Correlations in Random-Exchange $S = 1/2$ XXZ Chains: Breakdown of Universality

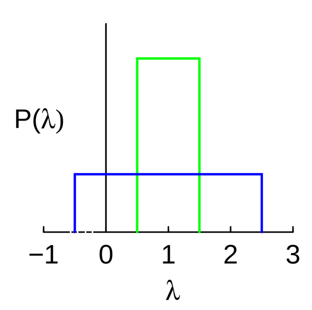
Kay Hamacher, Joachim Stolze (U Dortmund), Wolfgang Wenzel (FZ Karlsruhe), Gerhard Müller (URI), Heinrich Röder (LANL),

The *random-exchange-XXZ* chain (antiferromagnet)

$$H = J \sum_{i=1}^{N-1} \left[\lambda_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + \Delta S_i^z S_{i+1}^z \right]$$

$$S = \frac{1}{2} \quad ; \quad 0 \le \Delta \le 1 \quad ; \quad T = 0$$

λ_i random :



$1 - w \le \lambda \le 1 + w$

Aim: (average) ground-state correlations: $\langle S_i^\alpha S_j^\alpha \rangle$ $(\alpha = x, z)$

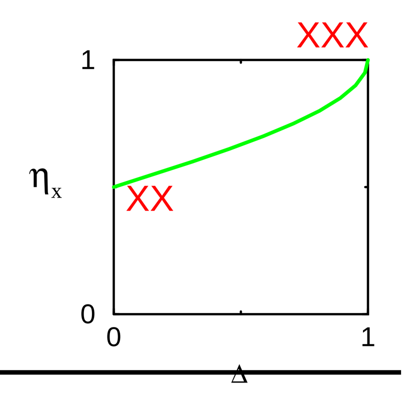
- $\Delta = 0$: XX chain:
  H = noninteracting lattice fermions with random hopping.
  Nevertheless, correlations are nontrivial.
- $w = 0$: *homogeneous* XXZ chain:
  Critical ground state: some analytical results.
- $\Delta \neq 0 \neq w \rightarrow$ DMRG

The critical phase (without randomness)

... shows power-law correlations in the ground state
(Luther, Peschel 1975):

$$|\langle S_i^\alpha S_j^\alpha \rangle| \sim |i - j|^{-\eta_\alpha}$$

$$\eta_x = \eta_z^{-1} = 1 - \pi^{-1} \arccos \Delta$$

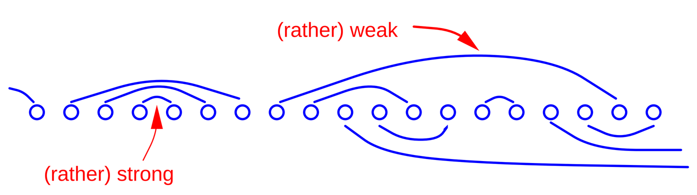


The *random-singlet* phase

RSRG treatment (D.S. Fisher 1992, 1994)

- The strongest bond of the chain is in its local ground state ($\rightarrow$ singlet pair); effective coupling of the two neighboring spins from perturbation theory.

$\Rightarrow$ "quasi-localized" random singlet phase:



(singlet pairs on all length scales)

- static correlations $\langle S_i^\alpha S_j^\alpha \rangle$ determined by many weakly coupled and few strongly coupled pairs (i, j).

Average correlation in the rs phase:

$$|\overline{\langle S_i^\alpha S_j^\alpha \rangle}^{\text{conf}}| \sim |i - j|^{-2} \qquad (\alpha = x, y, z)$$

Behavior like $|\langle S_i^z S_j^z \rangle|$ in the nonrandom XX-Model; but there $|\langle S_i^x S_j^x \rangle| \sim |i - j|^{-1/2}$, decaying much more slowly.
$\Rightarrow$ xx correlation should show drastic randomness dependence.

