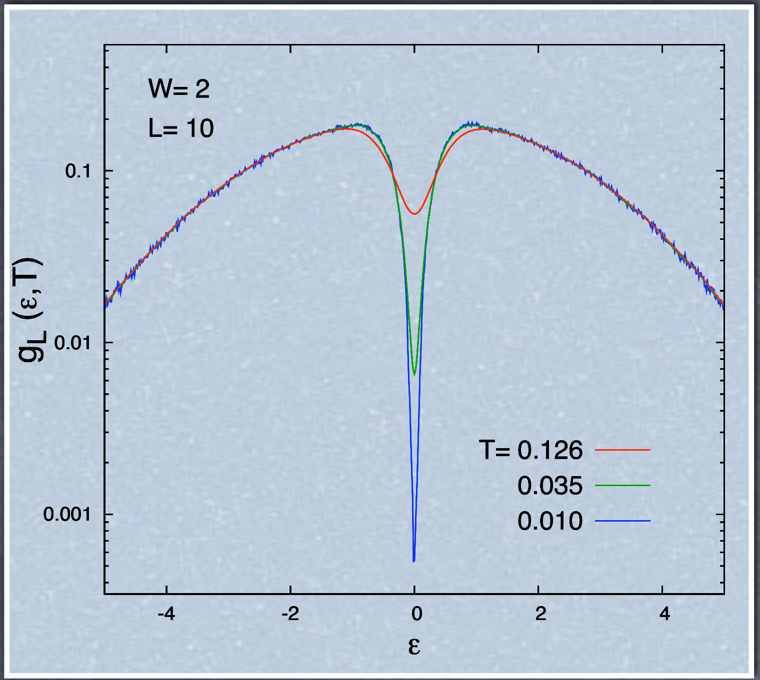

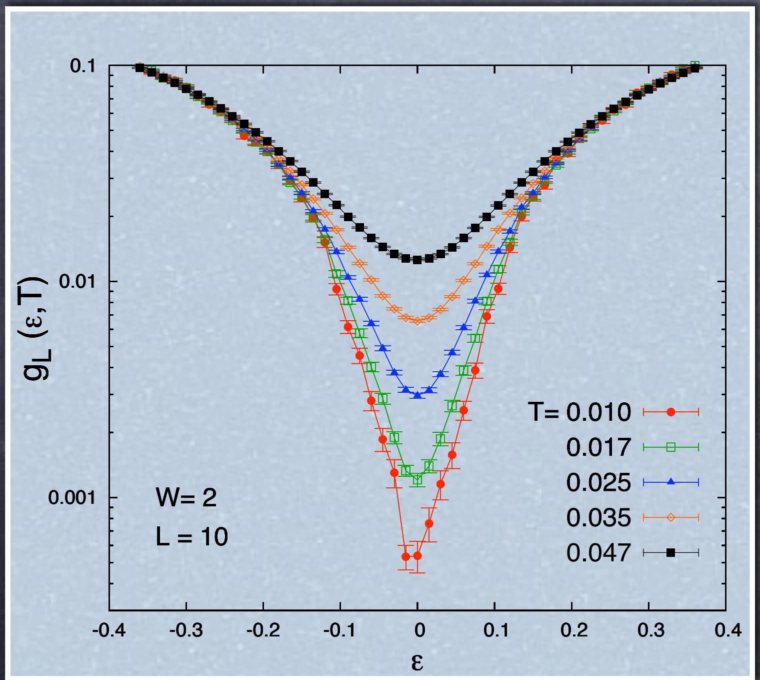

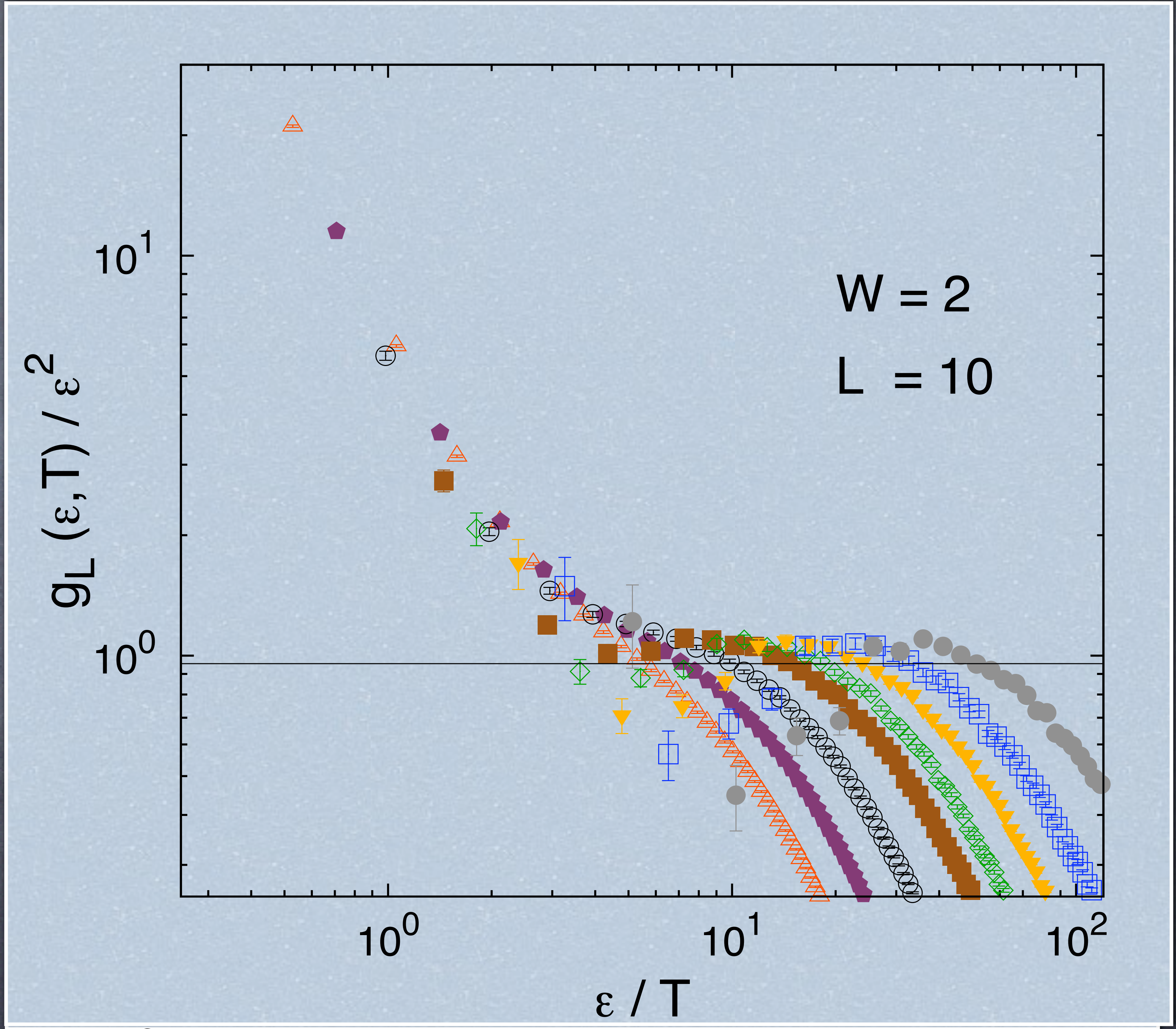

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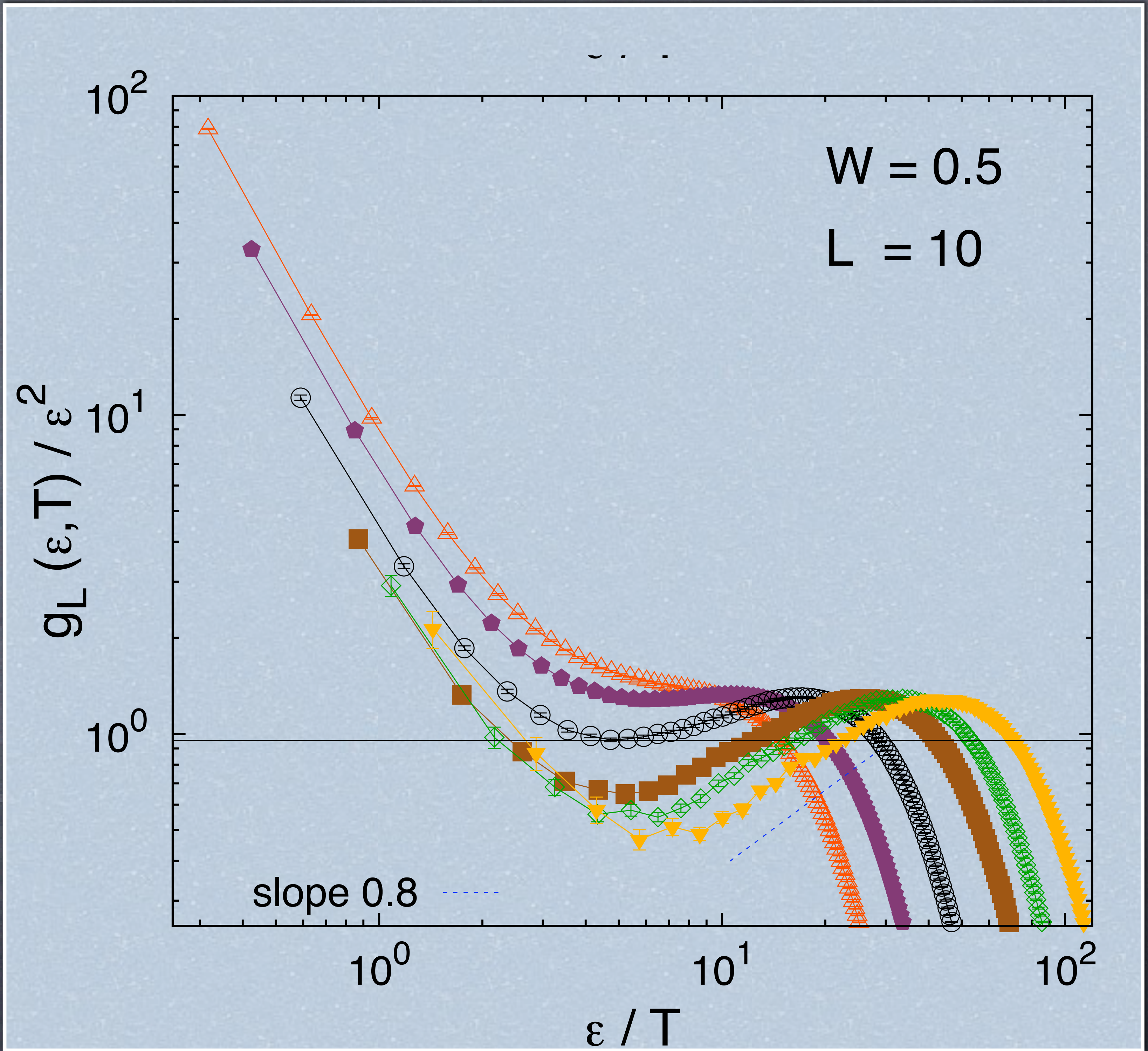

