Magnetic order in the easy-plane XXZ model

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Motivation

magnetic properties of low-D spin systems with anisotropy, e.g. high-T_c parent compounds: La_2CuO_4 & $Ca(Sr)CuO_2$

Hamiltonian

$$\mathcal{H} = \frac{J}{2}\Big[\sum_{\langle i,j\rangle_{x,y}} \left(S_i^+ S_j^- + \Delta S_i^z S_j^z\right) + R_z \sum_{\langle i,j\rangle_z} \left(S_i^+ S_j^- + \Delta S_i^z S_j^z\right)\Big]$$

easy-plane region: $-1 < \Delta < 1$
XY model: $\Delta = 0$

AFM interplane coupling $R_z = J_z/J < 1$
$\Rightarrow$ magnetic short-range order effects!
$\Rightarrow$ Néel transitions: effects of spatial and spin anisotropy!
$\Rightarrow$ quantum-classical crossover at $\Delta < 0$!

Methods

- Green's-function projection approach [1,2]
- exact diagonalizations (up to 36 sites; PBC)

Goal

- complete wave vector, T, Δ, and R_z dependences of transverse

$$\chi_{\mathbf{q}}^{+-}(\omega) = -\langle\langle S_{\mathbf{q}}^+ ; S_{-\mathbf{q}}^- \rangle\rangle_\omega$$

and longitudinal

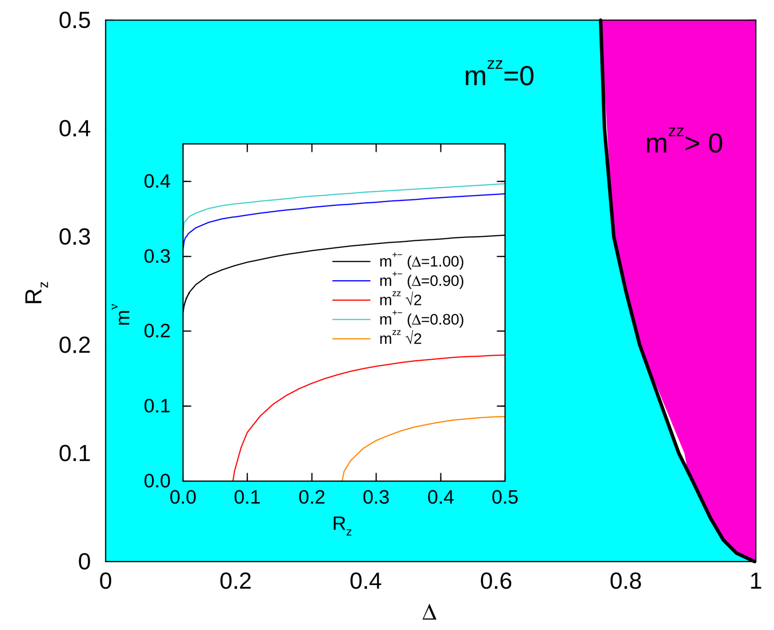
$$\chi_{\mathbf{q}}^{zz}(\omega) = -\langle\langle S_{\mathbf{q}}^z ; S_{-\mathbf{q}}^z \rangle\rangle_\omega$$

spin susceptibilities
- comparison with experiments: correlation length, Néel temperatures

