Very high precision determination of the low-energy parameters for the 2d quantum antiferromagnets

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Outline

- Introduction: Heisenberg-type models:
  - Heisenberg-type models are important and interesting from both experimental and theoretical perspectives
- Magnon chiral perturbation theory: the exact low-energy effective field theory for antiferromagnets
- A proposal of calculating the spinwave velocity c using the squares of winding numbers
- Monte Carlo results
- Conclusions

Introduction: Heisenberg-type models

- Heisenberg-type models have been studied in great detail both numerically and analytically during last 2 decades
- The reasons why these models have drawn a lot of attention is twofold:
  - Heisenberg-type models are relevant to real materials:
    - It is believed that spin-1/2 Heisenberg model on the square lattice is the correct model to describe the undoped cuprate which might become high T_c superconductors by doping charge carriers into these materials
    - Due to their relevance to real materials, even today research of Heisenberg-type models is still very active

Introduction: Heisenberg-type models

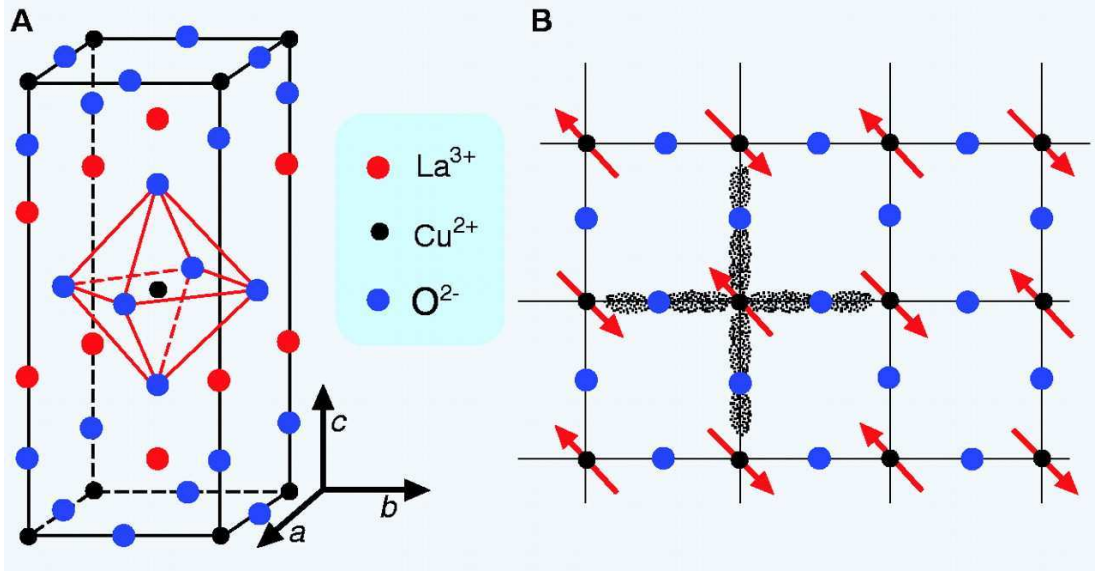
- The availability of efficient Monte Carlo algorithms:
  - With the increasing computing power as well as the advances in numerical Monte Carlo algorithms, the properties of Heisenberg-type models on non-frustrated lattices have been investigated with unprecedented numerical accuracy
  - Using a loop algorithm, the low-energy constants of spin-1/2 Heisenberg model on the square lattice are calculated with high precision (Ying and Wiese, 1994) :

    $$\mathcal{M}_s = 0.3074(4)/a^2, \ \hbar c = 1.68(1)Ja, \ \rho_s = 0.184(4)J$$

  - Experimental results:
    - Inelastic neutron scattering of spin wave velocity : $\hbar c = 0.85(3)$eVÅ
    - Raman scattering : $J = 0.1480(70)$K, $a = 3.79$Å
    - $\rightarrow$ $\hbar c = 1.75(9)Ja, \ \rho_s = 0.186(J)$
  - Because efficient Monte Carlo algorithms can be designed for Heisenberg-type models on non-frustrated lattices, these models are suitable for examining new ideas or testing theoretical predictions

Crystal structure of undoped Cuprates

The crystal structure of undoped cuprates:



- Layers are weakly coupled.
- The interactions in the CuO_2 planes are strong.
- The relevant physics is determined by the 2-dimensonal CuO_2 planes.
- Spontaneous magnetization : anti-parallel spins.

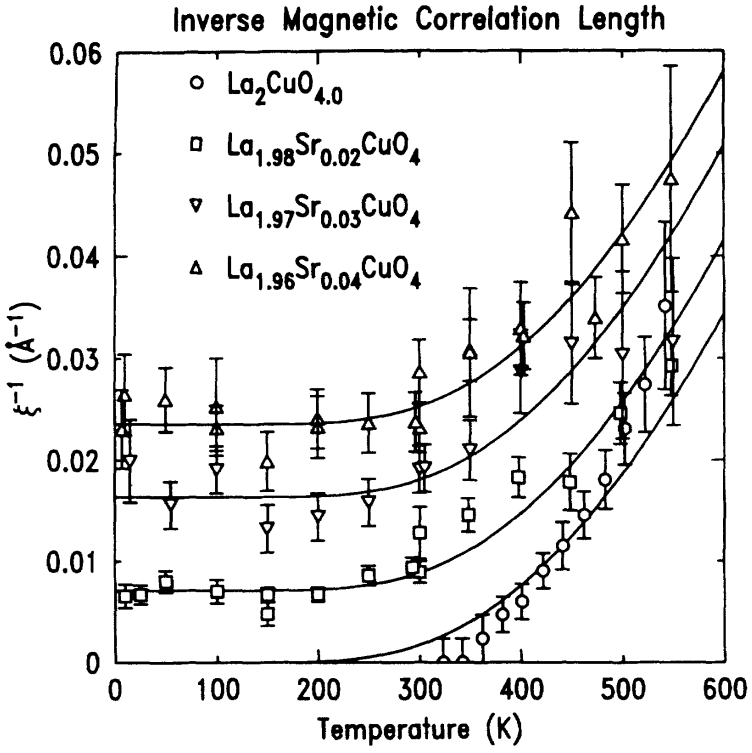
The Heisenberg Models

$$H = J \sum_{\langle xy \rangle} \vec{S}_x \cdot \vec{S}_y \, , J > 0 \, .$$

- Antiferromagnetic alignment of spins is prefered $\longrightarrow$ Heisenberg model on the square lattice indeed is the correct model to describe the properties of undoped cuprates
- Heisenberg-type models are important and interesting because of their relevance to real materials
- Spontaneous Symmetry Breaking (SSB): $SU(2)_s \longrightarrow U(1)_s$
- Goldstone's theorem : 2 massless excitations $\longrightarrow$ magnons

Antiferromagnetism in Real Materials at Low Doping

Keimeret et al. PRB 1992 :