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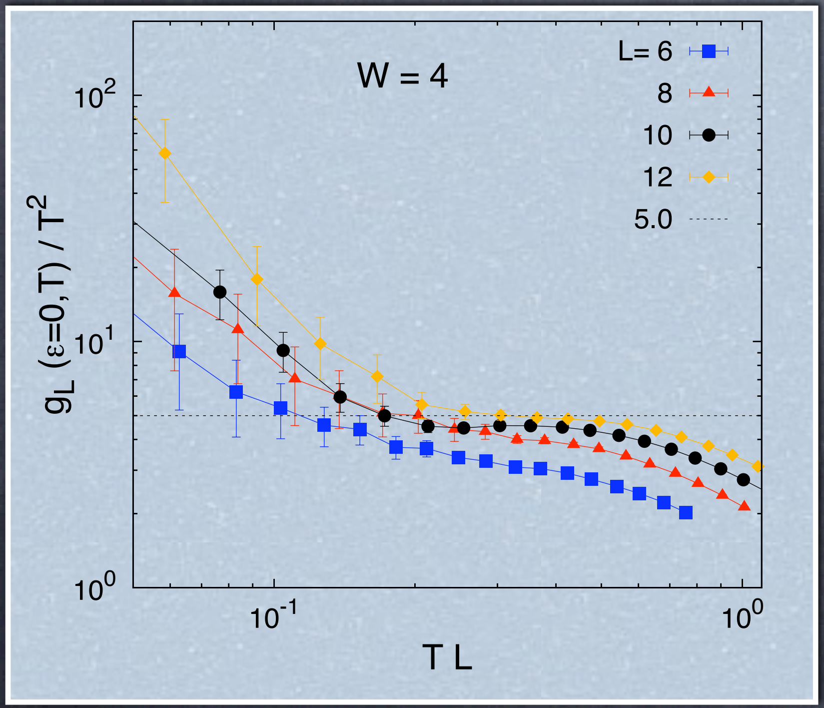
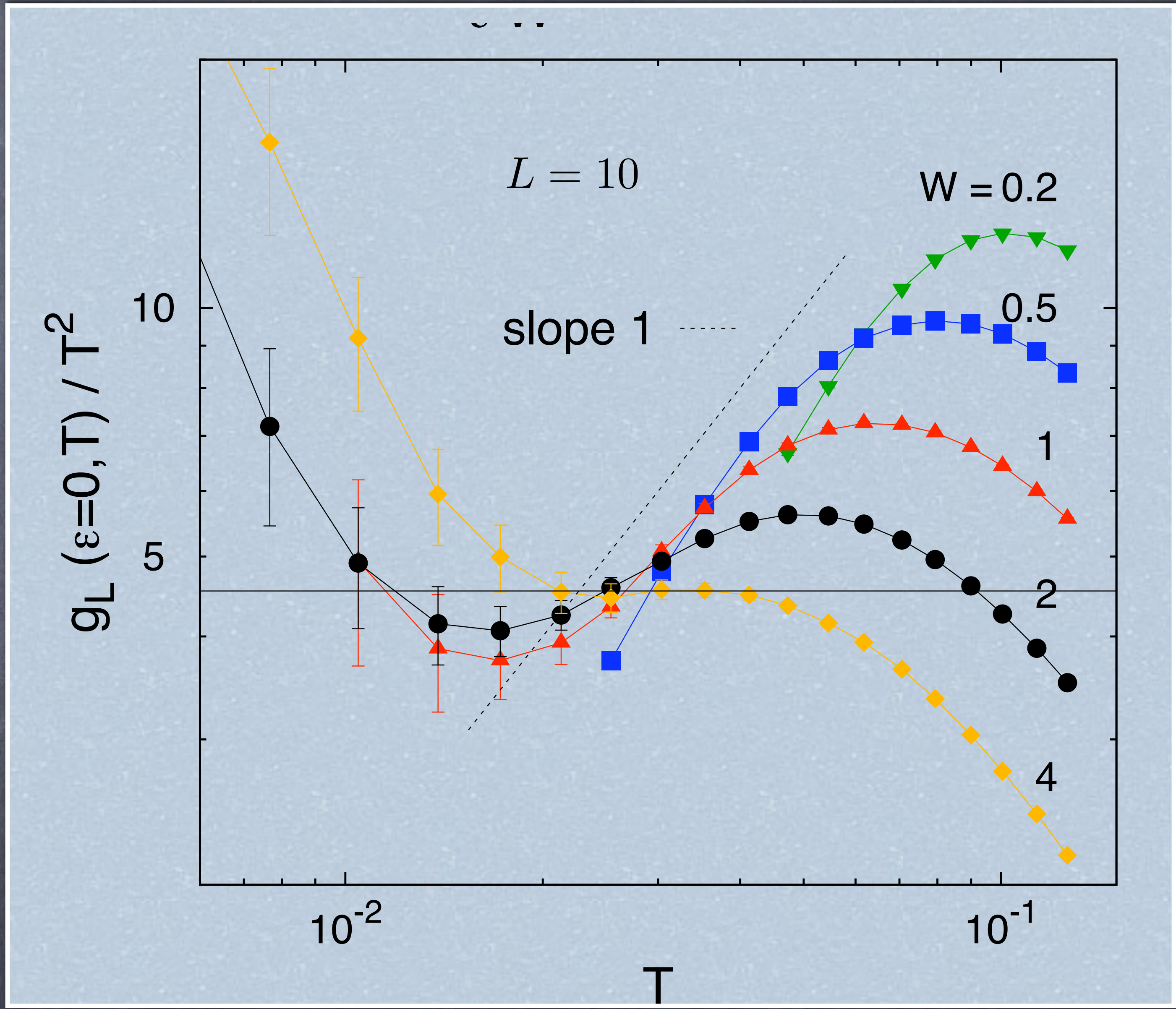
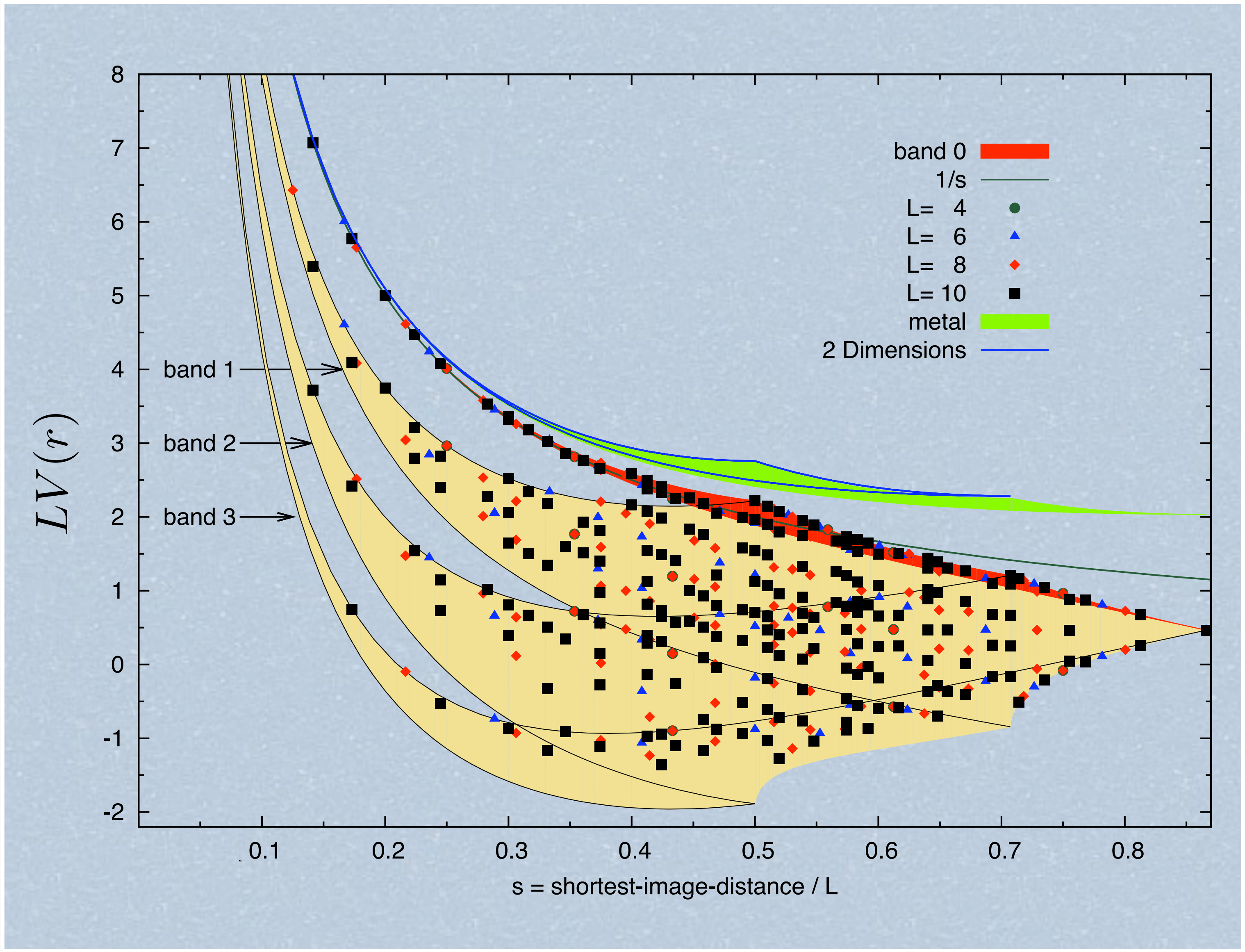