3D XXZ model

Ground-state long-range order

$R_z - \Delta$ phase diagram

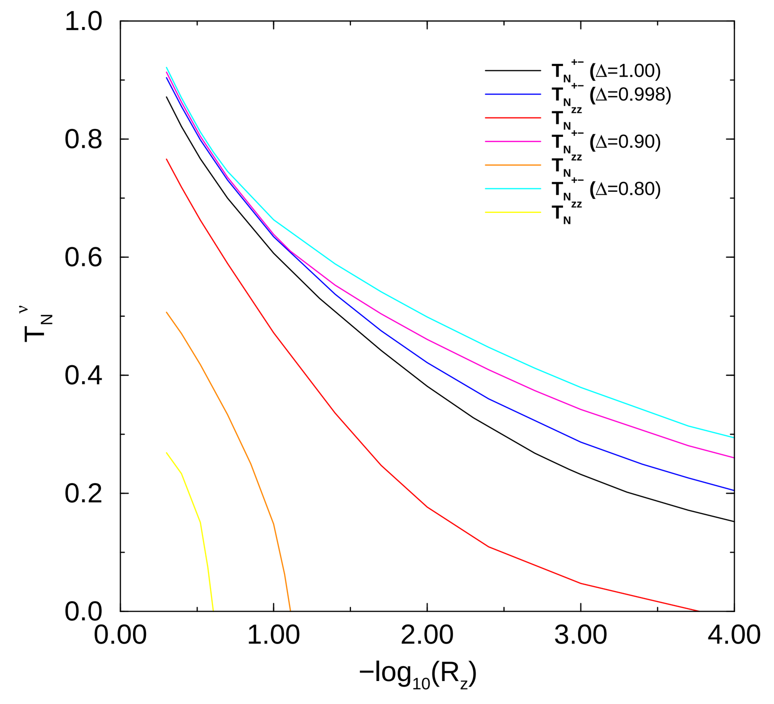


- phase I: $m^{+-} > 0$, $m^{zz} = 0$
- new phase II: $m^{+-} > 0$, $m^{zz} > 0$
- combined influence of spatial and spin anisotropy!
- phase boundary with:

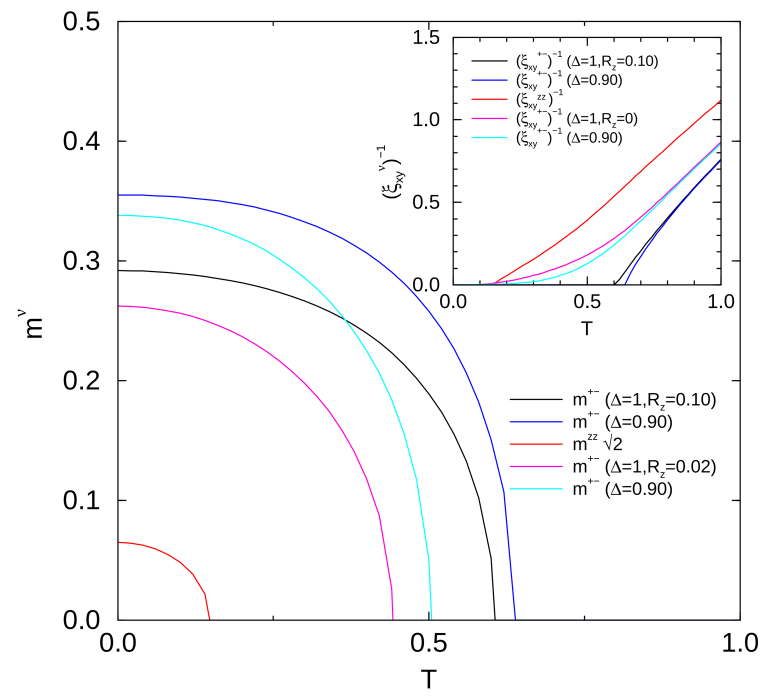
$$\lim_{R_z \to 0} \Delta_c(R_z) = 1 \quad \& \quad \lim_{\Delta \to 1} R_{z,c}(\Delta) = 0$$

