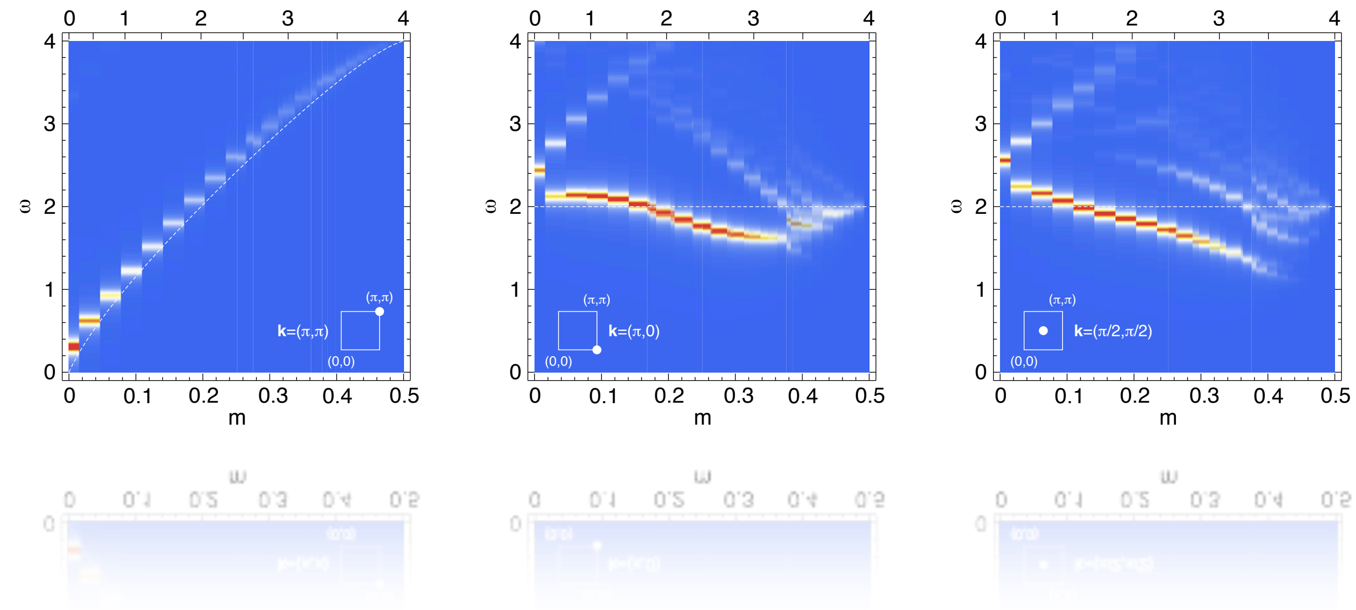


Exact Diagonalization:
A Smart Tool to Study New States of Quantum Matter

Andreas Läuchli,
“New states of quantum matter”
MPI für Physik komplexer Systeme - Dresden

http://www.pks.mpg.de/~aml
laeuchli@comp-phys.org

IPAM QS2009 Workshop, January 27, 2009

Outline

- Exact Diagonalization
- Dynamical Spin Correlations
  - Square Lattice AFM in a field
  - Kagome AFM
- “Tower of States” spectroscopy (continuous symmetry breaking)
  - Conventional magnetic vs spin nematic order
- Correlation Density Matrices
  - Concept
  - Applications to spin chains and the Kagome AFM

Outline

- Exact Diagonalization
- Dynamical Spin Correlations
  - Square Lattice AFM in a field
  - Kagome AFM
- "Tower of States" spectroscopy (continuous symmetry breaking)
  - Conventional magnetic vs spin nematic order
- Correlation Density Matrices
  - Concept
  - Applications to spin chains and the Kagome AFM

Exact Diagonalization: Main Idea

$$\mathcal{H}|\psi\rangle = E|\psi\rangle$$

Exact Diagonalization: Main Idea

- Solve the Schrödinger equation of a quantum many body system numerically

$$\mathcal{H}|\psi\rangle = E|\psi\rangle$$

Exact Diagonalization: Main Idea

- Solve the Schrödinger equation of a quantum many body system numerically

$$\mathcal{H}|\psi\rangle = E|\psi\rangle$$

- Sparse matrix, but for quantum many body systems the vector space dimension grows exponentially!

Exact Diagonalization: Main Idea

- Solve the Schrödinger equation of a quantum many body system numerically

$$\mathcal{H}|\psi\rangle = E|\psi\rangle$$

- Sparse matrix, but for quantum many body systems the vector space dimension grows exponentially!

- But if you want to get a maximum of physical information out of a finite system there is a lot more you can do, and the reward is a powerful:

Exact Diagonalization: Main Idea

- Solve the Schrödinger equation of a quantum many body system numerically

$$\mathcal{H}|\psi\rangle = E|\psi\rangle$$

- Sparse matrix, but for quantum many body systems the vector space dimension grows exponentially!