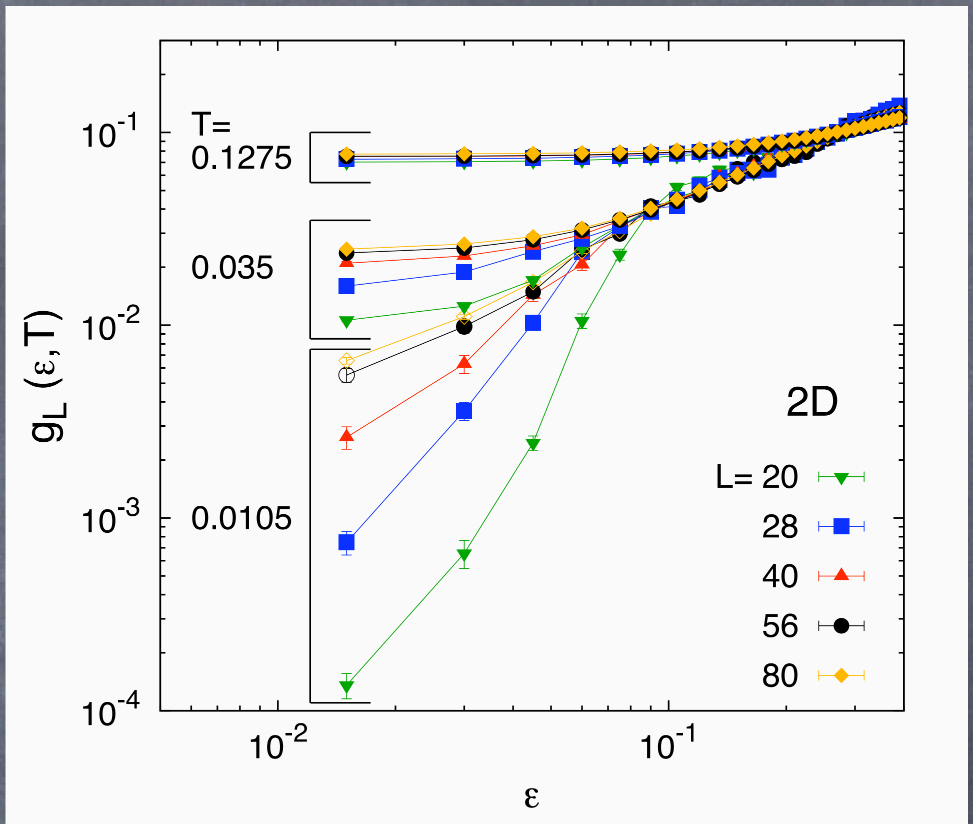


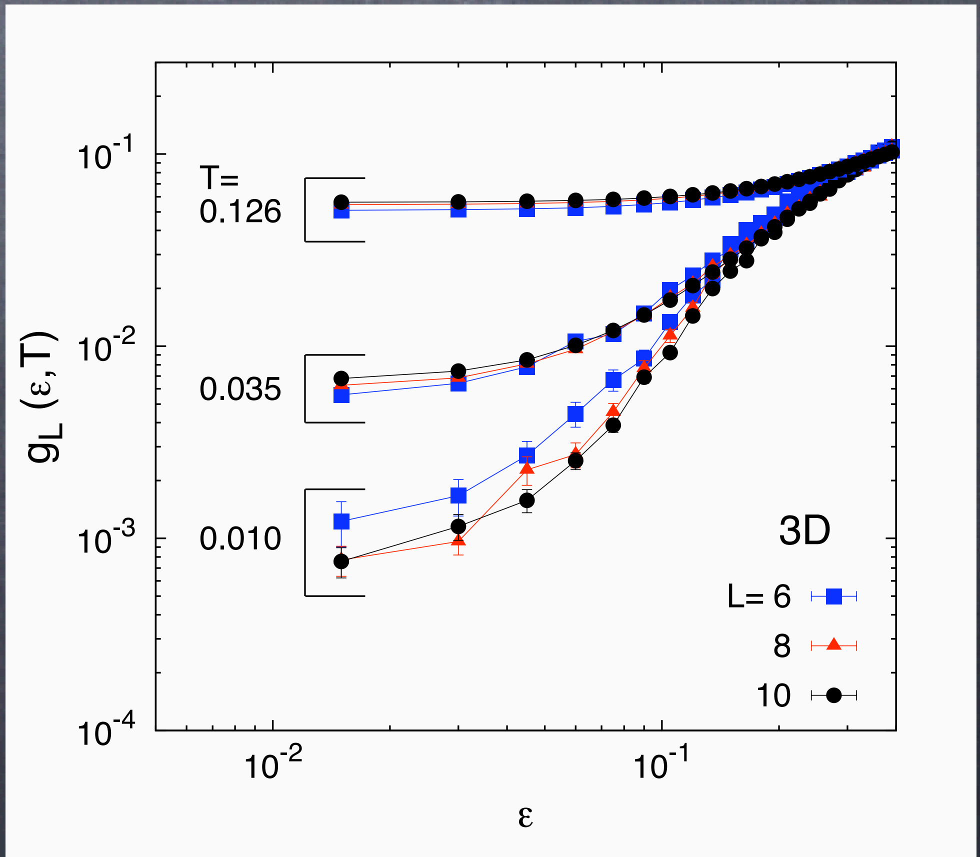
With an infinite periodic system, finite size effects are stronger in 2D than in 3D (with vacuum surrounding media)

$$\Delta E_{i\to j} = \epsilon_j - \epsilon_i - V(\mathbf{r}_{ij})$$

$$V(\mathbf{r}_{ij}) \equiv \frac{1}{|\mathbf{r}_{ij}|} - \sum_{\substack{\mathbf{m}\\ \mathbf{m}\neq 0}} \left[\frac{1}{|\mathbf{m}|} - \frac{1}{|\mathbf{r}_{ij}+\mathbf{m}|}\right] = \frac{1}{L}\tilde{V}\left(\frac{\mathbf{r}}{L}\right)$$