Finite-temperature results

transition temperatures T_N^ν vs. R_z



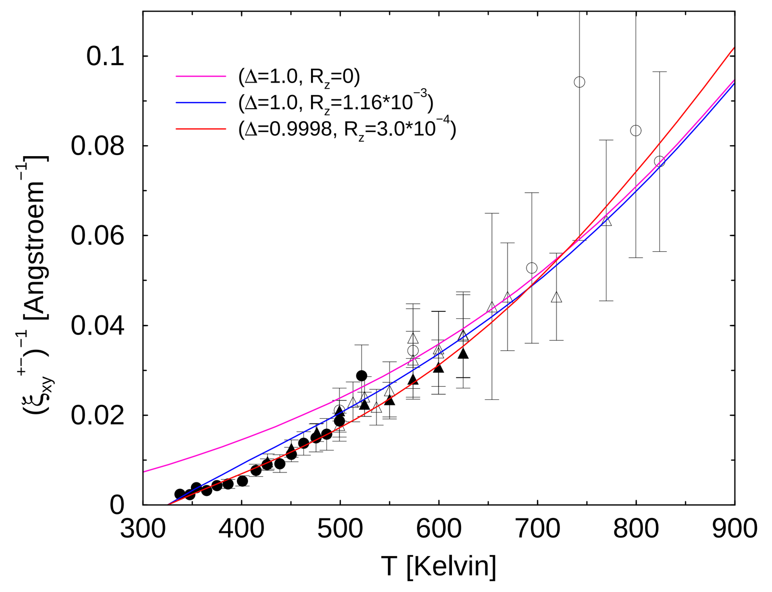
staggered magnetizations and correlation lengths



$\Rightarrow$ second-order transitions at T_N^{+-} and T_N^{zz}

Comparison with experiments $(R_z \ll 1)$

correlation length in La_2CuO_4 $(T_N^{+-} = 325\ \mathrm{K}[3])$
$\alpha_{xy} \equiv 1 - \Delta = 2 \times 10^{-4} \rightsquigarrow R_z = 3.0 \times 10^{-4}$ $[J = 117\ \mathrm{meV}]$



symbols – neutron scattering experiments [4]

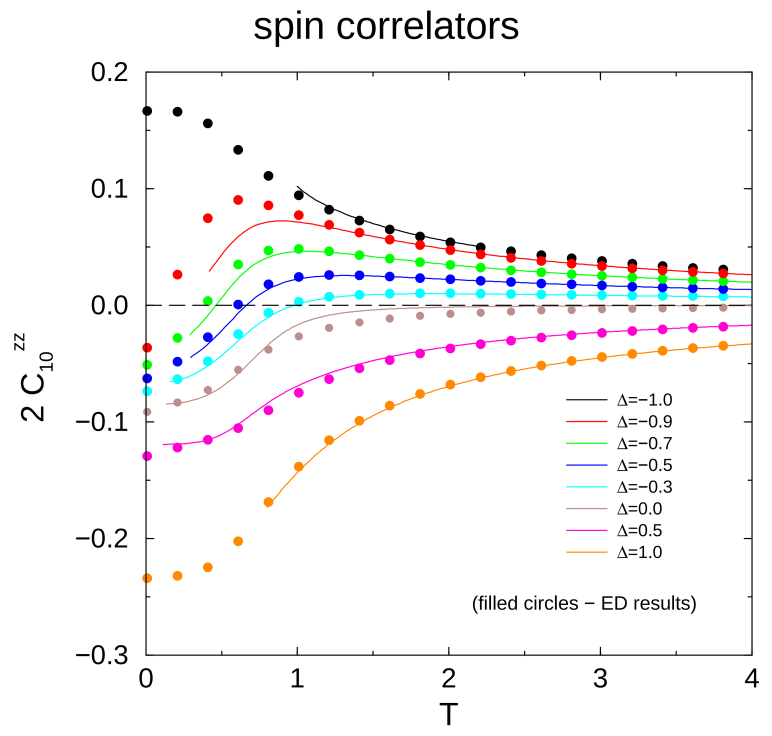
phase transition to longitudinal LRO
$(\mu^{zz} \equiv 2\mu_B m^{zz} > 0)$

Δ	La_2CuO_4	$Ca_{0.85}Sr_{0.15}CuO_2$
$\mu^{zz}(T=0)$	$6.5 \times 10^{-2}\ \mu_B$	$0.16\mu_B$
T_N^{zz}	35 K	190 K

$Ca_{0.85}Sr_{0.15}CuO_2$ $(T_N^{+-} = 540\ \mathrm{K}[5])$:
$\alpha_{xy} = 2 \times 10^{-4} \rightsquigarrow R_z = 5.0 \times 10^{-3}$ $[J = 125\ \mathrm{meV}]$
$\Rightarrow$ prediction has to be confirmed!