Numerical Methods

Jordan-Wigner mapping

Spins	Fermions
S_i^+, S_j^-	$\pm a_i^\dagger, \pm a_j$
S_i^z	$a_i^\dagger a_i - 1/2$
$\lambda_i J (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)$	$t\ (a_i^\dagger a_{i+1} + \text{h.c.})$ hopping
$\Delta J\ S_i^z S_{i+1}^z$	$V\ n_i n_{i+1}$ *interaction*
$h\ S_i^z$	$\mu\ n_i$ chemical potential

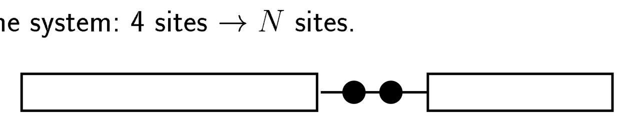
- XX case ($\Delta = 0$)
  i) Determine ground state of $\frac{N}{2}$ noninteracting fermions,
  ii) use Wick´s theorem to calculate *many-fermion* correlations:

$$\pm = \prod_k (1 - 2a_k^\dagger a_k)$$

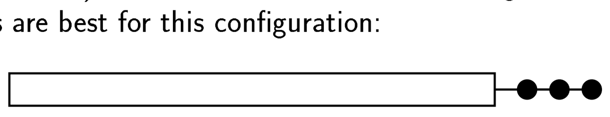
- XXZ case ($\Delta \neq 0$)
  Interacting fermions offer no advantage over spins.
  Use DMRG in spin space.

DMRG details

Mostly open bc´s, 50 states, $N = 80$
Build up the system: 4 sites $\rightarrow$ N sites.



Sweep back and forth until lowest energy converges.
Olson (64 states) and Davidson methods for diagonalization.
Correlations are best for this configuration:



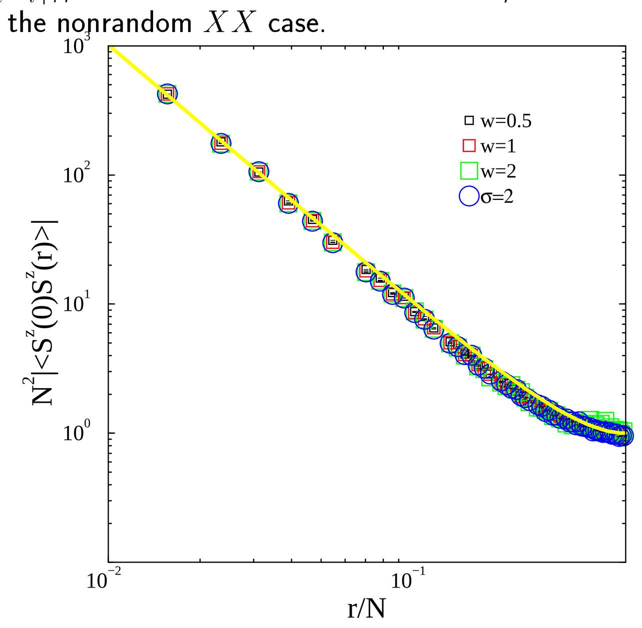
(Comparison to explicit diagonalization for small N at $\Delta \neq 0$ or free-fermion results at $\Delta = 0$ for larger N.)
Periodic bc´s require more states for convergence $\rightarrow$ prohibitive.
Average over 250...1000 replicas for every (Δ, w).
More than 13000 replicas; some cpu-hours each.
(Inhomogeneous IBM SP2)

The z correlation in the XX model

...scales according to the expected power law:

$$\langle S_i^z S_{i+r}^z \rangle = r^{-\eta_z} f(r/N) = N^{-\eta_z} \left(\frac{r}{N}\right)^{-\eta_z} f(r/n); \ \eta_z = 2$$