- But if you want to get a maximum of physical information out of a finite system there is a lot more you can do, and the reward is a powerful:

Quantum Mechanics Toolbox

Exact Diagonalization: Applications

Exact Diagonalization: Applications

- Quantum Magnets: nature of novel phases, critical points in 1D, dynamical correlation functions in 1D & 2D

Exact Diagonalization: Applications

- Quantum Magnets: nature of novel phases, critical points in 1D, dynamical correlation functions in 1D & 2D

- Fermionic models (Hubbard/t-J): gaps, pairing properties, correlation exponents, etc

Exact Diagonalization: Applications

- Quantum Magnets: nature of novel phases, critical points in 1D, dynamical correlation functions in 1D & 2D
- Fermionic models (Hubbard/t-J): gaps, pairing properties, correlation exponents, etc
- Fractional Quantum Hall states: energy gaps, overlap with model states, entanglement spectra

Exact Diagonalization: Applications

- Quantum Magnets: nature of novel phases, critical points in 1D, dynamical correlation functions in 1D & 2D
- Fermionic models (Hubbard/t-J): gaps, pairing properties, correlation exponents, etc
- Fractional Quantum Hall states: energy gaps, overlap with model states, entanglement spectra
- Quantum dimer models or other constrained models:
  → following talk by D. Poilblanc

Exact Diagonalization: Applications

- Quantum Magnets: nature of novel phases, critical points in 1D, dynamical correlation functions in 1D & 2D
- Fermionic models (Hubbard/t-J): gaps, pairing properties, correlation exponents, etc
- Fractional Quantum Hall states: energy gaps, overlap with model states, entanglement spectra
- Quantum dimer models or other constrained models:
  → following talk by D. Poilblanc
- Full Configuration Interaction in Quantum Chemistry

Exact Diagonalization: Applications

- Quantum Magnets: nature of novel phases, critical points in 1D, dynamical correlation functions in 1D & 2D
- Fermionic models (Hubbard/t-J): gaps, pairing properties, correlation exponents, etc
- Fractional Quantum Hall states: energy gaps, overlap with model states, entanglement spectra
- Quantum dimer models or other constrained models:
  → following talk by D. Poilblanc
- Full Configuration Interaction in Quantum Chemistry

Exact Diagonalization: Present Day Limits

low-lying eigenvalues, not full diagonalization

Exact Diagonalization: Present Day Limits

- Fractional quantum hall effect

  different filling fractions ν, up to 16-20 electrons

  up to 300 million basis states, up to 1 billion in the near future

low-lying eigenvalues, not full diagonalization

Exact Diagonalization: Present Day Limits

- Fractional quantum hall effect
  different filling fractions ν, up to 16-20 electrons
  up to 300 million basis states, up to 1 billion in the near future

- Spin S=1/2 models:
  40 spins square lattice, 39 sites triangular, 42 sites star lattice at $S^z=0$
  64 spins or more in elevated magnetization sectors
  up to 1.5 billion(=10^9) basis states with symmetries, up to 4.5 billion without

low-lying eigenvalues, not full diagonalization

Exact Diagonalization: Present Day Limits

- Fractional quantum hall effect
  different filling fractions ν, up to 16-20 electrons
  up to 300 million basis states, up to 1 billion in the near future

- Spin S=1/2 models:
  40 spins square lattice, 39 sites triangular, 42 sites star lattice at $S^z=0$
  64 spins or more in elevated magnetization sectors
  up to 1.5 billion(=10^9) basis states with symmetries, up to 4.5 billion without

- t-J models:
  32 sites checkerboard with 2 holes
  32 sites square lattice with 4 holes
  up to 2.8 billion basis states

low-lying eigenvalues, not full diagonalization

Exact Diagonalization: Present Day Limits

- Fractional quantum hall effect
  different filling fractions ν, up to 16-20 electrons
  up to 300 million basis states, up to 1 billion in the near future
- Spin S=1/2 models:
  40 spins square lattice, 39 sites triangular, 42 sites star lattice at $S^z=0$
  64 spins or more in elevated magnetization sectors
  up to 1.5 billion(=10^9) basis states with symmetries, up to 4.5 billion without
- t-J models:
  32 sites checkerboard with 2 holes
  32 sites square lattice with 4 holes
  up to 2.8 billion basis states
- Hubbard models
  20 sites square lattice at half filling, 20 sites quantum dot structure
  22-25 sites in ultracold atoms setting
  up to 80 billion basis states

low-lying eigenvalues, not full diagonalization

Frequency Dynamics (in 2D)

- Exact Diagonalization:

  numerically determine the low-lying eigenstates of the full many-body Schrödinger equation using Krylov-space techniques.

  - Ground state at different total S^z obtained by the Lanczos method

  - Dynamical correlations by the continued fraction method

$$S(Q,\omega)_\eta = -\frac{1}{\pi}\mathrm{Im}\langle GS|S(Q)^\dagger \frac{1}{\omega - H + E_{GS} + i\eta} S(Q)|GS\rangle$$

$$S(Q,\omega) = \sum_n |\langle\psi_n|S(Q)|GS\rangle|^2 \delta(\omega - E_n)$$

  - Typical dimensions dim=10^8 states, i.e. 64 sites and 200-500 iterations give a good spectrum

Frequency Dynamics (in 2D)