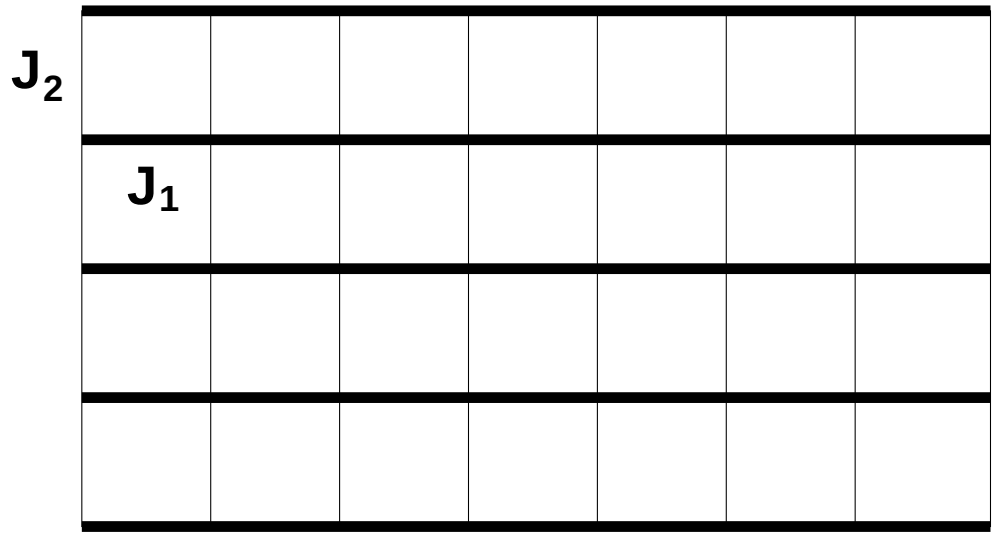
- Divergent magnetic correlation length ξ is a clear signal for massless excitation.
- Magnons dominate low-energy dynamics of lightly doped cuprates.

Spatially anisotropic Heisenberg models

- Isotropic Heisenberg model: J are the same for any 2 nearest neighboring spins
- A more general class of Heisenberg models: spatially anisotropic Heisenberg models
- Spatially Anisotropic Heisenberg Models are relevant to real materials as well:
  - Underdoped cuprate superconductor $YBa_2Cu_3O_{6.45}$
- Spatially Anisotropic Heisenberg Models are of theoretical interest and importance as well
- Efficient Monte Carlo algorithms can be designed to simulate spatially anisotropic Heisenberg models. Hence they are useful in examing theoretical predictions: phase transition induced by dimerization

Spatially Anisotropic Heisenberg Models

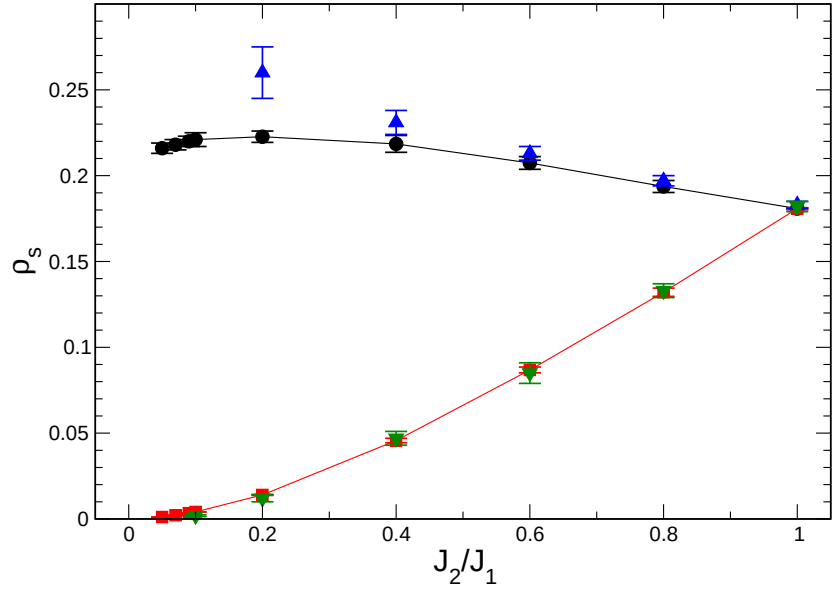
- As one increases the anisotropy, say decreasing the value of J_2, the original 2-D model will become decoupled Heisenberg chains eventually.
- Relevant to the underdoped cuprate superconductor $YBa_2Cu_3O_{6.45}$.



Spatially Anisotropic Heisenberg Models

- Pinning effects of the electronic liquid crystal direction in the underdoped cuprate superconductor $YBa_2Cu_3O_{6.45}$.
- A tiny in-plane lattice anisotropy lead to a much stronger energy in (1,0)-axis direction compared to that in (0,1)-axis.
- Using the method of series expansion, it is argued that : (Pardini, Singh, Katanin and Sushkov , PRB, 2008)
  - The anisotropic spin stiffness ρ_{s1} and ρ_{s2} will lead to a very strong pinning energy, hence provides a possible mechanism to explain the observed pinning effects.
  - The J_1/J_2 dependence of ρ_{s1}/ρ_{s2} in the weak anisotropic regime is given by $\rho_{s1}/\rho_{s2} = 1 + 1.8(J_1/J_2 - 1)$, which deviates from the intuitive expectation $\rho_{s1}/\rho_{s2} \sim J_1/J_2$.
  - Pinning energy per Cu is 5×10^{-2}MeV.
  - Significally larger than the pining energy per spin $\sim 1.5 \times 10^{-3}$MeV in La_2CuO_4.
- It is useful and important to have a relevant Monte Carlo study as well.

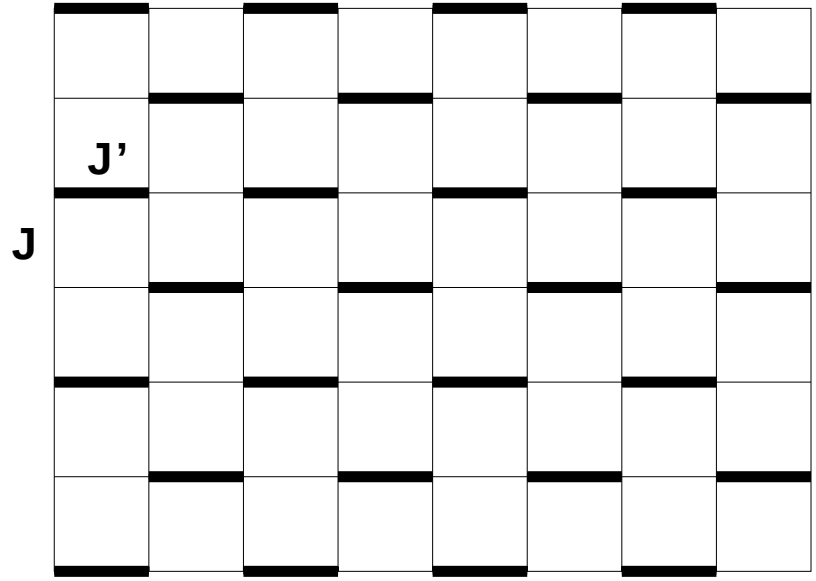
ρ_{s1} and ρ_{s2} as Functions of J_2/J_1



- While the black circles and red squares are the Monte Carlo results for ρ_{s1} and ρ_{s2}, respectively, the blue up triangles and green down triangles are the corresponding series expansion results of ρ_{s1} and ρ_{s2}, respectively. (**FJJ, Kampfer, Nyfeler, PRB 2009**)
- The anisotropic spin stiffness ρ_{s1} and ρ_{s2} indeed will lead to a very strong pinning energy, hence provides a possible mechanism to explain the observed pinning effects as claim by Pardini, Singh, Katanin and Sushkov.