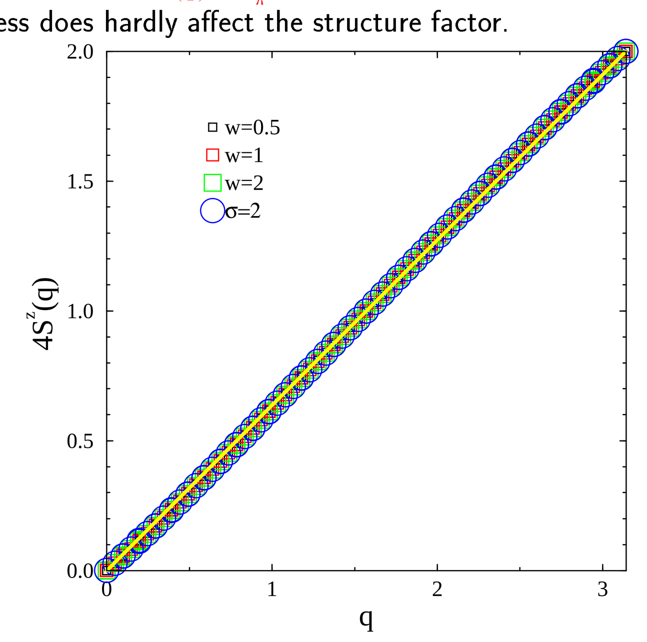
$\Rightarrow$ $N^{\eta_z} \langle S_i^z S_{i+r}^z \rangle$ should be a universal function of r/N for all N, which is known for the nonrandom XX case.



Gaussian and box distributions, $N = 32, 64, 128$.
Typical correlation does *not* scale (in this way).

The z structure factor in the XX model

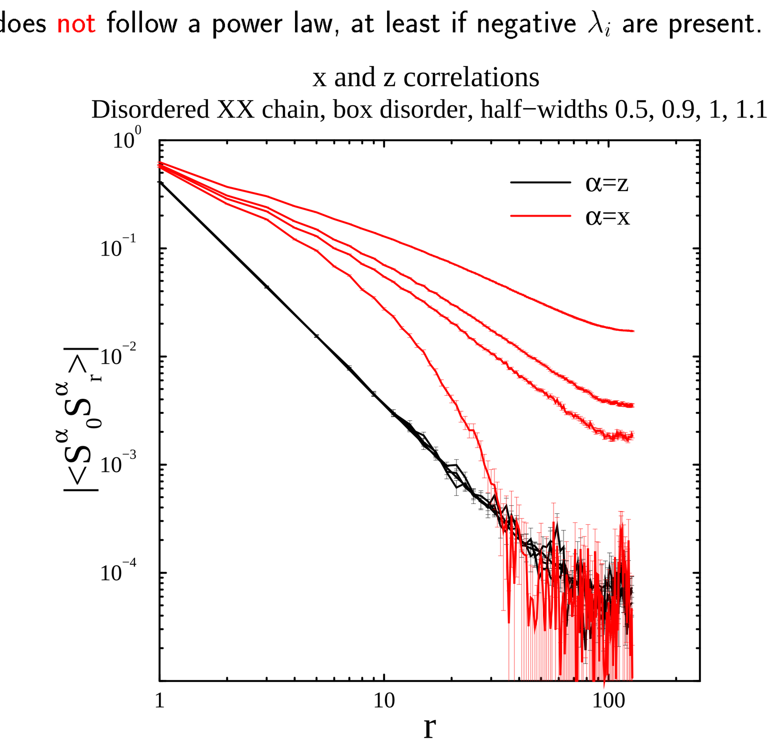
$S^z(q) = N^{-1} \sum_{r=0}^{N-1} \langle S_0^z S_r^z \rangle e^{iqr}$
nonrandom case $\Rightarrow$ $4S^z(q) = \frac{2q}{\pi}$
Randomness does hardly affect the structure factor.



Gaussian and box distributions, $N = 32, 64, 128$.