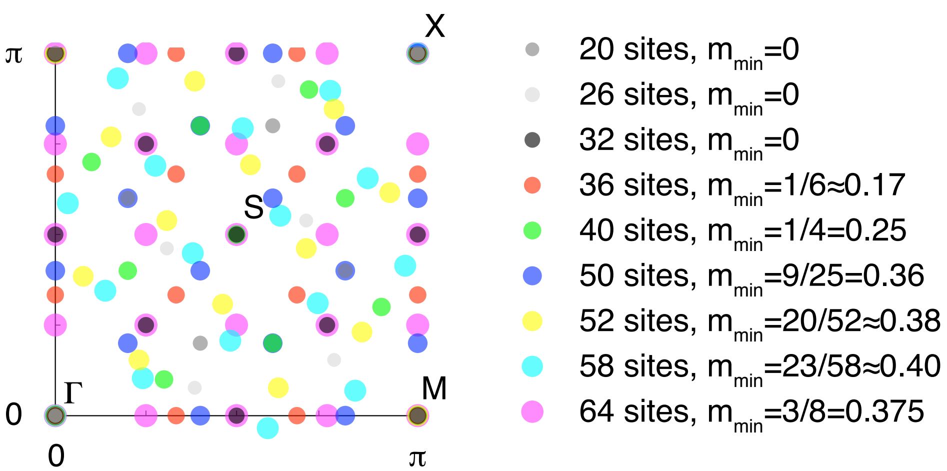
- Exact Diagonalization:

  numerically determine the low-lying eigenstates of the full many-body Schrödinger equation using Krylov-space techniques.

  - Ground state at different total S^z obtained by the Lanczos method
  - Dynamical correlations by the continued fraction method

$$S(Q,\omega)_\eta = -\frac{1}{\pi}\mathrm{Im}\langle GS|S(Q)^\dagger \frac{1}{\omega - H + E_{GS} + i\eta} S(Q)|GS\rangle$$

$$S(Q,\omega) = \sum_n |\langle \psi_n|S(Q)|GS\rangle|^2 \delta(\omega - E_n)$$



  - Typical dimensions dim=10^8 states, i.e. 64 sites and 200-500 iterations give a good spectrum

Frequency Dynamics (in 2D)

- Exact Diagonalization:

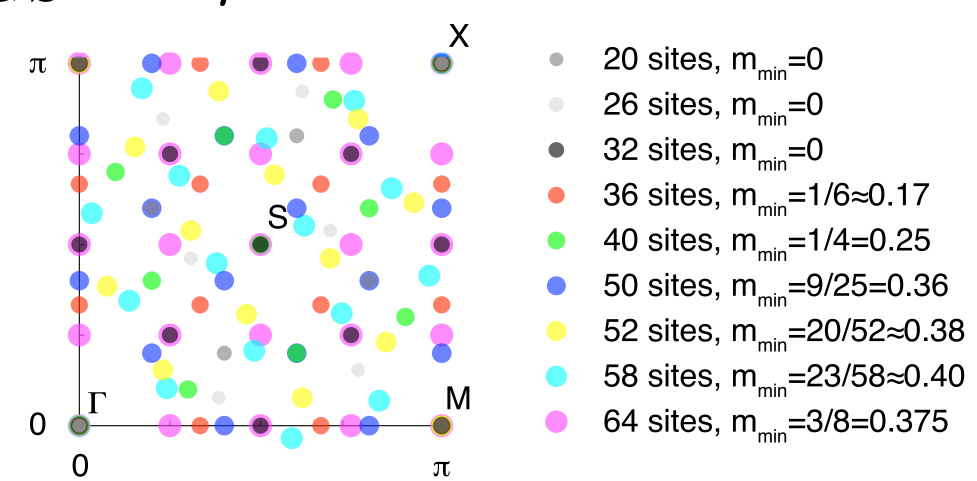
numerically determine the low-lying eigenstates of the full many-body Schrödinger equation using Krylov-space techniques.

- Ground state at different total S^z obtained by the Lanczos method

- Dynamical correlations by the continued fraction method

$$S(Q,\omega)_\eta = -\frac{1}{\pi}\mathrm{Im}\langle GS|S(Q)^\dagger \frac{1}{\omega - H + E_{GS} + i\eta} S(Q)|GS\rangle$$

$$S(Q,\omega) = \sum_n |\langle \psi_n|S(Q)|GS\rangle|^2 \delta(\omega - E_n)$$



- Typical dimensions dim=10^8 states, i.e. 64 sites and 200-500 iterations give a good spectrum