2D XXZ model

spin correlators

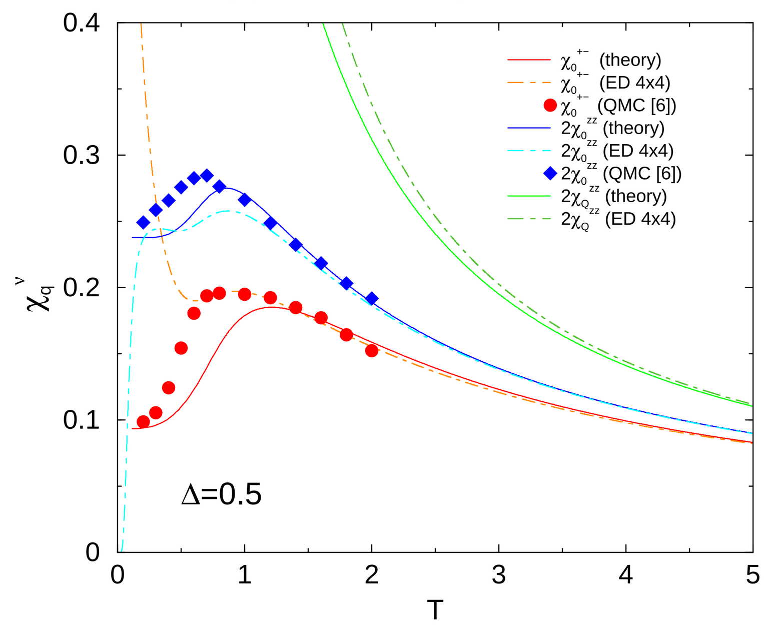


$\Rightarrow$ observation of a quantum-classical crossover
for $-1 < \Delta < 0$: sign change $C_{\mathbf{r}}^{zz} < 0 \rightarrow C_{\mathbf{r}}^{zz} > 0$ with increasing $T/\mathbf{r}$ ($\mathbf{r}/T$ fixed) at $T_0(\Delta;\mathbf{r})$

Δ	$T_0(\Delta;\mathbf{r})$ $\mathbf{r} = (1,0)$	$\mathbf{r} = (1,1)$	$\mathbf{r} = (2,0)$
-0.1	2.98 [2.540]	1.76	1.76 [1.520]
-0.3	0.96 [0.931]	0.74	0.72 [0.713]
-0.5	0.66 [0.605]	0.52 [0.527]	0.50 [0.476]
-0.7	0.46 [0.391]	0.36 [0.303]	0.34 [0.301]
-0.9	<0.2 [0.125]	<0.2 [0.106]	<0.2 [0.106]