The x correlation in the XX model

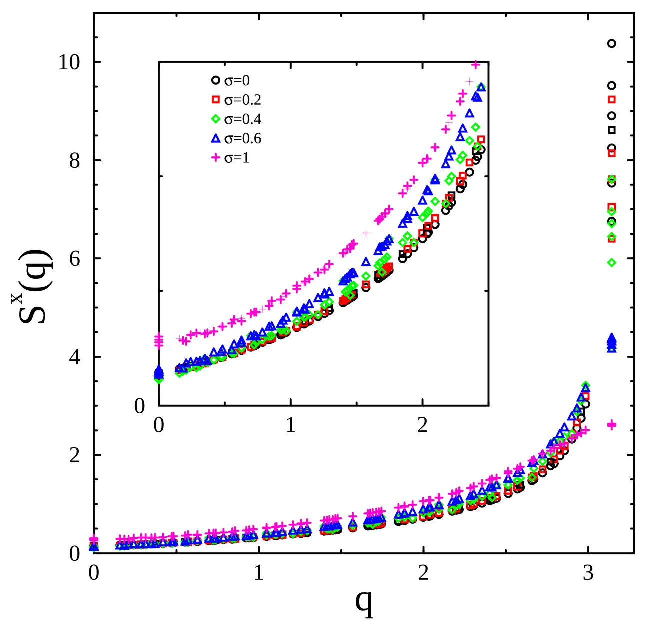
... does not follow a power law, at least if negative λ_i are present.



At $w = 1$ the x correlation *may* follow a r^{-2} law.
(Henelius and Girvin 1998)

The x structure factor in the XX model

- systematic variation with randomness, in contrast to the z structure factor
- finite-size effects only at $q = \pi$



$18 \le N \le 40$, Gauss (similar for box)

Exponential suppression of x correlations in a solvable model:

XXZ chain with random sign of the transverse coupling; this randomness can be gauged away almost completely.

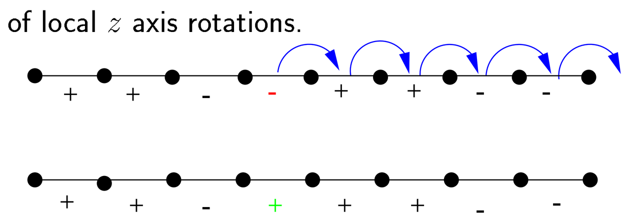
$$H_{RTS} = J \sum_{i=1}^{N-1} \left[t_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + \Delta S_i^z S_{i+1}^z \right]$$

$$P(t_i) = (1 - p)\delta(t_i - 1) + p\delta(t_i + 1)$$

Transformation:

$$U_T H_{RTS} U_T^\dagger = H_{XXZ}$$

composed of local z axis rotations.



Correlations:

$$U_T S_i^z U_T^\dagger = S_i^z$$

$\Longrightarrow$ z correlations of the RTS model are identical to those of the homogeneous XXZ model (power law), but

$$U_T S_i^x S_{i+r}^x U_T^\dagger = S_i^x S_{i+r}^x \prod_{l=i}^{i+r-1} t_l$$

$$\Longrightarrow \overline{\langle S_i^x S_{i+r}^x \rangle_{RTS}}^{\text{conf}} = \langle S_i^x S_{i+r}^x \rangle_{XXZ} (1 - 2p)^r$$