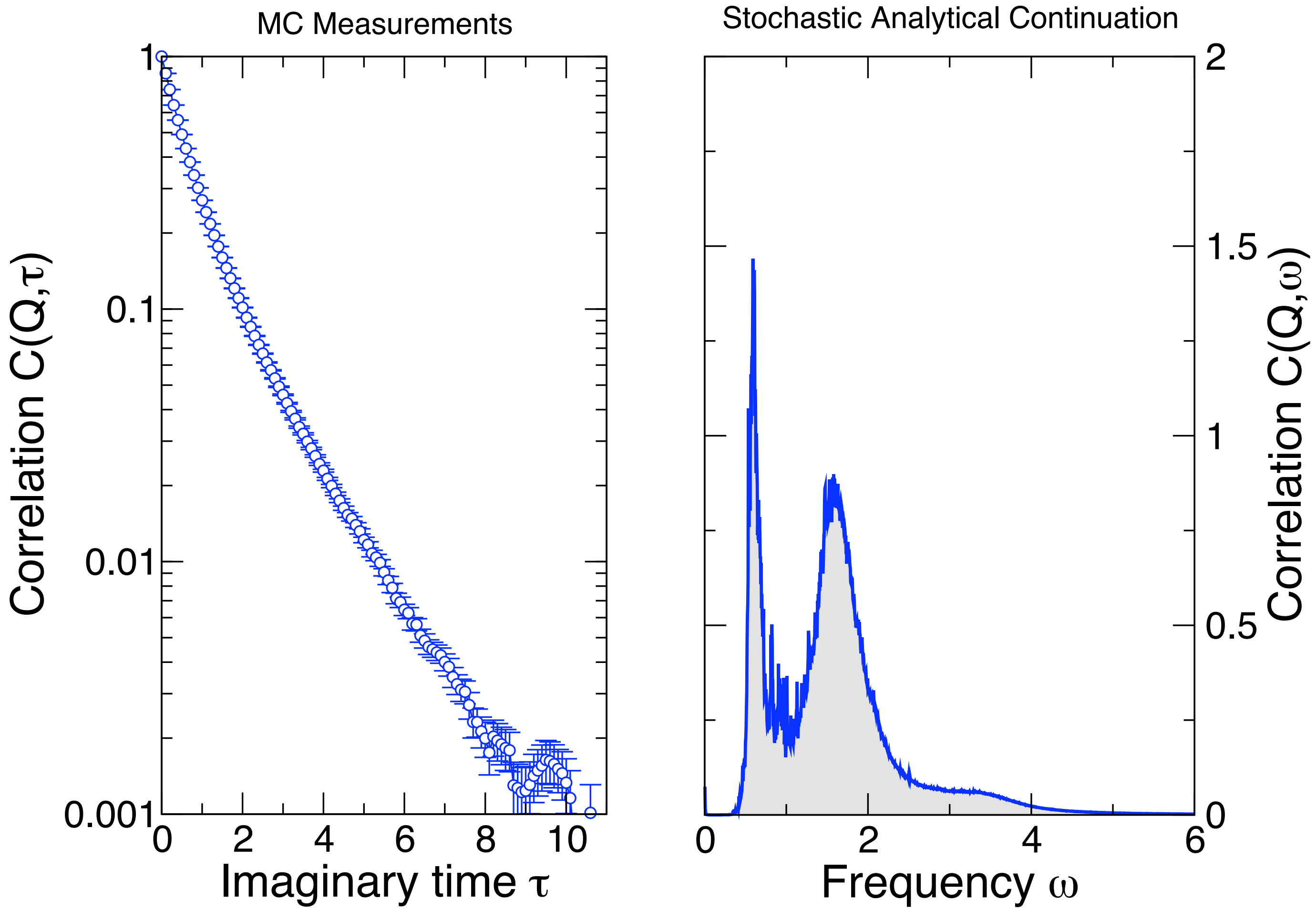
Numerical Approaches (in 2D)

- Quantum Monte Carlo:

  Highly efficient sampling of the partition function for unfrustrated quantum magnets using e.g. Stochastic Series Expansion (SSE) Sandvik ’91,’99

- Measures correlation functions in imaginary time

- Analytical continuation to real frequency needed (inverse Laplace transform): Maximum Entropy, Stochastic Analytical Continuation
  Jarrell & Gubernatis ’96, Sandvik ’98, Beach ’04



Numerical Approaches (in 2D)