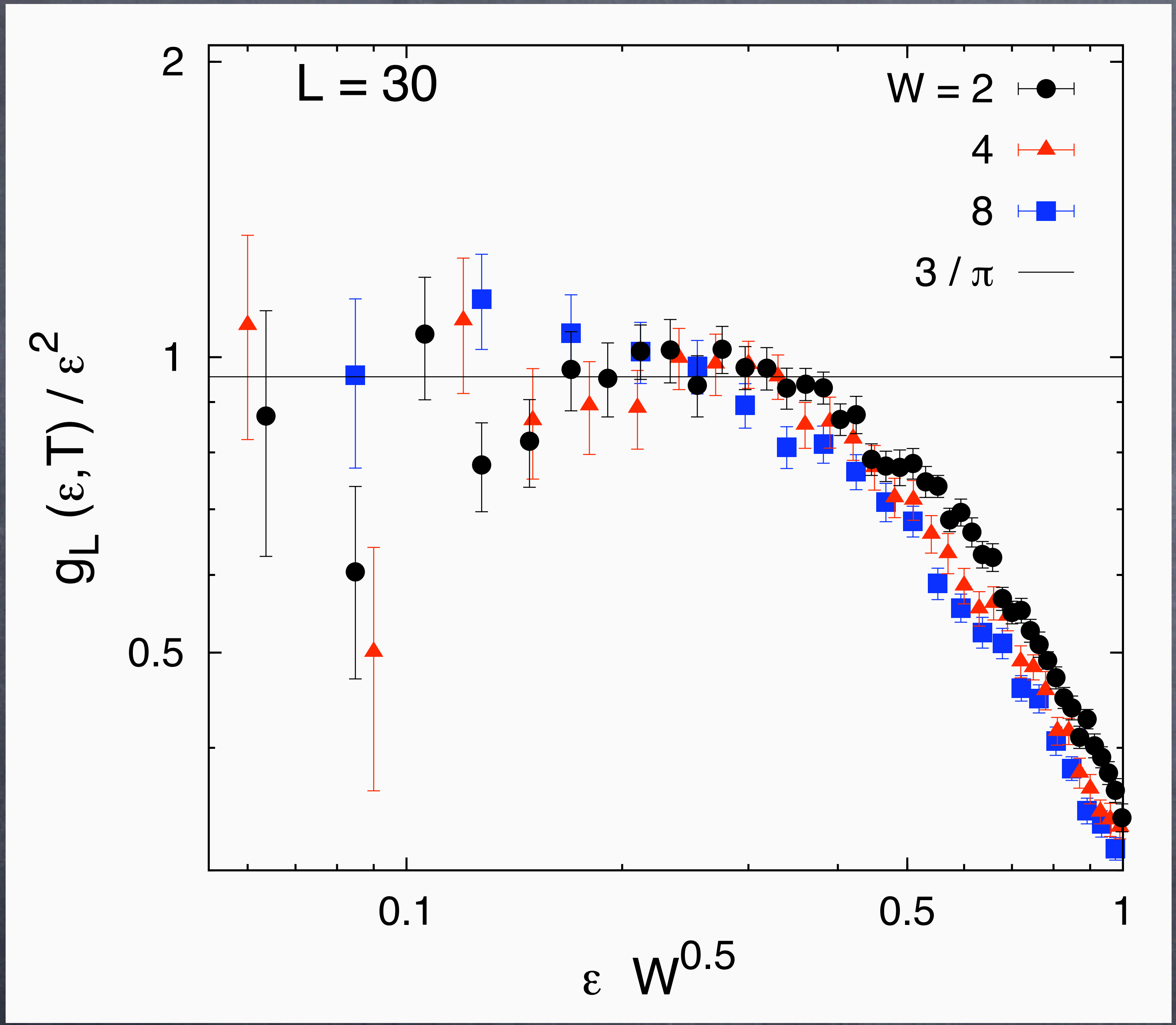


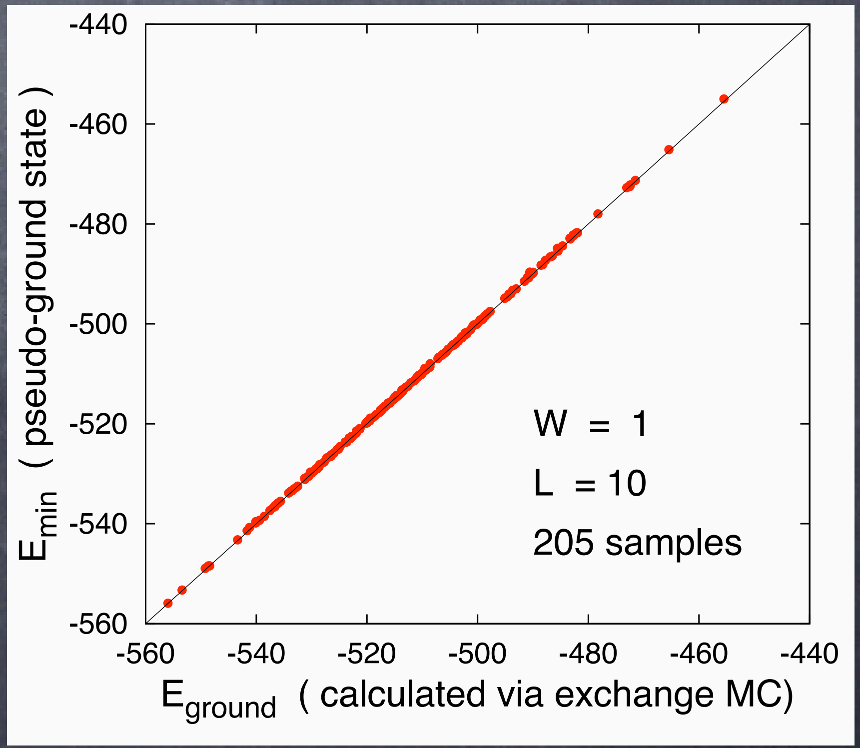




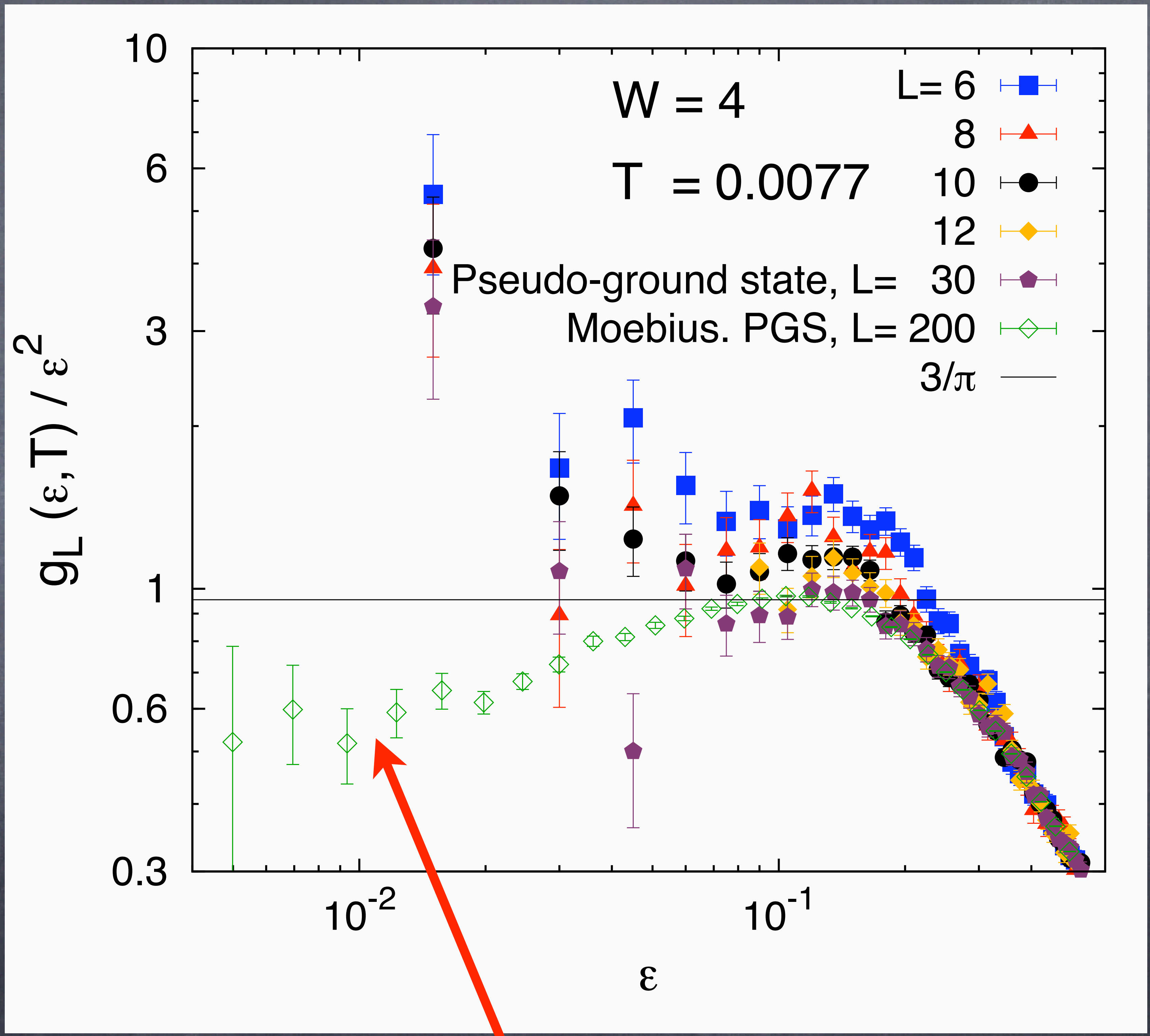
M.Goethe and MP, unpublished

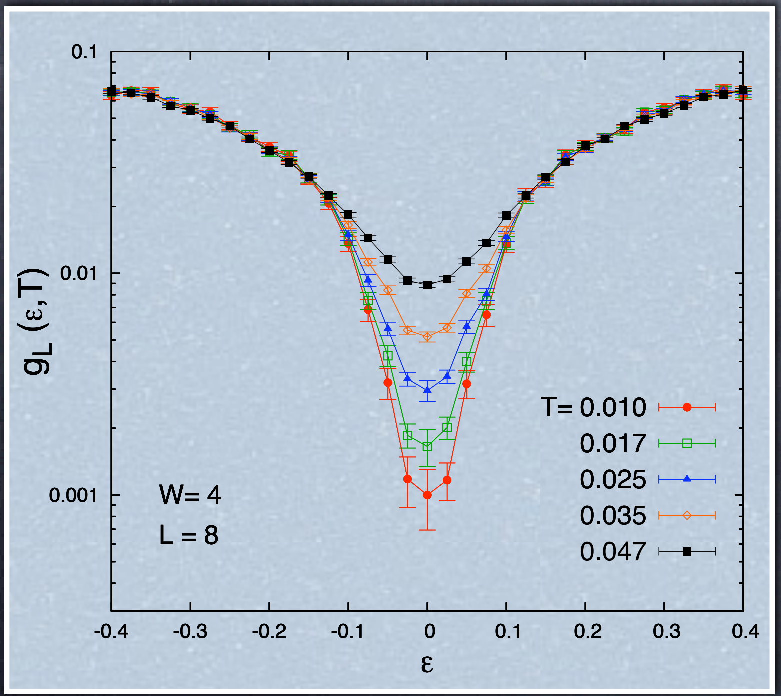
Pseudo-ground state calculations confirm our Monte Carlo results