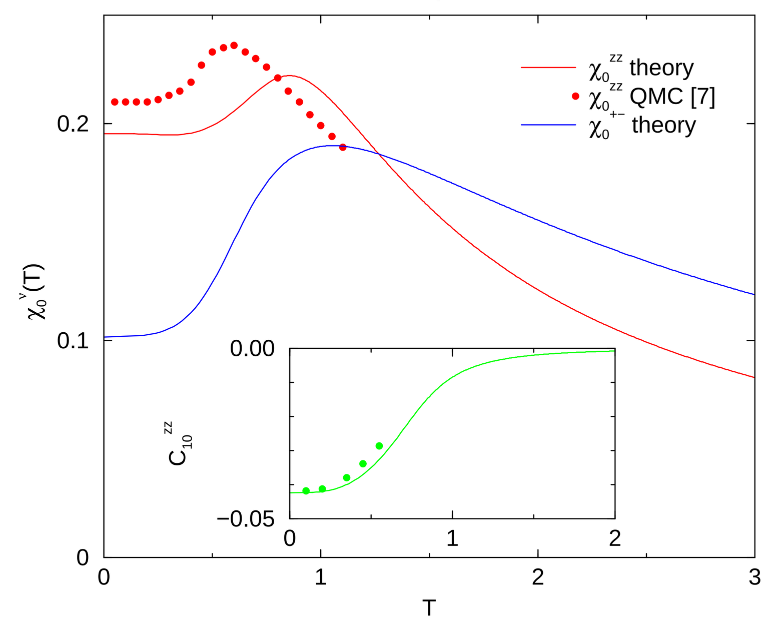
$[\ldots]$ - ED data for 4×4 lattice

temperature dependence of uniform and staggered susceptibilities



2D XY model

uniform susceptibilities

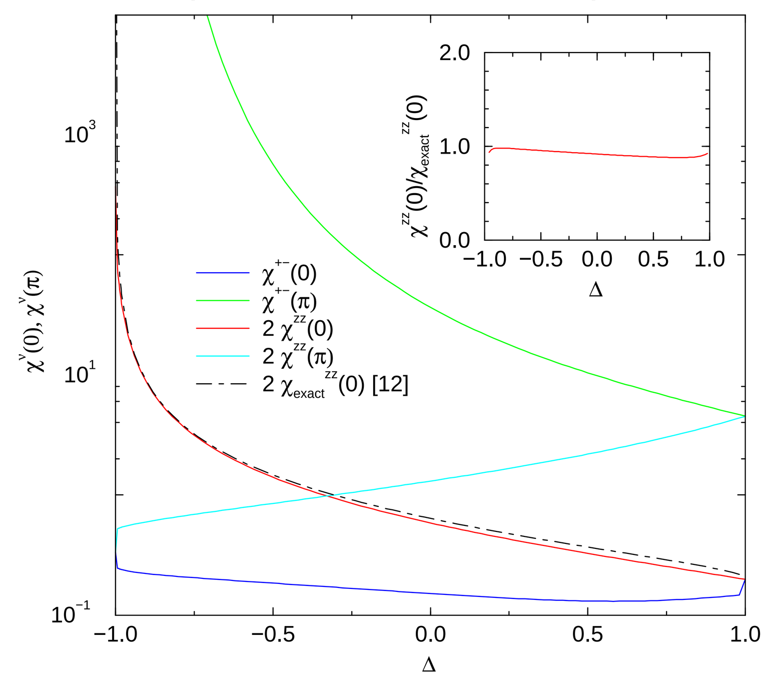


n	C_{n0}^{zz} (theory)	C_{n0}^{zz} (QMC data [8])
1	-4.197×10^{-02}	-4.118×10^{-02}
2	-1.838×10^{-03}	-1.828×10^{-03}
3	-5.88×10^{-04}	-6.78×10^{-04}
4	-1.51×10^{-04}	-1.68×10^{-04}
5	-4.7×10^{-05}	(no data)

$\Rightarrow$ quantum effects $\rightsquigarrow$ zz-correlations

1D XXZ model

zero-temperature uniform susceptibilities



Summary

- two Néel transitions with $T_N^{+-} > T_N^{zz}$ $\Leftarrow$ new!
- excellent agreement of $\xi_{xy}^{+-}(T)$ with experiments on La_2CuO_4
- complete calculation of all static magnetic properties in good agreement with numerical (ED, QMC) data
- quantum-classical crossover in the ferromagnetic region of the 2D easy-plane XXZ model
- maximum in uniform static susceptibilities as an effect of magnetic short-range order

Referenes

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Appendix: Green's-function theory