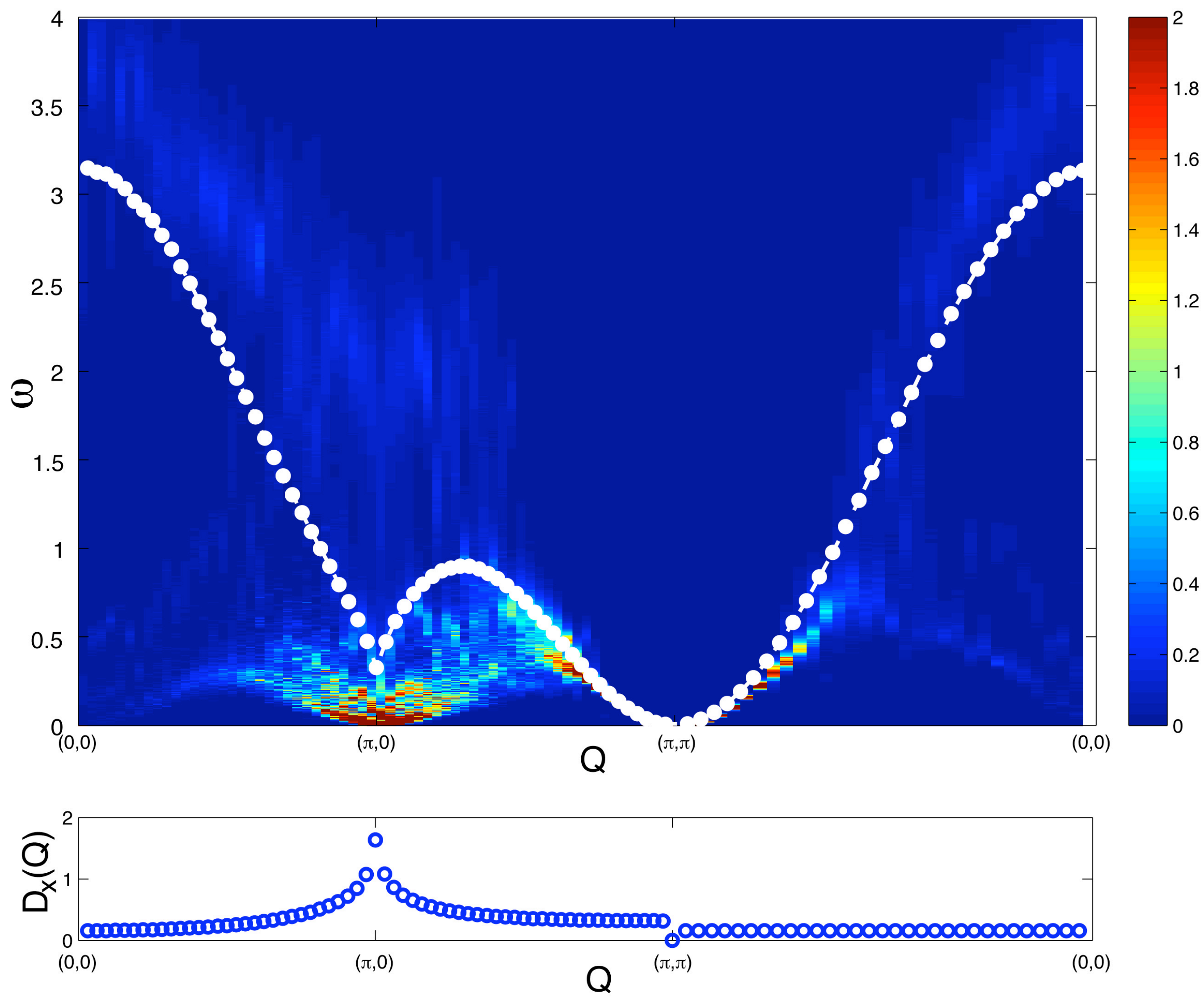
- Quantum Monte Carlo:

  Highly efficient sampling of the partition function for unfrustrated quantum magnets using e.g. Stochastic Series Expansion (SSE) Sandvik ’91,’99

- Measures correlation functions in imaginary time

- Analytical continuation to real frequency needed (inverse Laplace transform): Maximum Entropy, Stochastic Analytical Continuation

  Jarrell & Gubernatis ’96, Sandvik ’98, Beach ’04

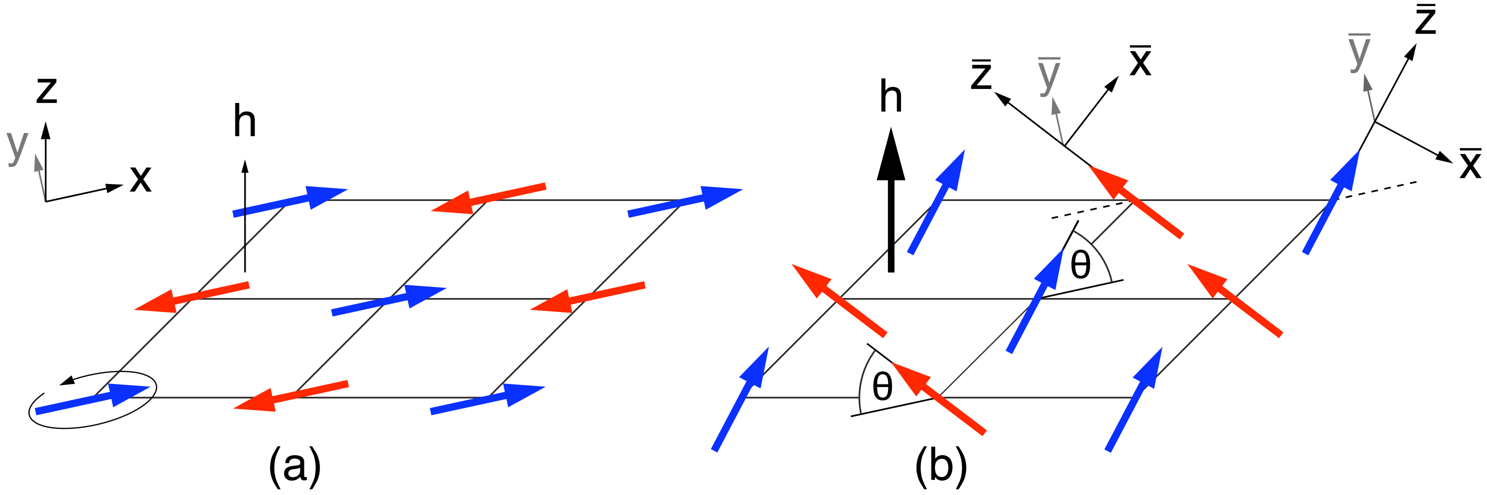


AML, Capponi, Assaad, JSTAT 08

Outline

- Exact Diagonalization
- Dynamical Spin Correlations
  - Square Lattice AFM in a field
  - Kagome AFM
- “Tower of States” spectroscopy (continuous symmetry breaking)
  - Conventional magnetic vs spin nematic order
- Correlation Density Matrices
  - Concept
  - Applications to spin chains and the Kagome AFM