Comparison with recent numerical work

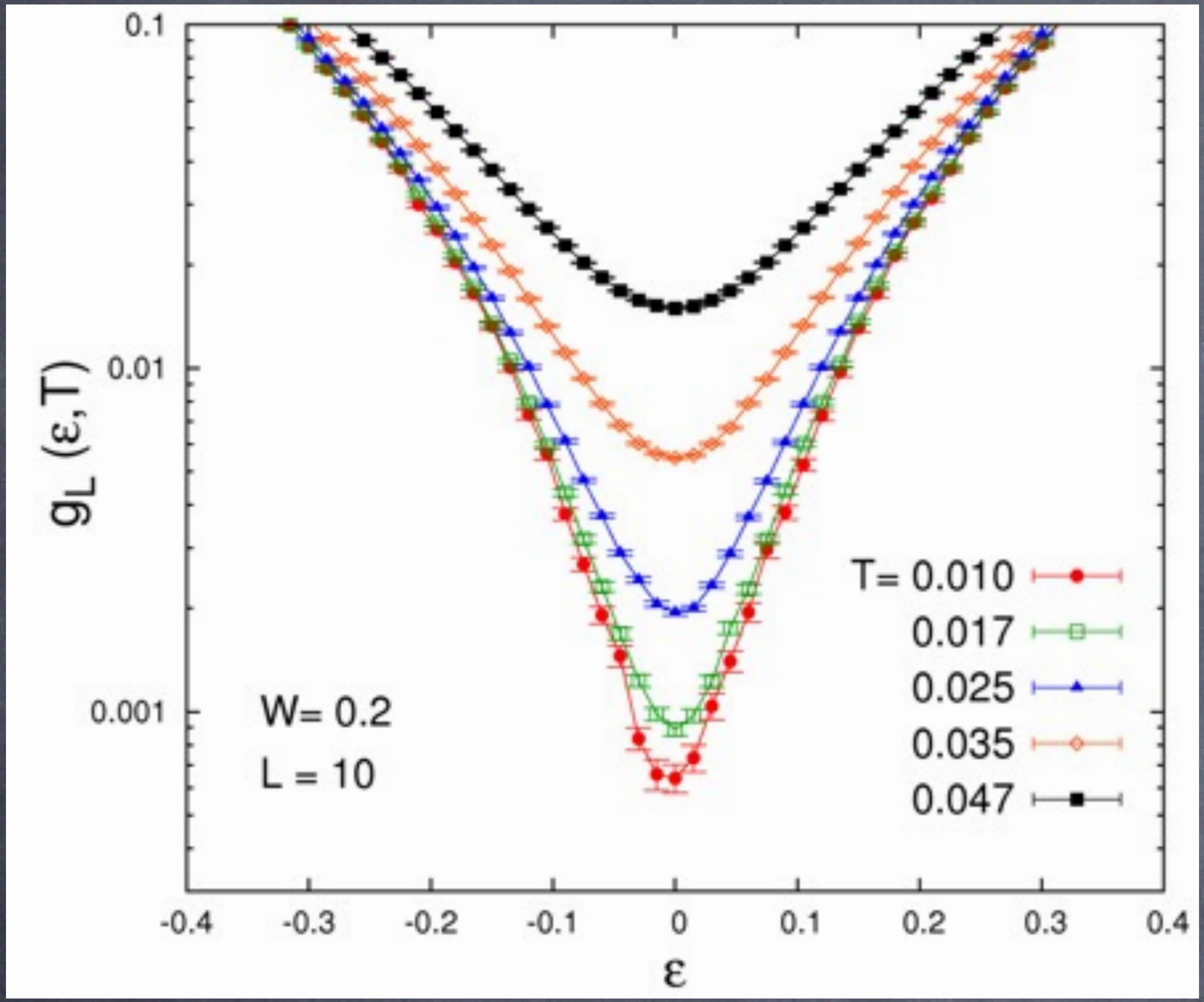




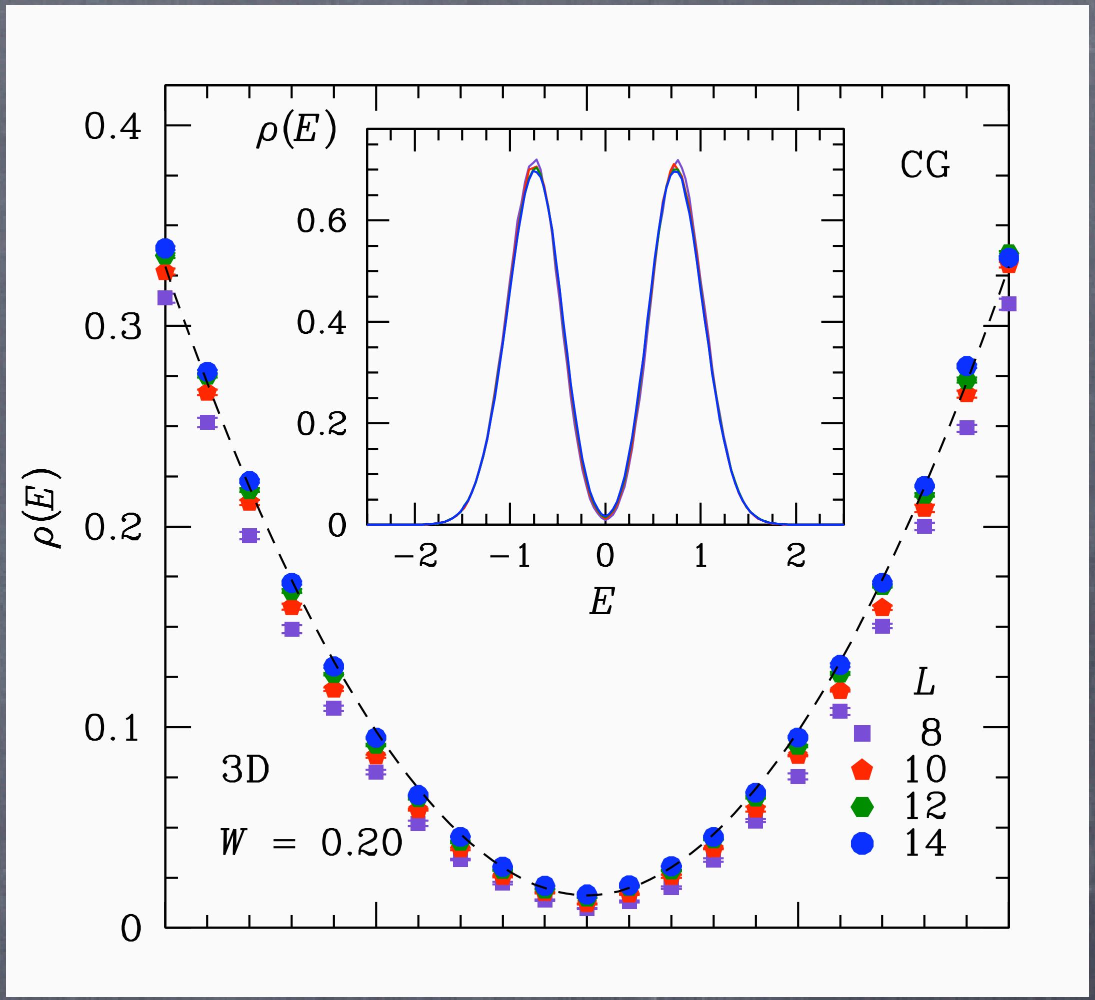
Unpublished data courtesy of Arnulf Möbius

Comparison with recent numerical work

Our data



Surer, Katzgraber, Zimanyi,
Allgood, Blatter, PRL 102, 067205



See also: Comment on the paper by Surer et al.
by Möbius and Richter Phys. Rev. Lett. 105, 039701 (2010)

Hardening of the Coulomb gap due to the "polaron shift"

- Efros (1976) considers the stability of sites + soft pairs. Assuming that soft pairs have a finite DOS $f(\omega)$ at low energy, he obtains:

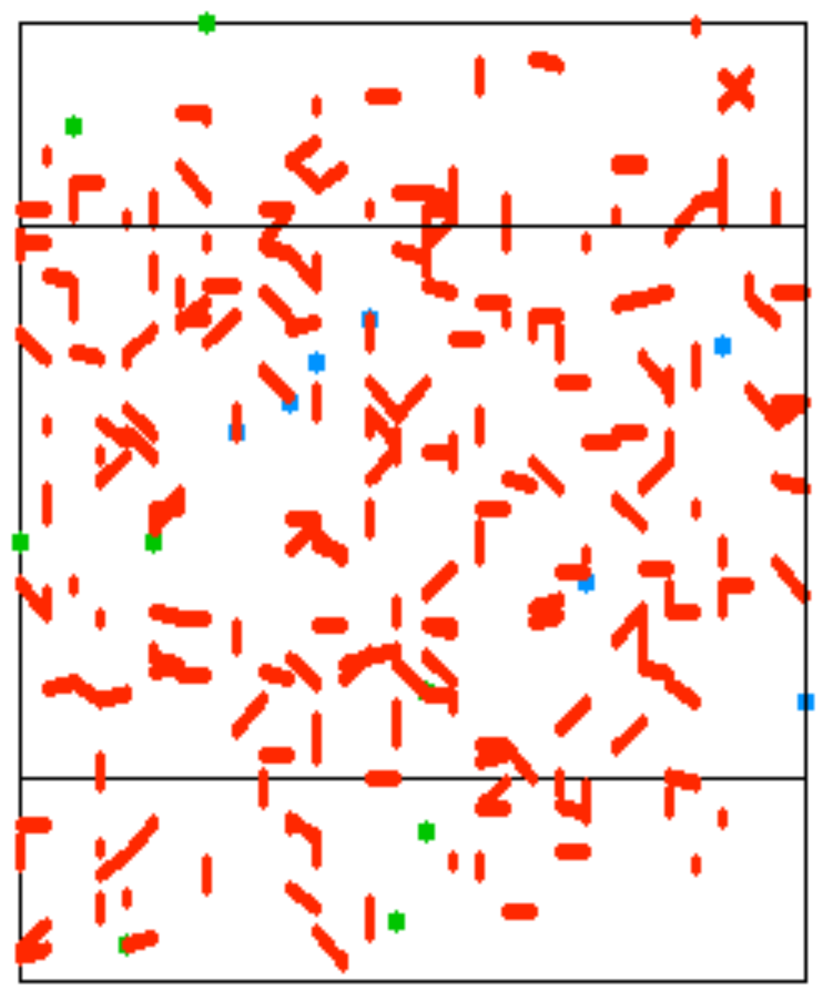
$$g(\epsilon) \leq g_0 \exp[-\left(\frac{a\Delta}{\epsilon}\right)^{\frac{1}{2}}]$$

- Baranovskii et al. (JETP, 1980) improved the argument and propose

$$g(\epsilon) \leq g_0 \exp[-\left(\frac{a\Delta}{\epsilon}\right)/(\ln(B/\epsilon))^{7/4}]$$

by considering:
- stability with respect to simultaneous flipping of many dipoles
- the angles in the dipolar interaction
- the depletion of the pair DOS due to dipole-dipole interaction, which gives $f(\omega) \propto \frac{1}{\ln(\Delta/\omega)}$

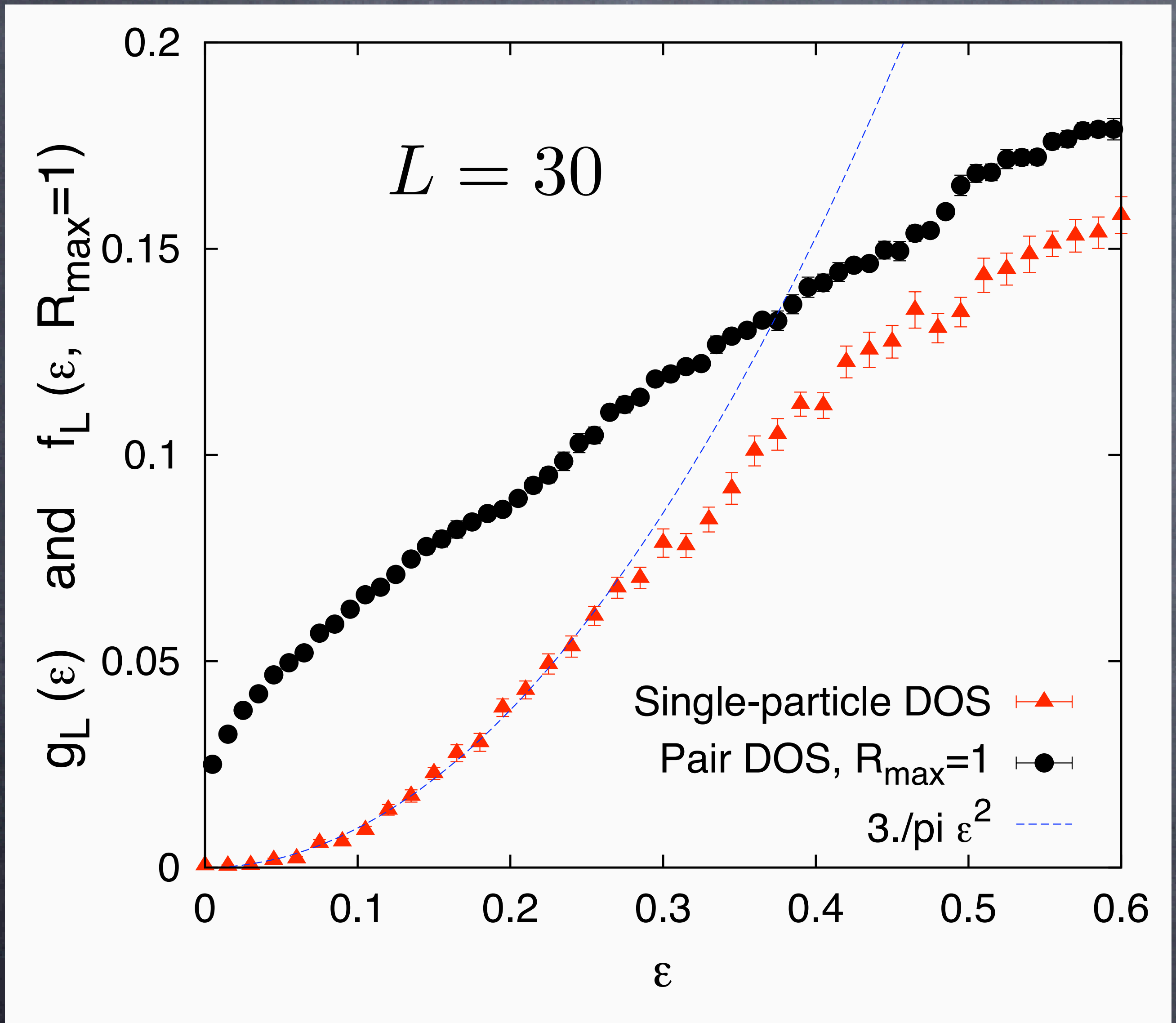
Why do we observe $g(\epsilon) \sim |\epsilon|^2$ then?