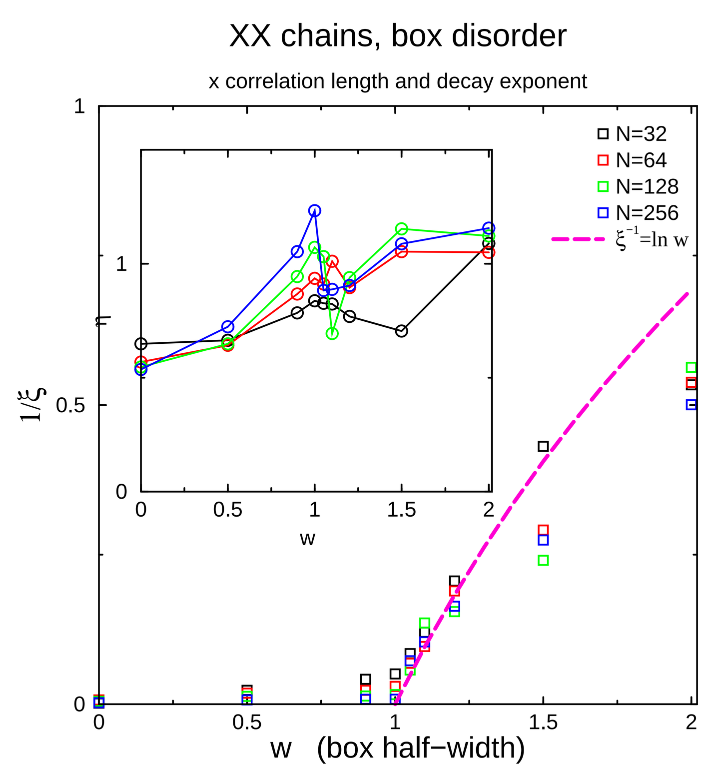
x correlation of the homogeneous model is multiplied by an exponential, with correlation length

$$\xi_x = \frac{-1}{\ln |1 - 2p|}$$

where p is the fraction of negative λ's. ξ_x diverges (with unit critical exponent) at the *randomness-induced quantum critical points* $p = 0$ and $p = 1$.
The quantum critical point $p = 0$ generalizes to less trivial models, as we show below.

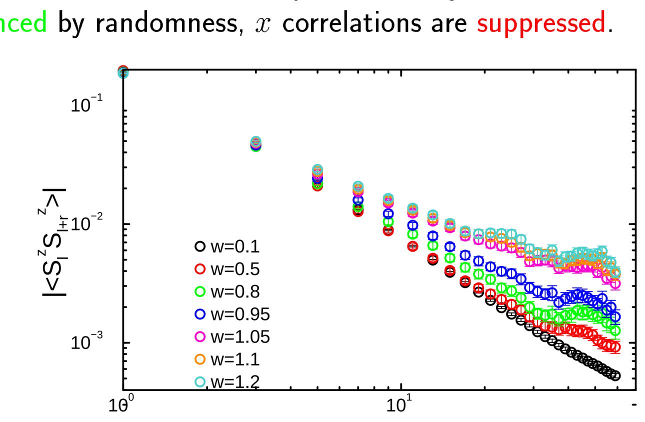
Critical point of the XX model with box-distributed λ

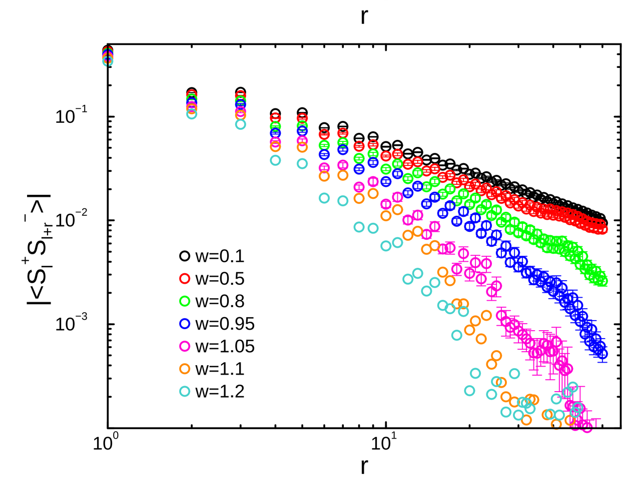
The decay exponent η fluctuates with the randomness w, but stays well below $\eta = 2$.
The correlation length shows the expected divergence as $w \rightarrow 1^+$.



Correlations of the $\Delta = 0.5$ XXZ model with box-distributed λ

Results from DMRG, 80 sites, open boundary conditions: z correlations are enhanced by randomness, x correlations are suppressed.