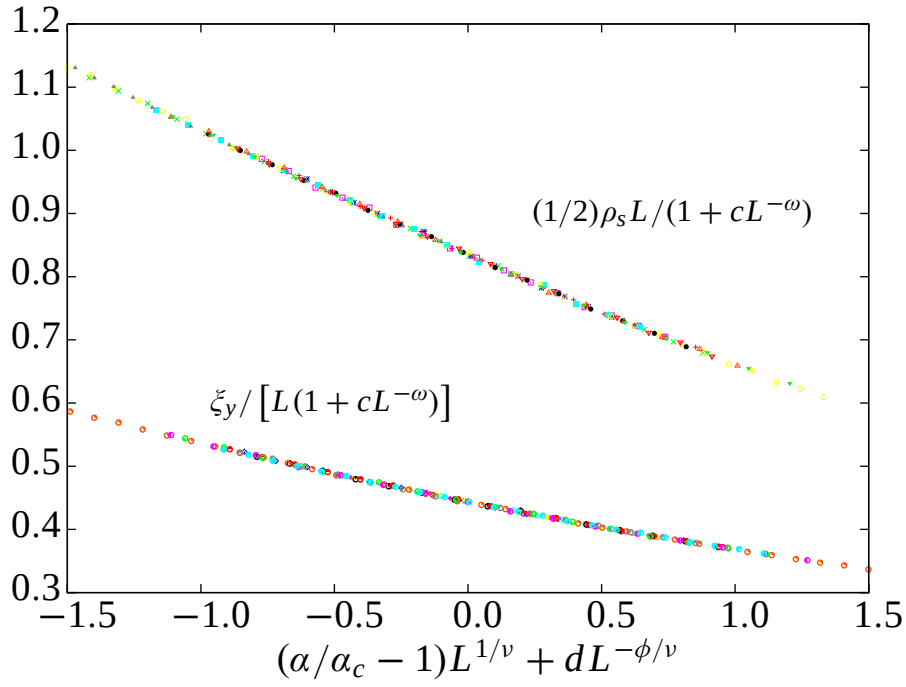
Spatially Anisotropic Heisenberg Models

- Phase transition induced by dimerization as one increases J'
- An unconventional phase transition other than the theoretically predicted $O(3)$ class! (S. Wenzel et al., RPL, 2008)
- $\nu = 0.689(5)$ v.s. $\nu = 0.7112(5)$ (Campostrini et al., PRB 2002)



An unconventional Phase Transition?

- $\nu = 0.689(5)$ instead of the $O(3)$ value $\nu = 0.7112(5)$ (S. Wenzel et al., RPL, 2008)
- Data collapse $\mathcal{O}_L(a/a_c) = (1 + cL^{-\omega})g((a/a_c - 1)L^{1/\nu} + dL^{-\phi/\nu})$:



- Several efforts have been devoted to understand this issue, but puzzle remains.

The Heisenberg Models

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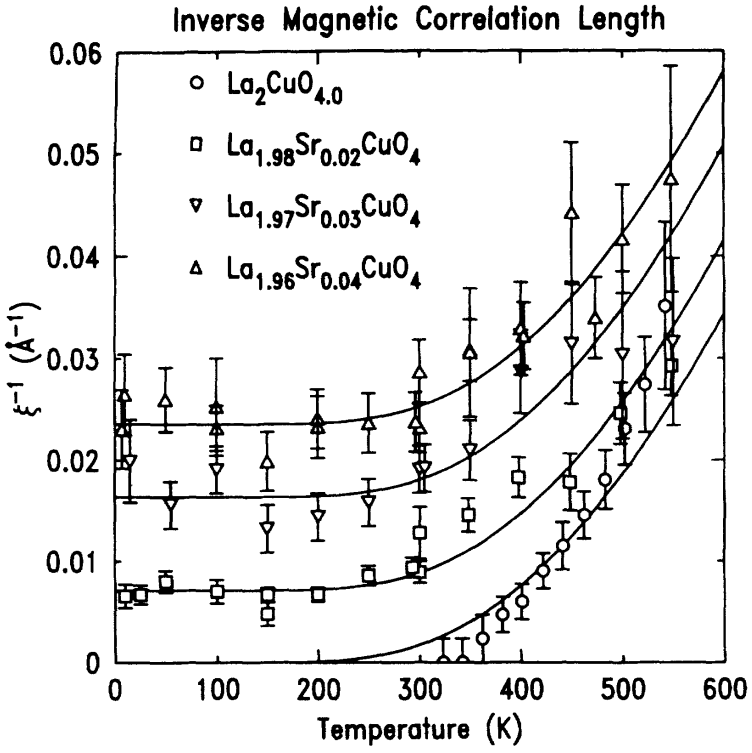

- Divergent magnetic correlation length ξ is a clear signal for massless excitation.
- Magnons dominate low-energy dynamics of lightly doped cuprates.

Effective Field Theory on One Slide

Consider a system with the spontaneous symmetry breaking pattern: $G \to H$, where H is the unbroken subgroup of G. Let n = dim$G$ - dim$H$,

- The low-energy physics of the system is governed by n massless Goldstone bosons.
- The full effective Lagrangian is systematically expressed in term of small parameters.
- In particular, the resulting effective Lagrangian must respect all the symmetries of the underlying physics system.
- The dynamics of the system is determined by the numerical values of the low-energy constants appearing in the effective Lagrangian.
  - The effective field theory is universal.
  - The dynamics is determined by the material-specific low-enrgy constants.

- Chiral Perturbation Theory for QCD : $SU(2)_R \times SU(2)_L \to SU(2)_V$.
  - 3 Golstone bosons : 3 pions.
  - Small parameters: momentum p/Λ_χ and m_π/Λ_χ.
  - Low-energy constants : F_π, $\langle\bar{\psi}\psi\rangle$.....

Magnon Chiral Perturbation Theory

Spontaneous symmetry breaking : $SU(2)_s \rightarrow U(1)_s$.

- Two Goldstone bosons (magnons) described by

$$\vec{e}(x) = \big(e_1(x), e_2(x), e_3(x)\big) \in S^2 = SU(2)_s/U(1)_s$$

  with $x = (x_1, x_2, t)$.

- Low-energy effective Lagrangian [a] :

$$\mathcal{L} = \frac{\rho_s}{2}(\partial_i \vec{e} \cdot \partial_i \vec{e} + \frac{1}{c^2}\partial_t \vec{e} \cdot \partial_t \vec{e}) + \cdots$$

  ρ_s: spin stiffness, c: spin wave velocity.

- Since the low-energy dynamics is completely determined by the numerical values of the corresponding low-energy parameters, it will be of great interest and importance to calculate these low-energy parameters accurately.