Square Lattice Heisenberg Antiferromagnet



weak (zero) field

finite field

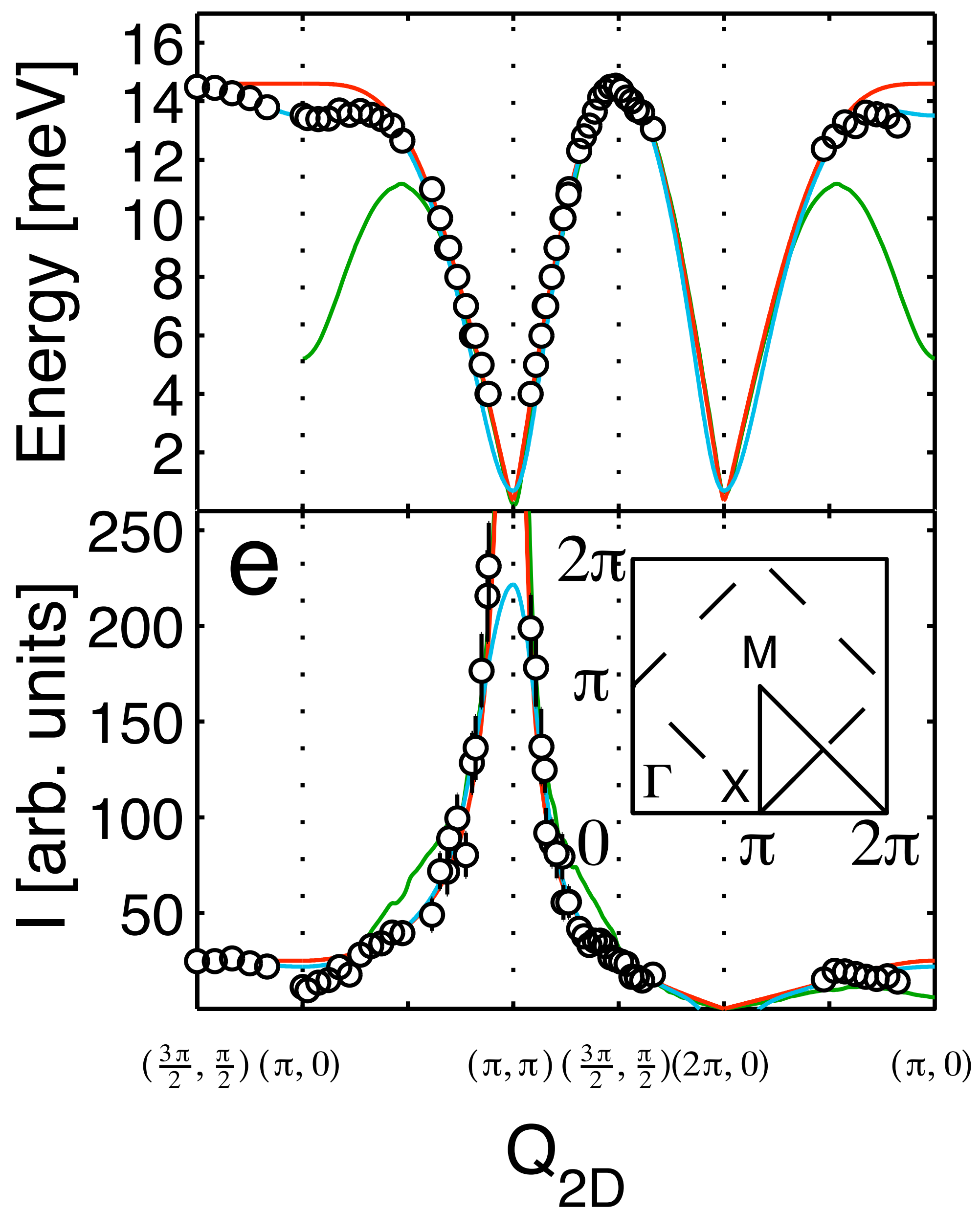
$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^z$$

A. Lüscher, AML, arXiv:0812.3420

Excitation Spectrum of a Square Lattice S=1/2 Antiferromagnet in a Field

Excitation Spectrum of a Square Lattice S=1/2 Antiferromagnet in a Field

- The zero field case is well understood both theoretically and experimentally (Series Expansions; QMC + MaxEnt; Experiments on CTFD, Ronnow '02/Christensen '07)



Excitation Spectrum of a Square Lattice S=1/2 Antiferromagnet in a Field

- The zero field case is well understood both theoretically and experimentally (Series Expansions; QMC + MaxEnt; Experiments on CTFD, Ronnow '02/Christensen '07)
- In a magnetic field the situation is much less clear:

Excitation Spectrum of a Square Lattice S=1/2 Antiferromagnet in a Field

- The zero field case is well understood both theoretically and experimentally (Series Expansions; QMC + MaxEnt; Experiments on CTFD, Ronnow '02/Christensen '07)
- In a magnetic field the situation is much less clear:
  - Theory: two conflicting predictions:
    M.E. Zhitomirsky & A.L. Chernyshev (PRL 99)
    interacting spin wave theory → magnons decay above a threshold field of approximately 3/4 of the saturation field.