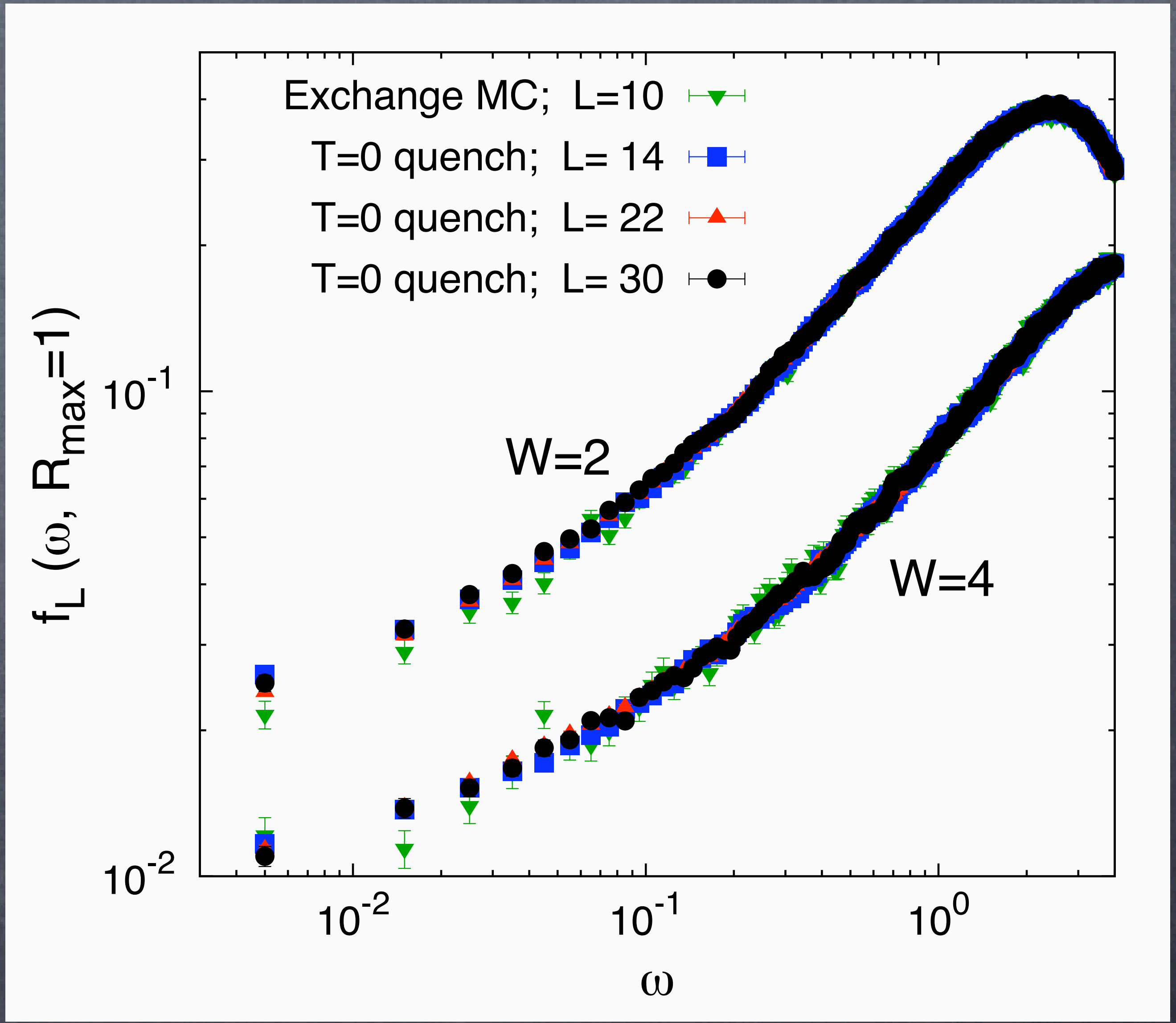


Soft sites (|energy| < 0.1) and soft dipoles (|energy| < 0.1; size <= 3)
in a L=30 sample

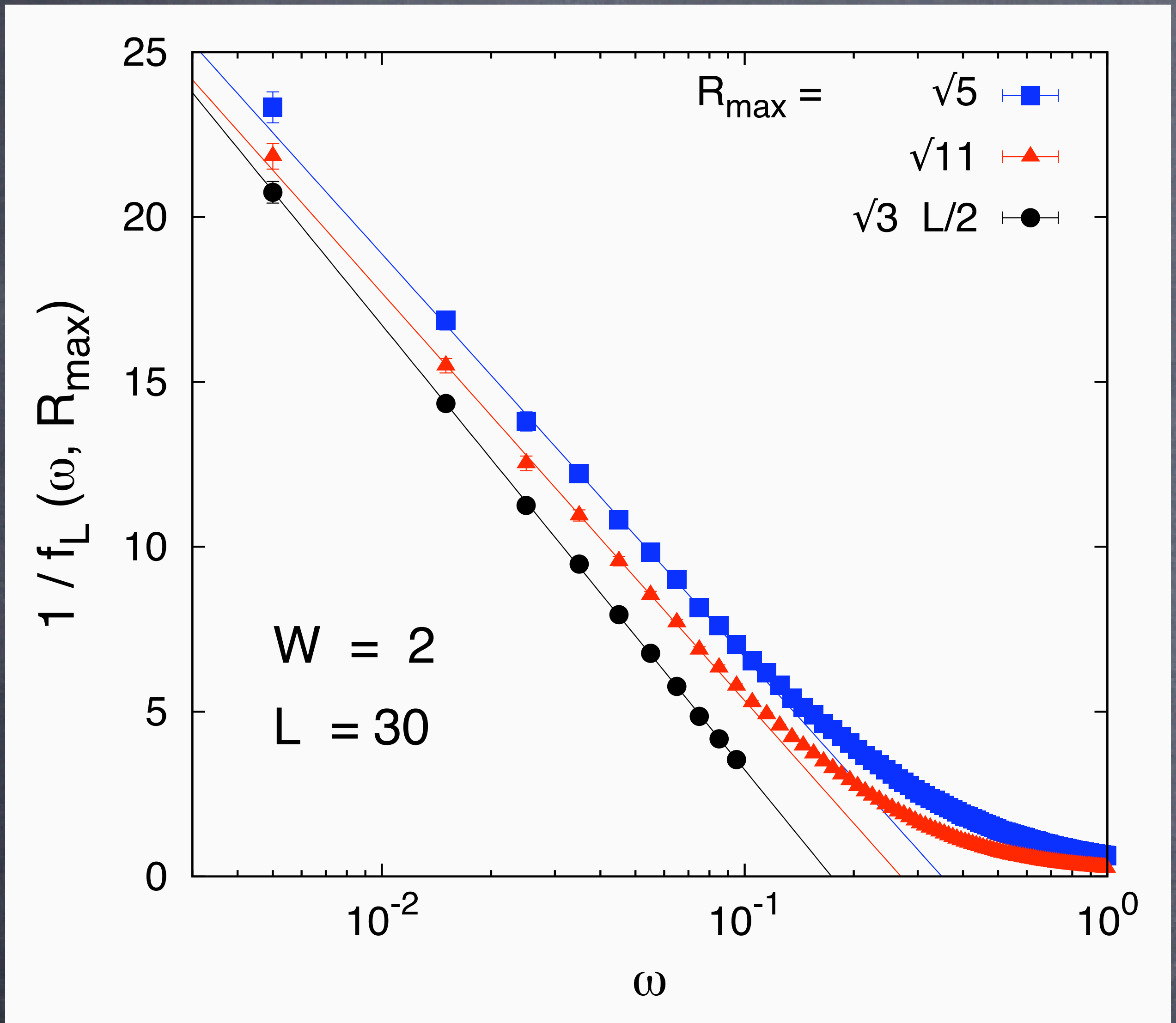
$$\omega_{ij} = \epsilon_j - \epsilon_i - 1/r_{ij} \qquad h_L(\omega, r) = \frac{1}{N} \sum_{(ij), r_{ij}=r} [\, \langle \delta(\omega - \omega_{ij}) \rangle \,]_{av}$$

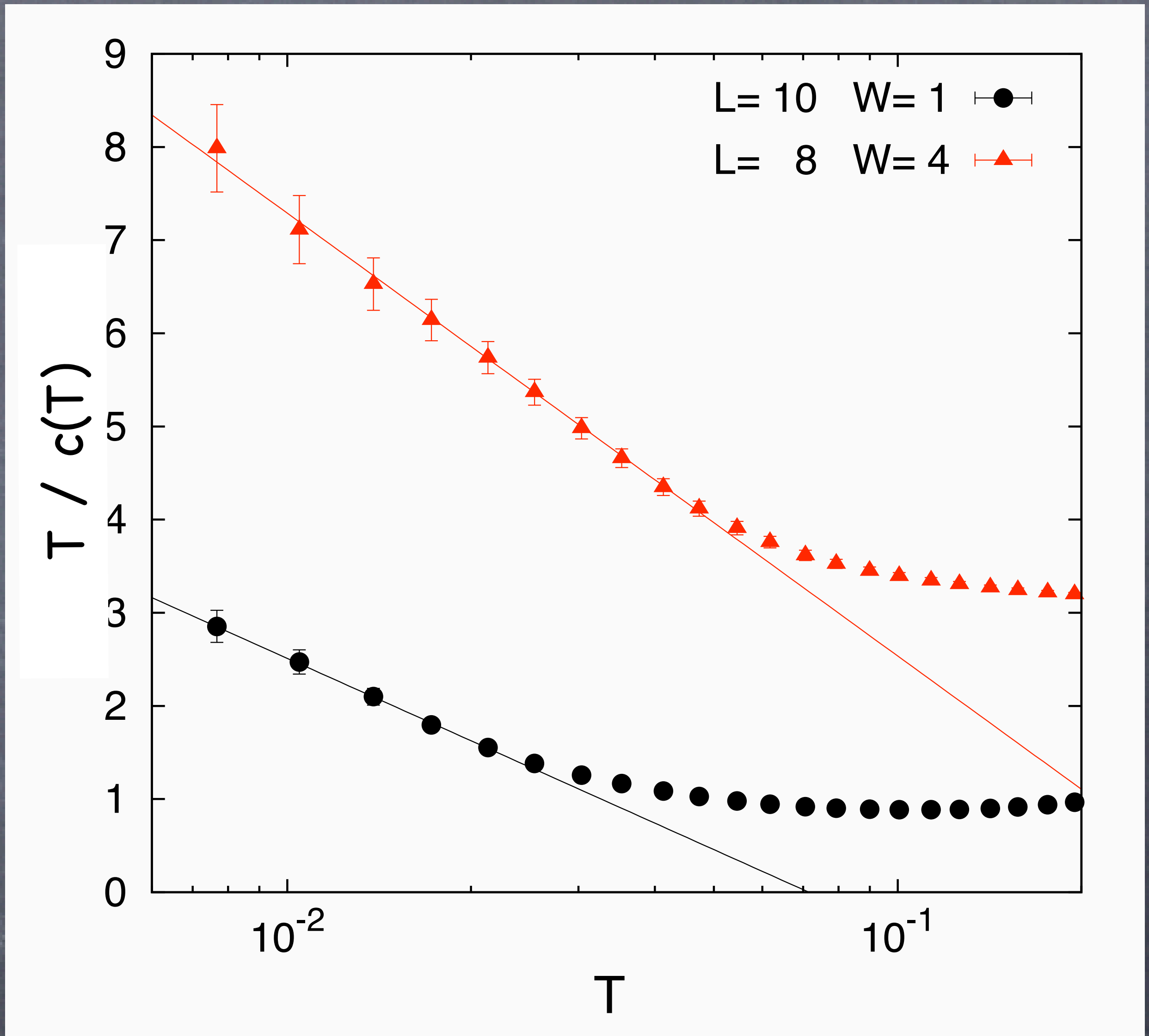
$$f_L(\omega, R) = \sum_{r \leq R} h_L(\omega, r)$$