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[a] Chakravarty, Halperin, and Nelson, PRB (1989), Hasenfratz and Niedermayer, Phys. Lett. B (1991).

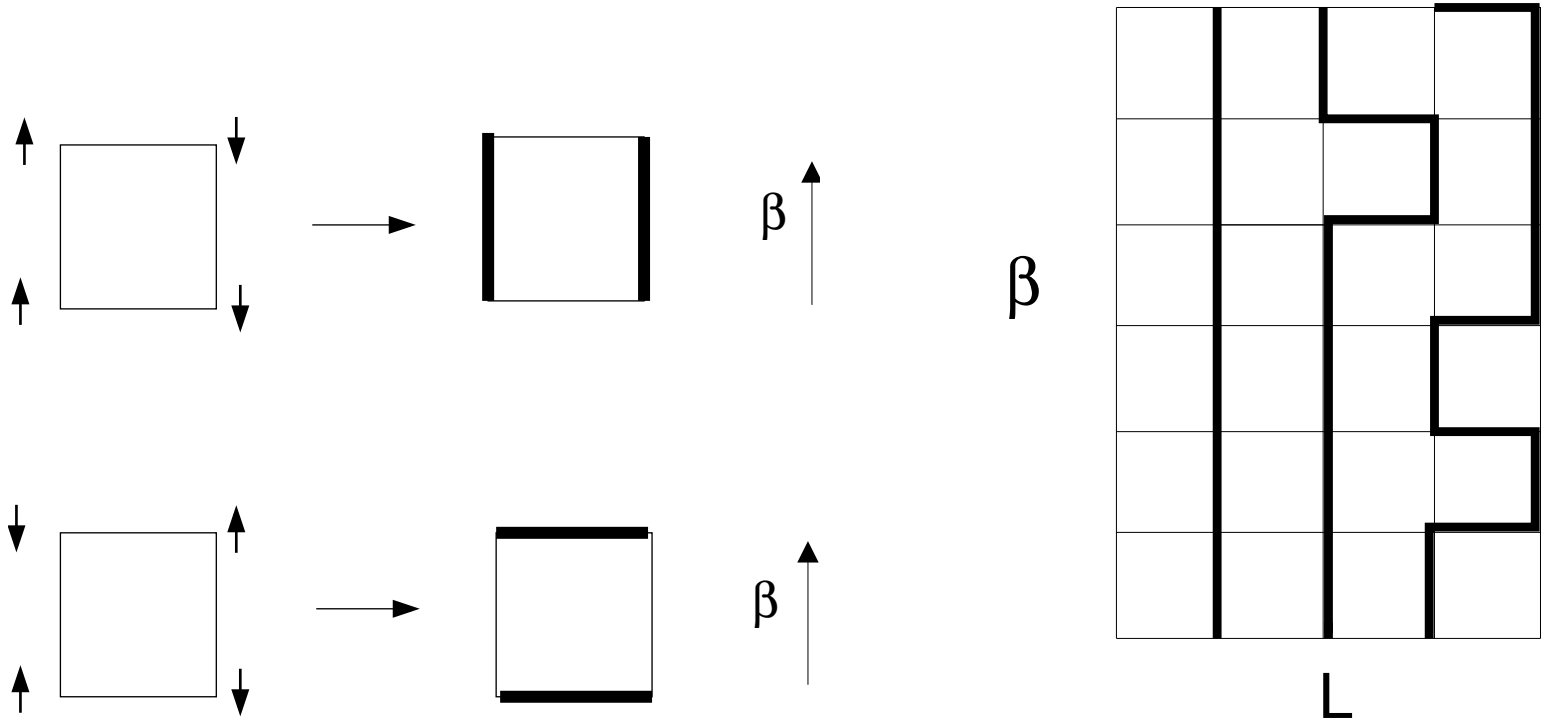
Monte Carlo method

- Methods of studying the properties of antiferromagnets: spin wave theory, series expansion, DMRG, quantum Monte Carlo...
- Monte Carlo is one non-perturbative and exact method
- Given a Hamiltonian H,
  - $$< A >= \frac{1}{Z} \mathrm{Tr}\left(Ae^{-\beta H}\right), \quad Z = \mathrm{Tr}\left(e^{-\beta H}\right)$$
    $$Z = \sum_a \sum_{n=0}^{\infty} \frac{\beta^n}{n!} < a|(-H)^n|a >$$
  - Each term in the summation of Z is called the Boltzmann weight of the configuration $|a >$.
  - Generating (sampling) the configurations according to their Boltzmann weight.

Monte Carlo method

- Generating (sampling) the configurations according to their Boltzmann weight:
  - Detailed Balance
  - Egordicity
- Local update: Heat bath, Metropolis... $\longrightarrow$ critical slowing down, say, a very long autocorrelation time
- Global update: Cluster algorithms... $\longrightarrow$ no critical slowing down
- Existng Monte Calro algorithms for simulating quantum spin sysetms: Loop, SSE, Worm...

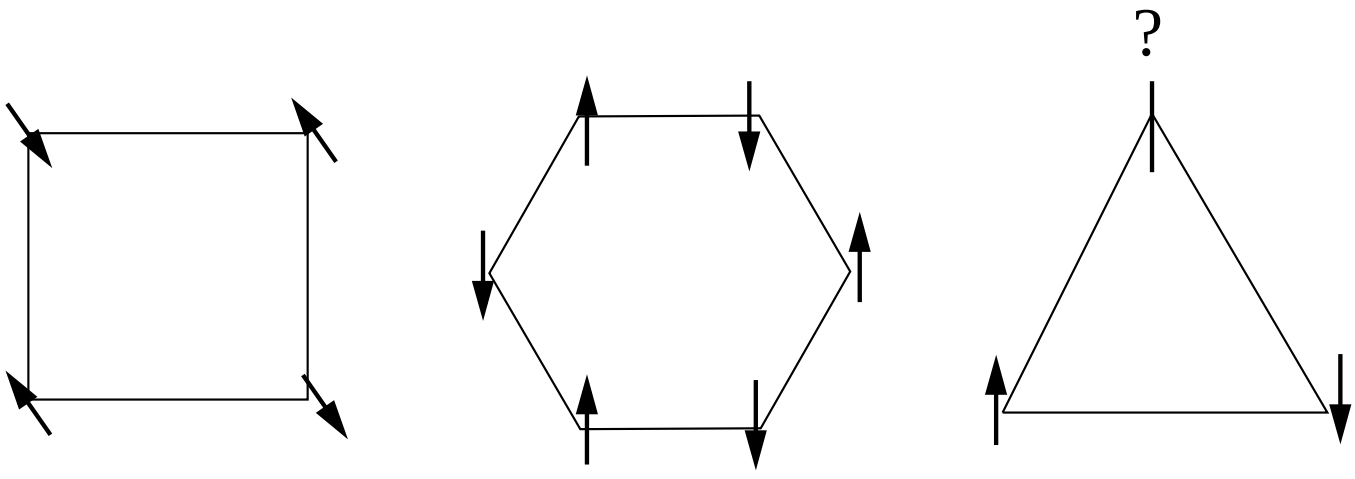
Cluster algorithms



- For each cluster, 0.5 probability to flip the spins along this cluster

Monte Carlo method

- Monte Carlo is a very powerful first principles non-perturbative method for study strongly correlated systems
- Sign problem on geometrically frustrated lattice!