    O. Syljuåsen & P.A. Lee (PRL 02)
    π - flux state mean-field calculations → no evidence for magnon decay, however low energy spectral weight in a region where spin wave theory predicts none.

Excitation Spectrum of a Square Lattice S=1/2 Antiferromagnet in a Field

- The zero field case is well understood both theoretically and experimentally (Series Expansions; QMC + MaxEnt; Experiments on CTFD, Ronnow '02/Christensen '07)
- In a magnetic field the situation is much less clear:
  - Theory: two conflicting predictions:
    M.E. Zhitomirsky & A.L. Chernyshev (PRL 99)
    interacting spin wave theory → magnons decay above a threshold field of approximately 3/4 of the saturation field.

    O. Syljuåsen & P.A. Lee (PRL 02)
    π - flux state mean-field calculations → no evidence for magnon decay, however low energy spectral weight in a region where spin wave theory predicts none.
  - Experiments: not yet performed (or on the way ?) ...

Excitation Spectrum of a Square Lattice S=1/2 Antiferromagnet in a Field

- The zero field case is well understood both theoretically and experimentally (Series Expansions; QMC + MaxEnt; Experiments on CTFD, Ronnow '02/Christensen '07)

- In a magnetic field the situation is much less clear:

  - Theory: two conflicting predictions:
    M.E. Zhitomirsky & A.L. Chernyshev (PRL 99)
    interacting spin wave theory → magnons decay above a threshold field of approximately 3/4 of the saturation field.

    O. Syljuåsen & P.A. Lee (PRL 02)
    π - flux state mean-field calculations → no evidence for magnon decay, however low energy spectral weight in a region where spin wave theory predicts none.

  - Experiments: not yet performed (or on the way ?) ...