- basis: $\mathbf{A}_1 = (S_{\mathbf{q}}^+, i\dot{S}_{\mathbf{q}}^+)^T$ & $\mathbf{A}_2 = (S_{\mathbf{q}}^z, i\dot{S}_{\mathbf{q}}^z)^T$

$$\langle\langle \mathbf{A}; \mathbf{A}^\dagger \rangle\rangle_\omega = [\omega - \mathfrak{M}'\mathfrak{M}^{-1}]^{-1}\mathfrak{M}$$

with $\mathfrak{M} = \langle[\mathbf{A}, \mathbf{A}^\dagger]\rangle$ and $\mathfrak{M}' = \langle[i\dot{\mathbf{A}}, \mathbf{A}^\dagger]\rangle$

- dynamic spin susceptibilities ($\nu = +-,\ zz$):

$$\chi_{\mathbf{q}}^\nu(\omega) = -\frac{M_{\mathbf{q}}^\nu}{\omega^2 - (\omega_{\mathbf{q}}^\nu)^2}$$

where

$$\begin{aligned} M_{\mathbf{q}}^{+-} &= -4[C_{1,0,0}^{+-}(1-\Delta\gamma_{\mathbf{q}}) + 2C_{1,0,0}^{zz}(\Delta - \gamma_{\mathbf{q}})] \\ &\quad -2R_z[C_{0,0,1}^{+-}(1 - \Delta\cos q_z) \\ &\quad +2C_{0,0,1}^{zz}(\Delta - \cos q_z)]\,, \\ M_{\mathbf{q}}^{zz} &= -4C_{1,0,0}^{+-}(1-\gamma_{\mathbf{q}}) - 2R_z C_{0,0,1}^{+-}(1 - \cos q_z)\,, \end{aligned}$$

$$\gamma_{\mathbf{q}} = (\cos q_x + \cos q_y)/2,$$

$$C_{nml}^\nu \equiv C_{\mathbf{r}}^\nu,\ C_{\mathbf{r}}^{+-} = \langle S_0^+ S_{\mathbf{r}}^- \rangle,\ C_{\mathbf{r}}^{zz} = \langle S_0^z S_{\mathbf{r}}^z \rangle,$$

$$C_{\mathbf{r}}^\nu = \frac{1}{N}\sum_{\mathbf{q}} \frac{M_{\mathbf{q}}^\nu}{2\omega_{\mathbf{q}}^\nu}[1 + 2p(\omega_{\mathbf{q}}^\nu)]\,\mathrm{e}^{i\mathbf{q}\mathbf{r}}$$

with $p(\omega_{\mathbf{q}}^\nu) = (\mathrm{e}^{\omega_{\mathbf{q}}^\nu/T} - 1)^{-1}$
and $\mathbf{r} = n\mathbf{e}_x + m\mathbf{e}_y + l\mathbf{e}_z$

- decoupling of products of 3 spins in $-\ddot{S}_i^+$ and $-\ddot{S}_i^z$ along the NN sequence $\langle i,j,l\rangle$ by use of vertex parameters [9]:

$$\begin{aligned} S_i^+ S_j^+ S_l^- &= \alpha_{1x,1z}^{+-}\langle S_j^+ S_l^- \rangle S_i^+ + \alpha_2^{+-}\langle S_i^+ S_l^- \rangle S_j^+\,, \\ S_i^z S_j^+ S_l^- &= \alpha_{1x,1z}^{zz}\langle S_j^+ S_l^- \rangle S_i^z\,, \\ S_i^+ S_j^z S_l^- &= \alpha_2^{zz}\langle S_i^+ S_l^- \rangle S_j^z \end{aligned}$$

$$\bullet i \quad \underbrace{\bullet j \quad \bullet l}_{\alpha_{1x}^{+-}} \qquad\qquad \underbrace{\bullet i \quad \bullet j \quad \bullet l}_{\alpha_2^{+-}}$$

$$-\ddot{S}_{\mathbf{q}}^+ = (\omega_{\mathbf{q}}^{+-})^2 S_{\mathbf{q}}^+ \quad \text{and} \quad -\ddot{S}_{\mathbf{q}}^z = (\omega_{\mathbf{q}}^{zz})^2 S_{\mathbf{q}}^z$$