Simulations and Observables

- We use a loop algorithm to simulate the quantum Heisenberg model.
- Staggered susceptibility χ_s and uniform susceptibility χ_u:

$$\chi_s = \frac{1}{L_1 L_2} \int_0^\beta dt \, \frac{1}{Z} \mathrm{Tr}[M_s^3(0) M_s^3(t) \exp(-\beta H)],$$

$$\chi_u = \frac{1}{L_1 L_2} \int_0^\beta dt \, \frac{1}{Z} \mathrm{Tr}[M^3(0) M^3(t) \exp(-\beta H)].$$

β : inverse temperature, L_i : spatial box size in the x_i-direction,

$Z = \mathrm{Tr} \exp(-\beta H)$: partition function,

$\vec{M}_s = \sum_x (-1)^x \vec{S}_x$: staggered magnetization (order parameter).
$\vec{M} = \sum_x \vec{S}_x$: uniform magnetization.

Both χ_s and χ_u can be measured very efficiently with loop algorithm.

Simulations and Observables

The cubical regime : $\beta c \approx L$[a]

$$\chi_s = \frac{\mathcal{M}_s^2 L^2 \beta}{3}\left\{1 + 2\frac{c}{\rho_s L l}\beta_1(l) + \left(\frac{c}{\rho_s L l}\right)^2\left[\beta_1(l)^2 + 3\beta_2(l)\right] + ...\right\},$$

$$\chi_u = \frac{2\rho_s}{3c^2}\left\{1 + \frac{1}{3}\frac{c}{\rho_s L l}\widetilde{\beta}_1(l) + \frac{1}{3}\left(\frac{c}{\rho_s L l}\right)^2\left[\widetilde{\beta}_2(l) - \frac{1}{3}\widetilde{\beta}_1(l)^2 - 6\psi(l)\right] + ...\right\}.$$

$\mathcal{M}_s$: staggered magnetization density per unit area.
$\beta_i(l)$, $\widetilde{\beta}_i(l)$, $\psi(l)$: shape coefficients of the space-time box depending on $l = (\frac{\beta c}{L})^{1/3}$.

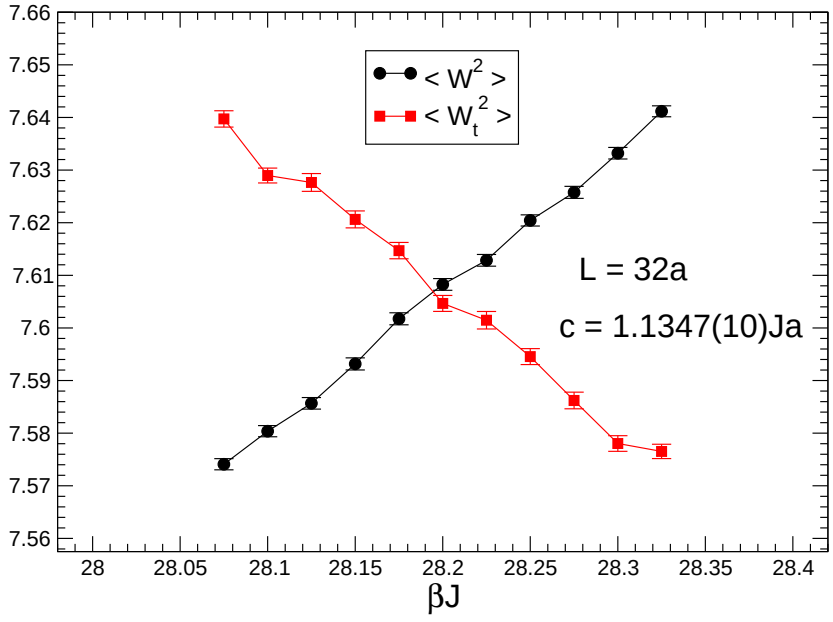
[a] Hasenfratz and Niedermayer, Z. Phys. B (1993).

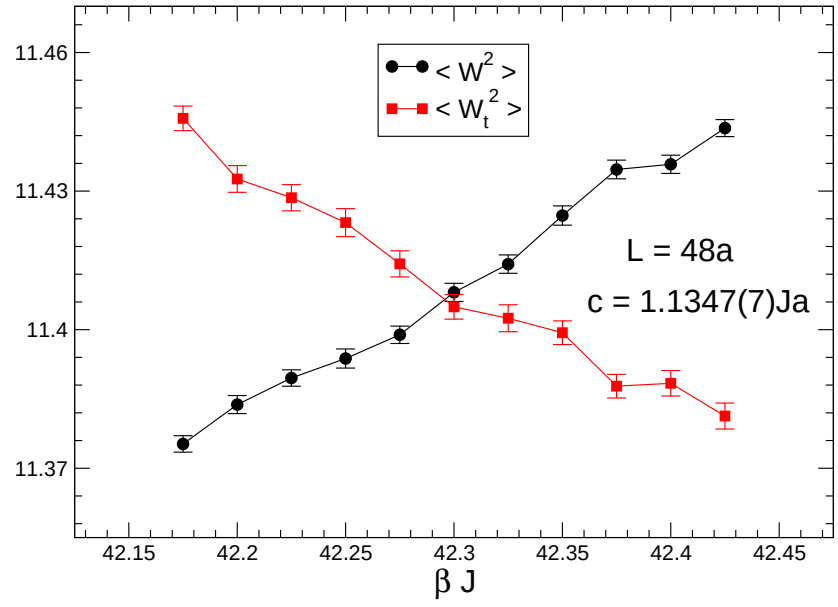
Extraction of the Low-Energy Parameters

- ρ_s and c are strongly correlated. Hence they cannot be determined very precisely by fitting the data to their theoretical predictions: $\rho_s = 1.84(4)J$, $c = 1.68(1)Ja$.
- It will be desirable to measure one of these low-energy parameters by another method.
- We will focus on the low-energy parameter c.
- Conventionally, c can be determined by $\chi = \rho/c^2$. Here χ and ρ are the bulk values of susceptibility and spin stiffness, respectively.
- Extrapolations of finite volume data of χ and ρ to their bulk values will introduce systematic errors as well.
- Therefore it will be important to determine c using a more direct method.
- Motivated by the cubical regime, we propose that c can be calculated by L/β, here L and β are the box size and inverse temperature so that the spatial and temporal winding number squareds take the same values in the Monte Carlo simulations. (**FJJ, PRB 2011**)