specific heat



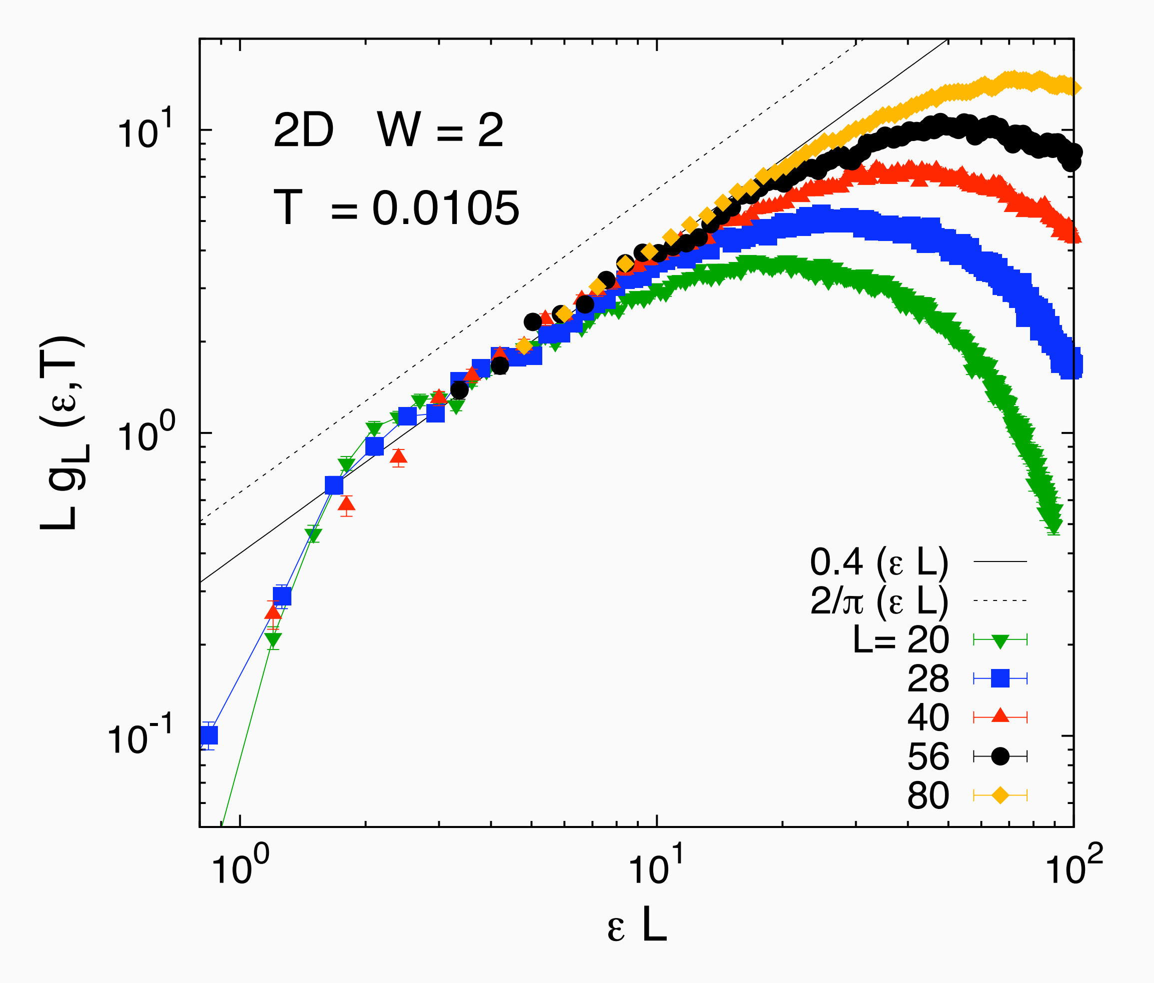


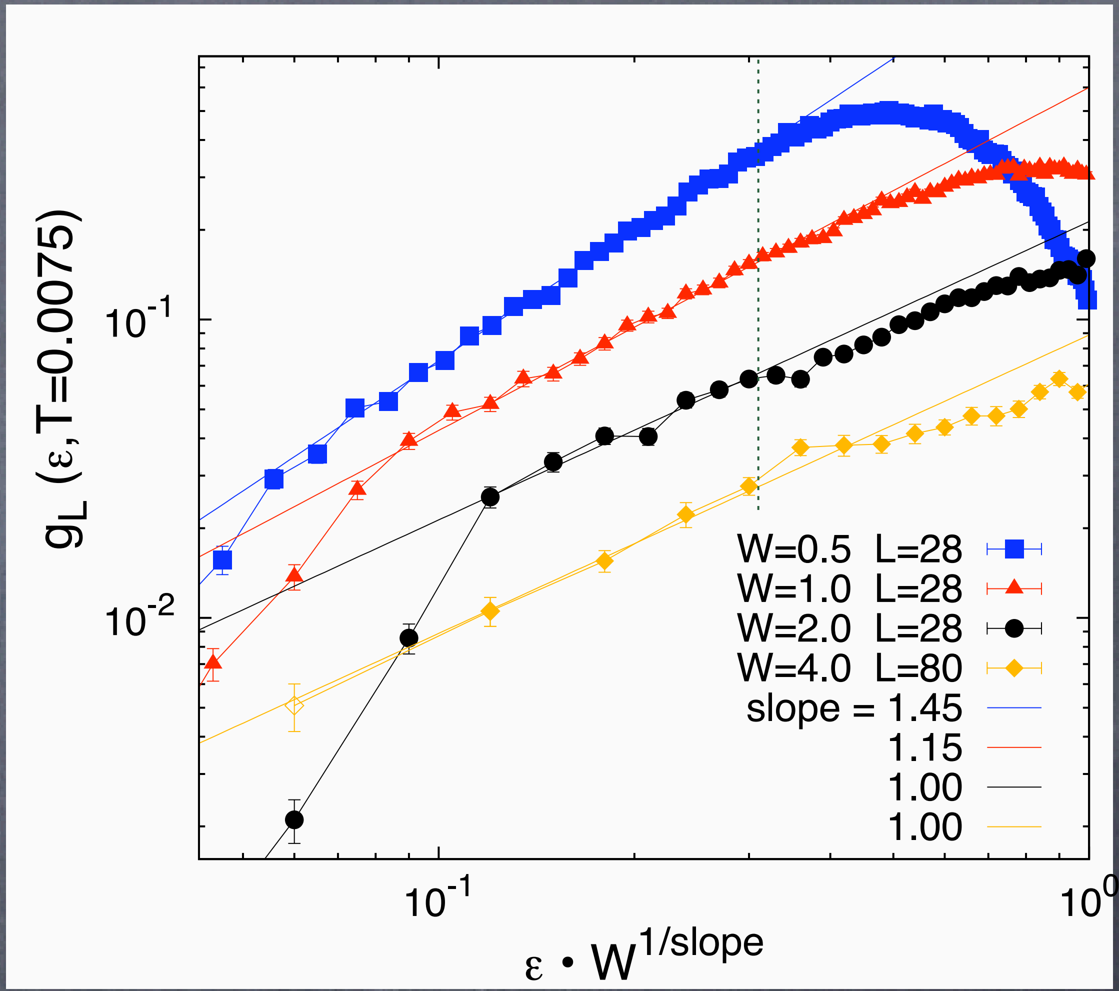
Summary

- no evidence for an equilibrium glass phase in 3D
- similar correlations in 2D and 3D
- characterization of the charge order phase transition
- saturated ES bound in 3D and 2D
- hardening of the gap only at unmeasurably small scales

Thank you

Results in two dimensions agree with $\delta = 1$ with crossover to larger δ at small disorder





M.Goethe and MP, unpublished

Crossover in 2D already observed by Pikus and Efros (1994)

Phase transition fluid / charge-ordered phase

	γ/ν	$\bar{\gamma}/\nu$	β/ν	ν
Coulomb glass	1.69(17)	2.89(9)	0.06(4)	1.11(12)
RFIM	1.44(12)	2.93(11)	0.011(4)	1.37(9)

← A. Middleton & D.S.Fisher, PRB 2002

$\beta/\nu, \;\; \bar{\gamma}/\nu$ from quotient method for $M_s, \;\; \bar{\chi}_L = N[\langle {m_s}^2 \rangle]_{av}$

γ/ν from divergence of $\chi_{|m_s|} = N[\langle m_s^2 \rangle - \langle |m_s| \rangle^2]_{av}$

ν from mod. hyperscaling $\nu = \dfrac{2-\alpha}{d+\gamma/\nu - \bar{\gamma}/\nu}$ assuming $\alpha = 0$

Transition in RFIM universailty class

-> Interaction is effectively short-range