- spectra $\omega_{\mathbf{q}}^\nu$:

$$\begin{aligned} (\omega_{\mathbf{q}}^{zz})^2 &= 2(1-\gamma_{\mathbf{q}})\Big[1 + 2\alpha_2^{zz}(C_{2,0,0}^{+-} + 2C_{1,1,0}^{+-}) \\ &\quad -2\Delta\alpha_{1x}^{zz}C_{1,0,0}^{+-}(1 + 4\gamma_{\mathbf{q}})\Big] \\ &\quad +R_z^2(1 - \cos q_z)\Big[1 + 2\alpha_2^{zz}C_{0,0,2}^{+-} \\ &\quad -2\Delta\alpha_{1z}^{zz}C_{0,0,1}^{+-}(1+2\cos q_z)\Big] \\ &\quad +8R_z\Big[\alpha_2^{zz}C_{1,0,1}^{+-}(2-\gamma_{\mathbf{q}}-\cos q_z) \\ &\quad +\Delta\alpha_{1z}^{zz}C_{0,0,1}^{+-}\gamma_{\mathbf{q}}(\cos q_z - 1) \\ &\quad +\Delta\alpha_{1x}^{zz}C_{1,0,0}^{+-}\cos q_z(\gamma_{\mathbf{q}} - 1)\Big] \end{aligned}$$

- LRO: $\lim_{T \to T_N^\nu}[\chi_{\mathbf{Q}}^\nu]^{-1} = 0$;
  $\omega_{\mathbf{Q}}^\nu = 0$ at $T \le T_N^\nu$

$\Rightarrow$ magnetization $(\mathbf{Q} = (\pi,\pi,\pi))$:

$$(m^\nu)^2 = \frac{1}{N}\sum_{\mathbf{r}} C_{\mathbf{r}}^\nu \mathrm{e}^{-i\mathbf{Q}\mathbf{r}} = C^\nu$$

- C^ν – condensation part in

$$C_{\mathbf{r}}^\nu = \frac{1}{N}\sum_{\mathbf{q}\neq\mathbf{Q}} \frac{M_{\mathbf{q}}^\nu}{2\omega_{\mathbf{q}}^\nu}\mathrm{e}^{i\mathbf{q}\mathbf{r}} + C^\nu \mathrm{e}^{i\mathbf{Q}\mathbf{r}}$$

- determination of vertex parameters:
  - $\alpha_2^{+-}(T)$ & $\alpha_{1x}^{zz}(T)$: sum rules $C_0^{+-} = 1/2$ & $C_0^{zz} = 1/4$)
  - $\alpha_{1z}^{zz}(T)$: $(c_z/c_{xy})^2 = R_z C_{0,0,1}^{+-}/C_{1,0,0}^{+-}$
  - $\alpha_{1x}^{+-}(0)$: data for ground-state energy ε [2,6,10,11]
    $\alpha_{1x}^{+-}(T)$: $\frac{\alpha_{1x}^{+-}(T)-1}{\alpha_{1x}^{zz}(T)-1} = \mathrm{const.}$
  - $\alpha_2^{zz}(0)$: data for $\partial\varepsilon/\partial\Delta$
    $\alpha_2^{zz}(T)$: $\frac{\alpha_2^{zz}(T)-1}{\alpha_{1x}^{zz}(T)-1} = \mathrm{const.}$
  - $\alpha_{1z}^{+-}(T)$: ansatz $\frac{\alpha_{1z}^{+-}(T)}{\alpha_{1x}^{+-}(T)} = \frac{\alpha_{1z}^{zz}(T)}{\alpha_{1x}^{zz}(T)}$