Determining c using the squares of winding numbers

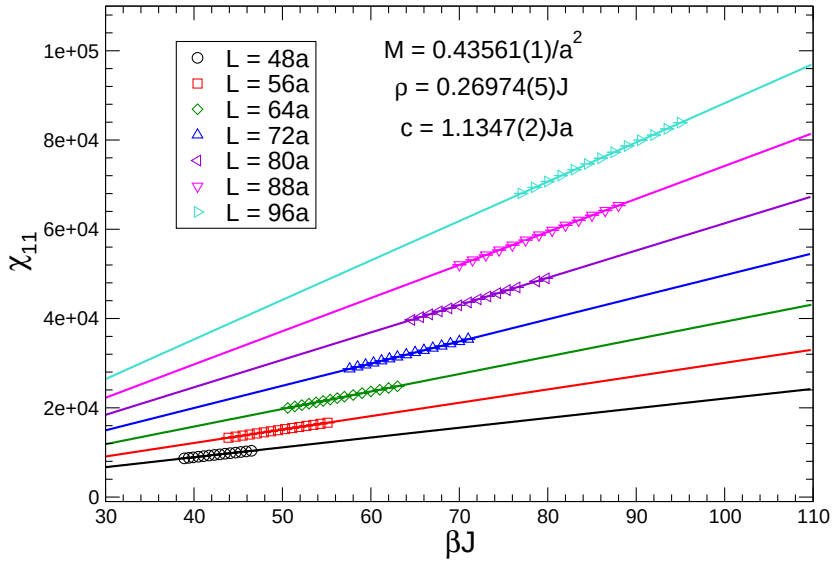
- The c for quantum XY model calculated from the squares of spatial and temporal winding numbers is given by $c = 1.1348(5)Ja$

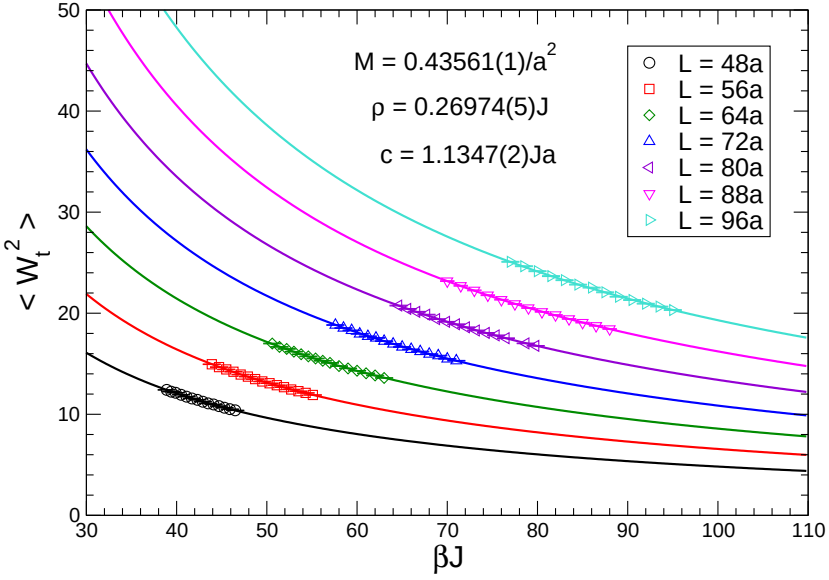




Determining c from chiral fits of χ_{11} and χ

- A simultaneous fit of χ_{11}, χ (and ρ) obtained in the cubical regime to their finite-lattice and -temperature predictions (a constant) from magnon chiral perturbation theory leads to $\mathcal{M} = 0.43561(1)/a^2$, $\rho = 0.26974(5)J$ and $c = 1.1347(2)Ja$
- The $c = 1.1347(2)Ja$ calculated from chiral fits agree excellently with the $c = 1.1348(5)Ja$ obtained using the squares of winding numbers

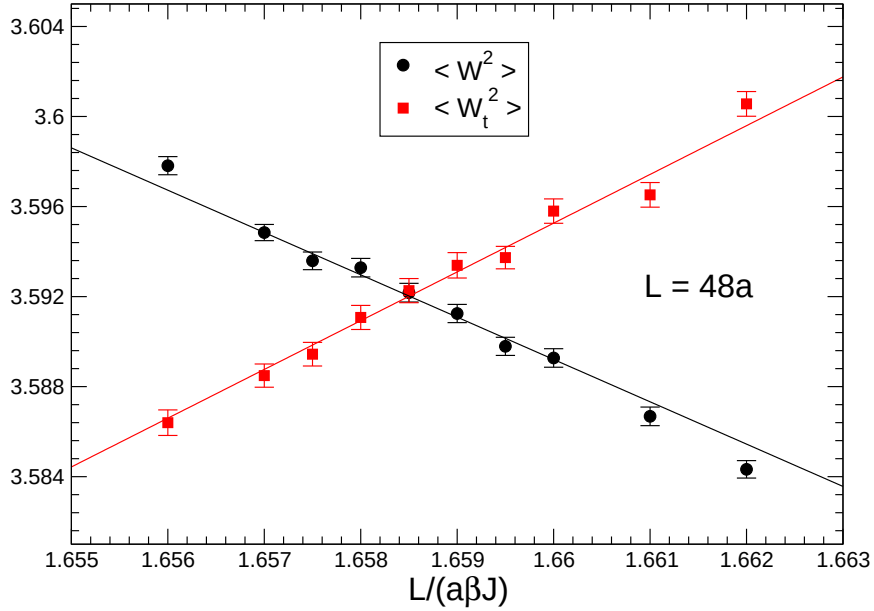




Low-Energy Parameters for Quantum Antiferromagnets

- After verifying the validity of the method of calculating c using the squares of (temporal and spatial) winding numbers, we turn to calculating the low-energy parameters for quantum antiferromagnets.

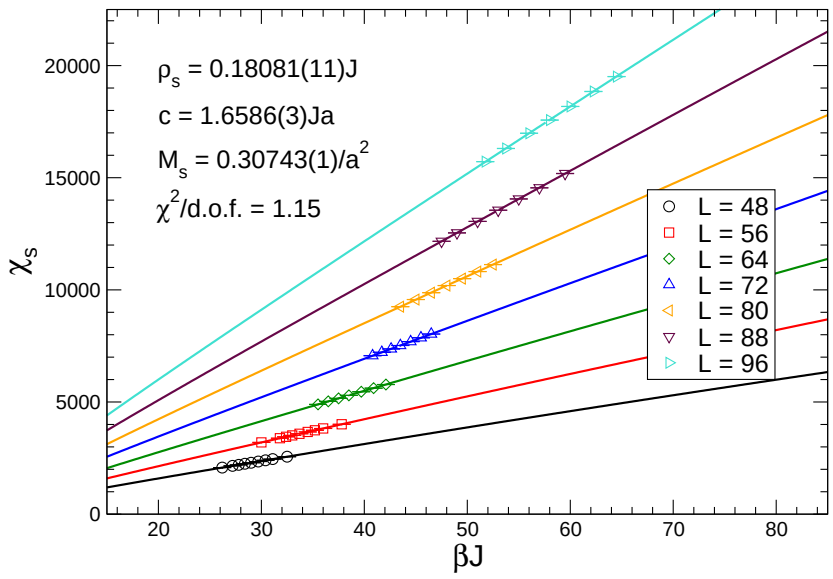
- The numerical value for c of quantum antiferromagnets are determined with very high precision: $c = 1.6586(3)Ja$