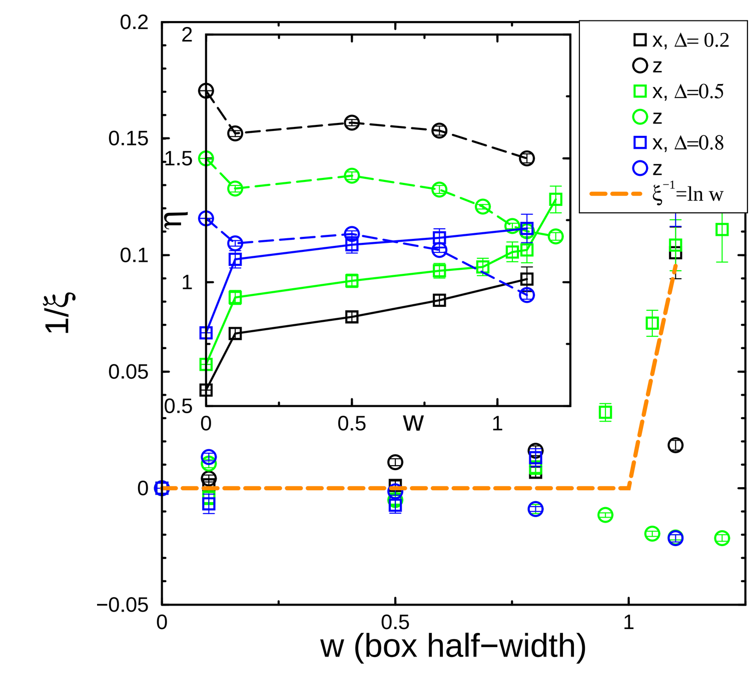


Critical point of the XXZ model with box-distributed λ

Results from DMRG, 80 sites, open boundary conditions:
exponential/algebraic fit for $r \le 60$:

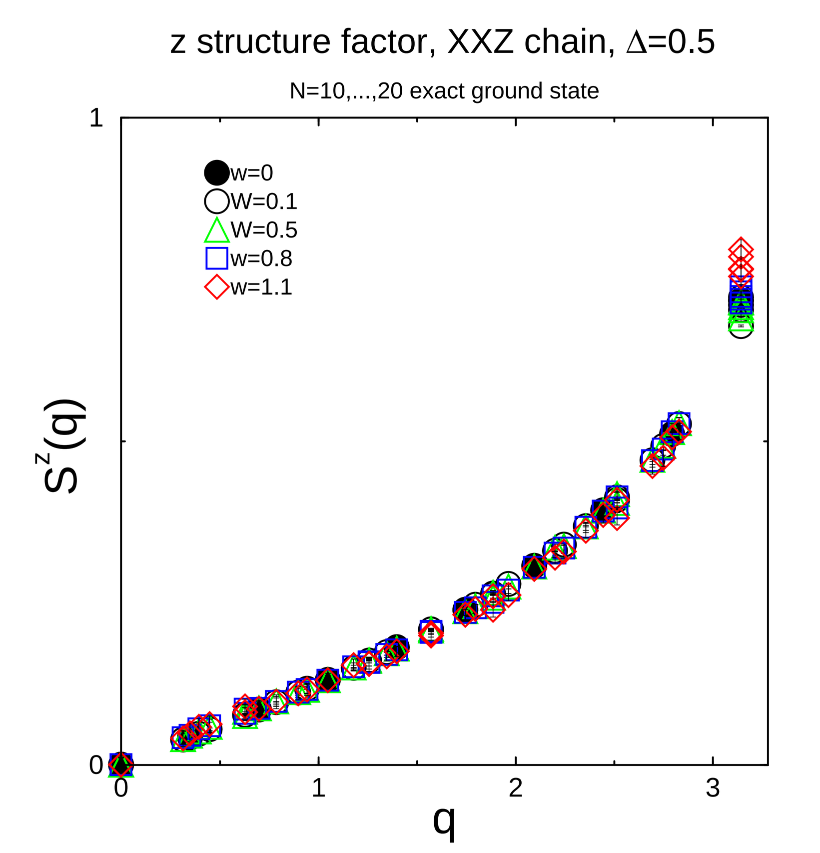
$$\langle S_i^\alpha S_{i+r}^\alpha \rangle \sim r^{-\eta_\alpha} \exp(-r/\xi_\alpha).$$