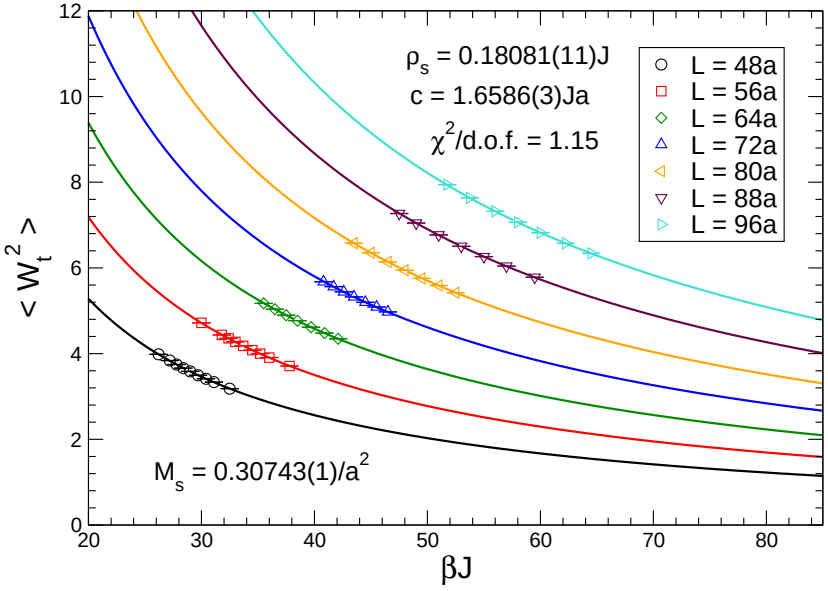


Low-Energy Parameters for Quantum Antiferromagnets

- Using $c = 1.6586(3)Ja$ the numerical values for $\mathcal{M}_s$ and ρ_s are calculated to unprecedented numerical accuracy (**FJJ and Wiese, PRB 2011**):

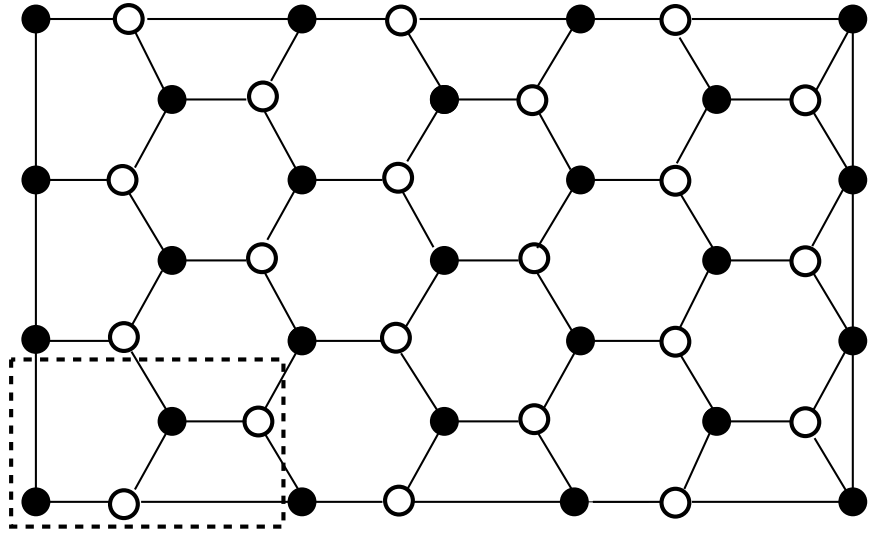
$$\mathcal{M}_s = 0.37043(1)/a^2, \quad \rho_s = 0.18081(11)J$$





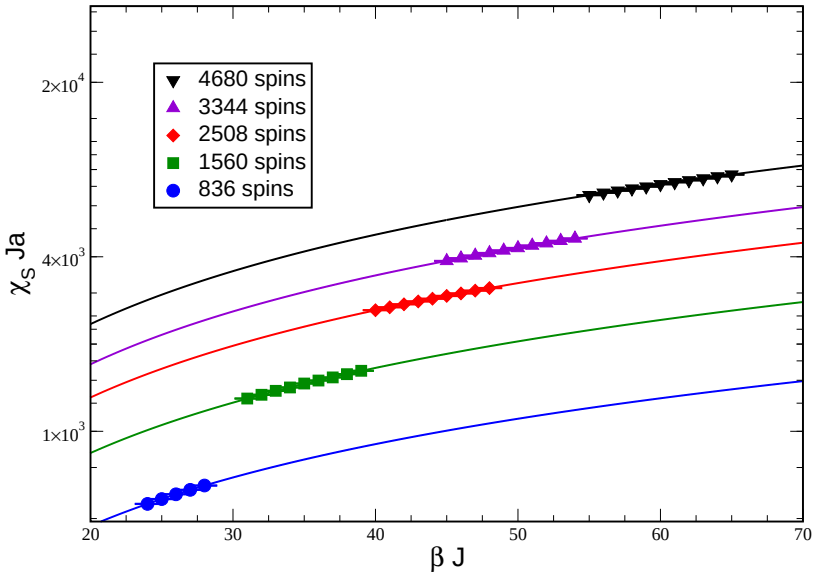
Quantum Antiferromagnets on the Honeycomb Lattice

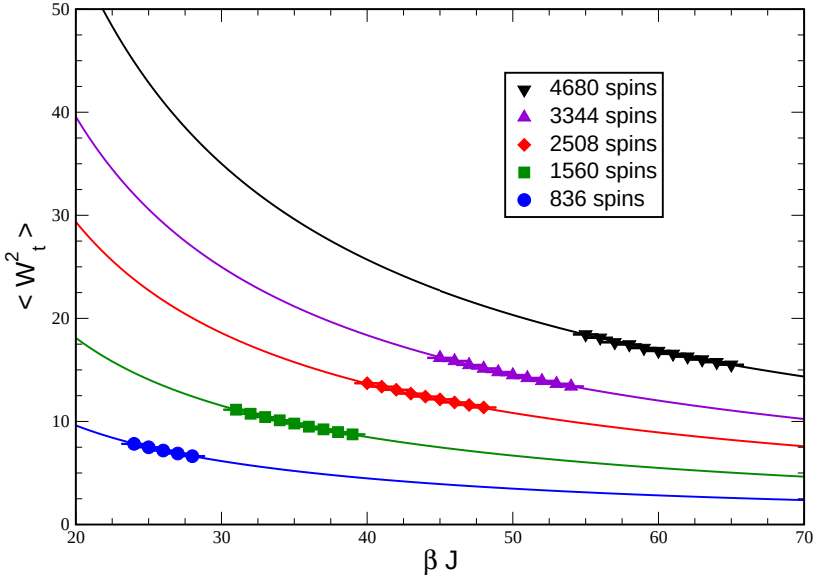
- Quantum antiferromagnets on the honeycomb lattice
  - $InCu_{2/3}V_{1/3}O_3$ (spin-1/2), $Bi_4Mn_4O_{12}(NO_3)$ (spin-3/2), $Na_{1/3}CoO_2 \cdot yH_2O$ (spin-1/2),....



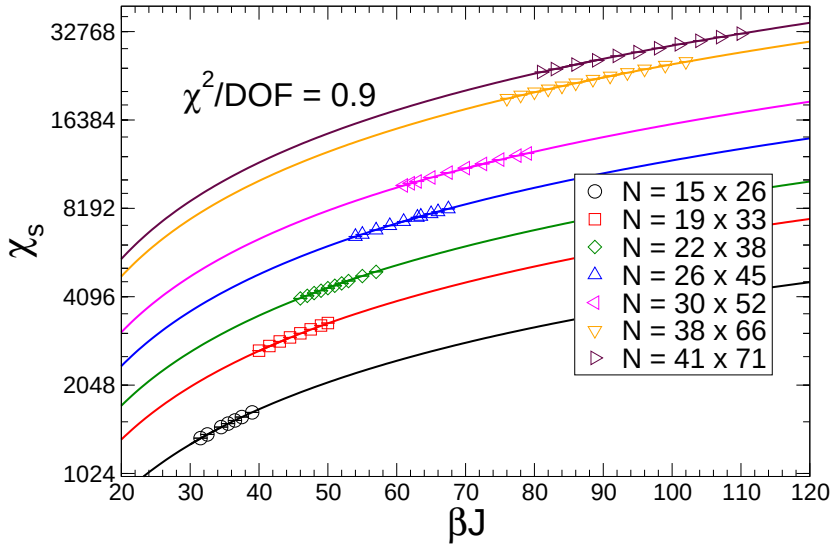
Quantum Antiferromagnets on the Honeycomb Lattice

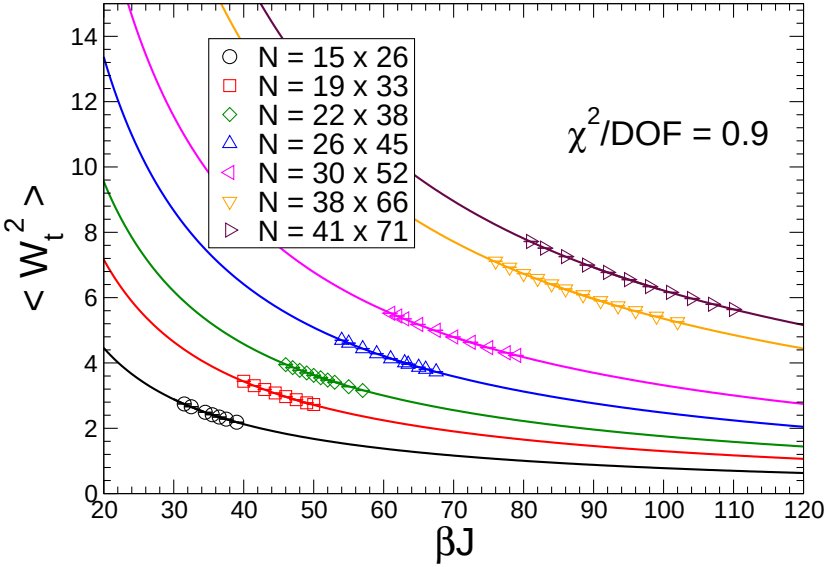
- $\mathcal{M}_s = 0.2688(3), \quad \rho_s = 0.102(2)J, \quad c = 1.297(16)Ja$ **(FJJ, Kampfer, Nyfeler, Wiese, PRB 2008)**





$\mathcal{M}_s = 0.26882(3), \quad \rho_s = 0.1012(2)J, \quad c = 1.2906(8)Ja$





Calculations on the Cylindrical Regime

- The results presented so far are done on the cubical regime: $\beta c \sim L$.
- Finite lattice expression from magnon choral perturbation theory for χ_s at very low temperature (cylindrical regime, $\beta c \gg L$) is available as well:

$$\chi_s = \frac{2}{3}\frac{\mathcal{M}_s^2 \rho_s L^4}{c^2}\left(1 + 3a\frac{c}{\rho_s L} + ...\right)$$

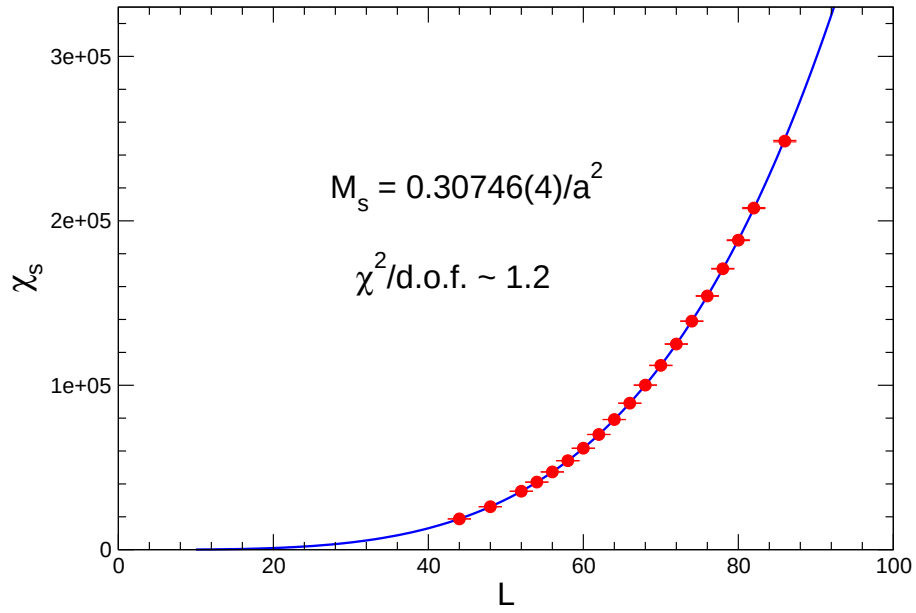
- $\mathcal{M}_s$ and ρ_s can also be calculated in the cylindrical regime.
- An analysis on the cylindrical regime provides a great opportunity to examine the robustness and predictive power of magnon chiral perturbation theory.

Calculations on the Cylindrical Regime

- A fit of χ_s data at very low temperature to their theoretical prediction leads to (**FJJ and Wiese, PRB 2011**)

$$\mathcal{M}_s = 0.30746(4)/a^2, \ \rho_s = 0.18081(11)J,$$

which agrees quantitatively with our earlier results obtained in the cubical regime.



Conclusions

- (Quantum) Heisenberg-type models are interesting and important:
  - Relevance to real materials.
  - Suitable for exploring new ideas.
  - Even today, new discoveries in experiments might be explained by these (simple) models.
- Low-energy dynamics of quantum antiferromagnets are completely determined by the numerical values of the corresponding low-energy parameters.
- We propose that c can be calculated from the squares of winding numbers.
- Verify our proposal by simulating the Quantum XY models.
- The numerical values for the low-energy parameters of the quantum antiferromagnets are determined with unprecedented numerical accuracy:

$$\mathcal{M}_s = 0.37043(1)/a^2, \quad \rho_s = 0.18081(11)J, \quad c = 1.6585(3)Ja.$$

Conclusions

- The consistence between the values of $\mathcal{M}_s$ obtained in the cubical and cylindrical regimes demonstrates the robustness of magnon chiral perturbation theory in understanding the low-energy dynamics of quantum antiferromagnets.