- Decay exponents are non-universal: $\eta_x \neq \eta_z \neq 2$.
- Correlation length ξ_x diverges as $w \rightarrow 1^+$, ξ_z does not.



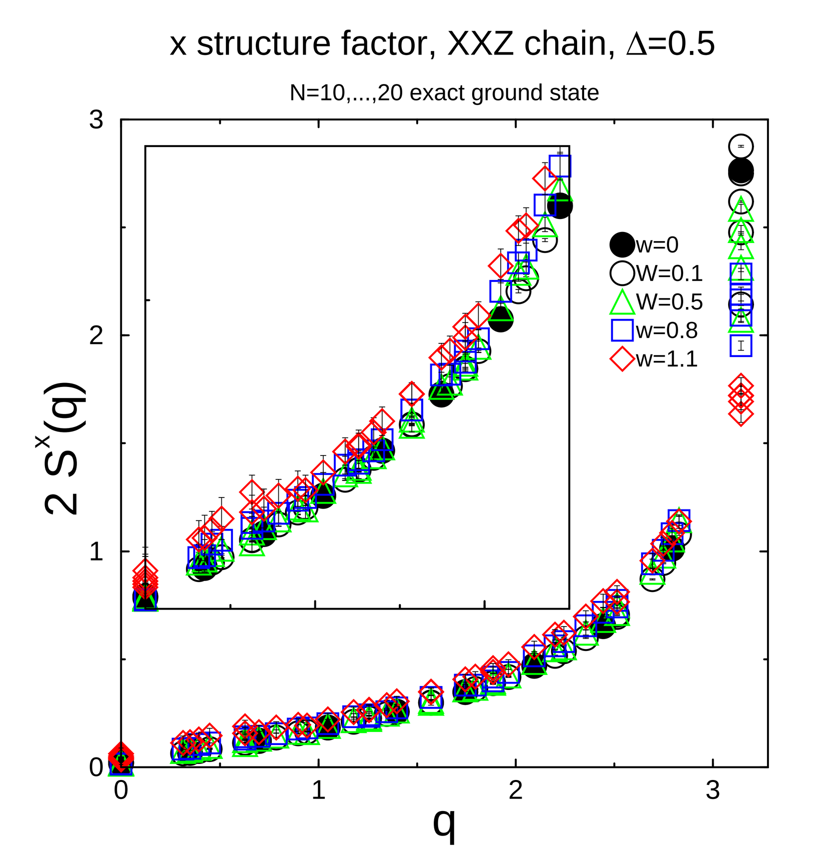
The z structure factor of the XXZ model ($\Delta = 0.5$)

Almost no dependence on N or w.
Obviously nonlinear, different from the XX case, in contrast to the random-singlet picture.



The x structure factor of the XXZ model ($\Delta = 0.5$)

Grows with w, except at $q = \pi$.



Conclusions

Correlations in random-exchange XXZ chains are non-universal.

- In the XX chain the z correlations behave as predicted by the RSRG: Randomness-independent power law with $\eta_z = 2$.
- In the XXZ chain the z correlations do not behave as predicted by the RSRG: power law with $\eta_z \neq 2$.
- x correlations *may* obey a power law as long as all couplings $\lambda > 0$.
- If negative couplings are allowed, x correlations are suppressed exponentially.
- Fundamental differences between x and z correlations in the random XX chain:
  z correlations vanish for even distances and are strictly positive for odd distances.
  x correlations alternate strictly, if only positive couplings are present and in general do not vanish.