  - Numerical simulation can help to settle this issue

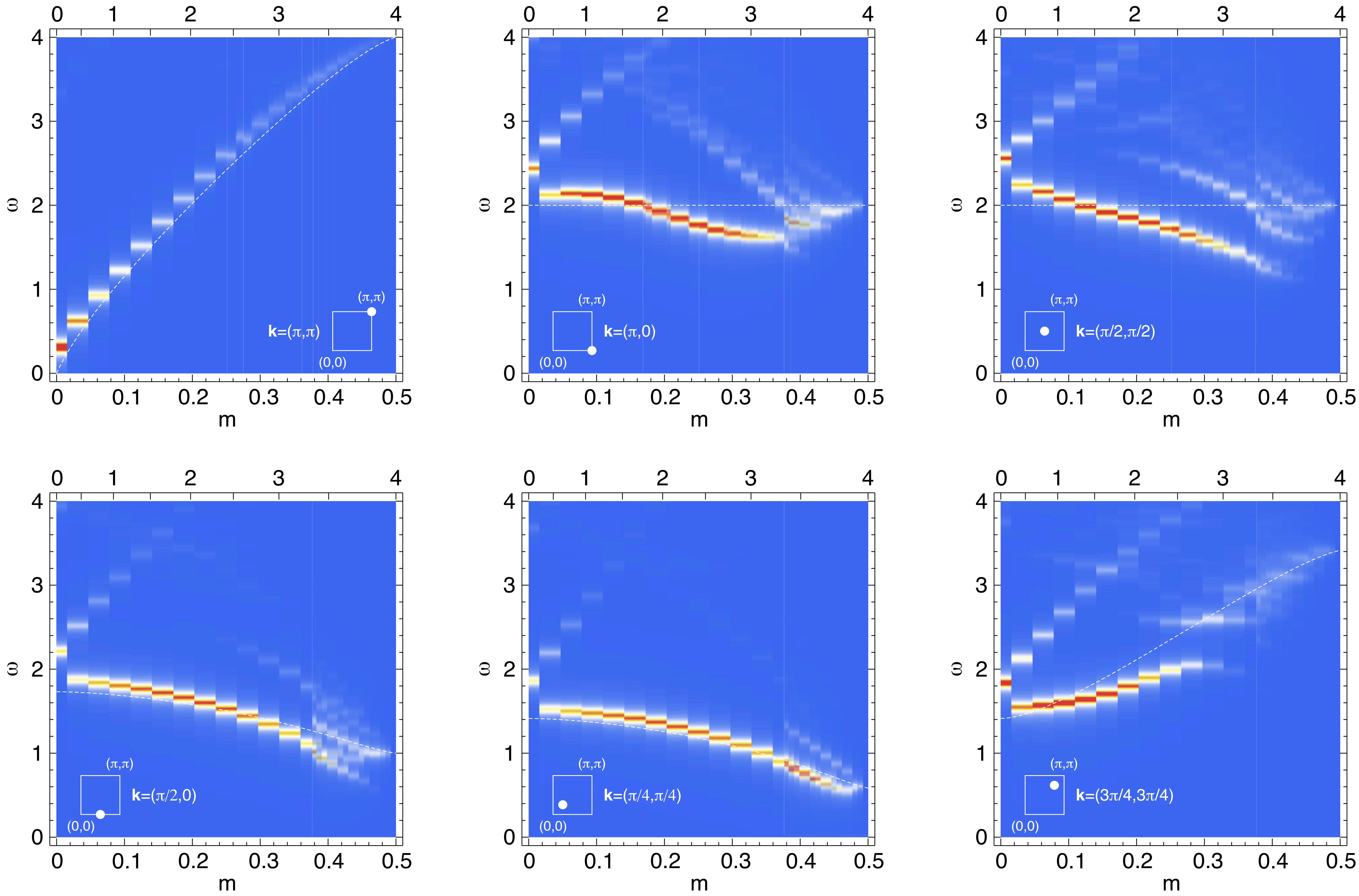
Dynamical Spin Correlations in a Field

- In a magnetic field the SU(2) symmetry is reduced to U(1)
- The relevant spin correlators are
  - The longitudinal response: $S^{zz}(Q,\omega)$
  - The transverse response:

$$S^{xx}(Q,\omega) = S^{yy}(Q,\omega) = \frac{1}{4}\left[S^{+-}(Q,\omega) + S^{-+}(Q,\omega)\right]$$

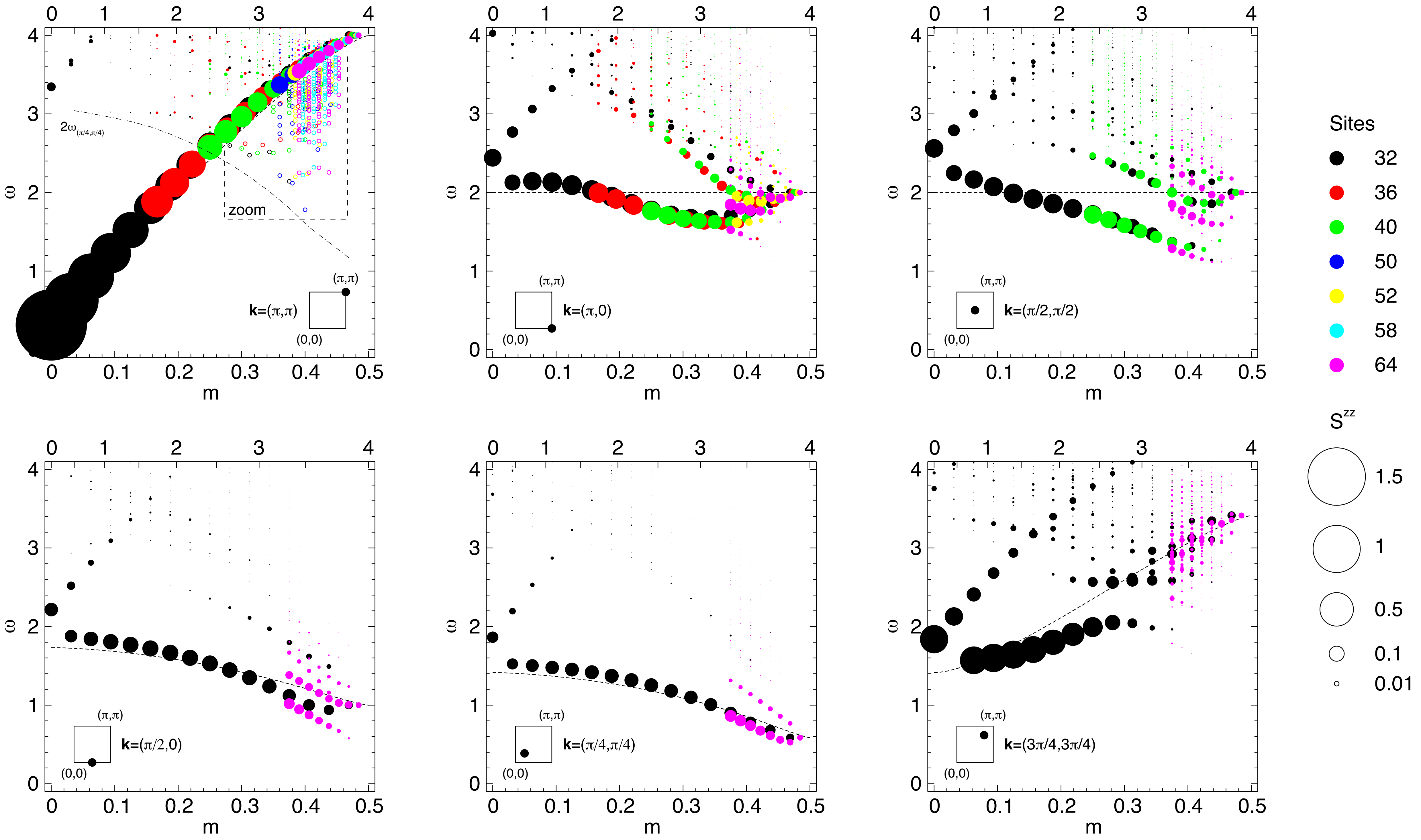
- In the present case the transverse response is to a very good approximation equal to the longitudinal response shifted by (π,π).

Predicted INS Spectra as a function of field



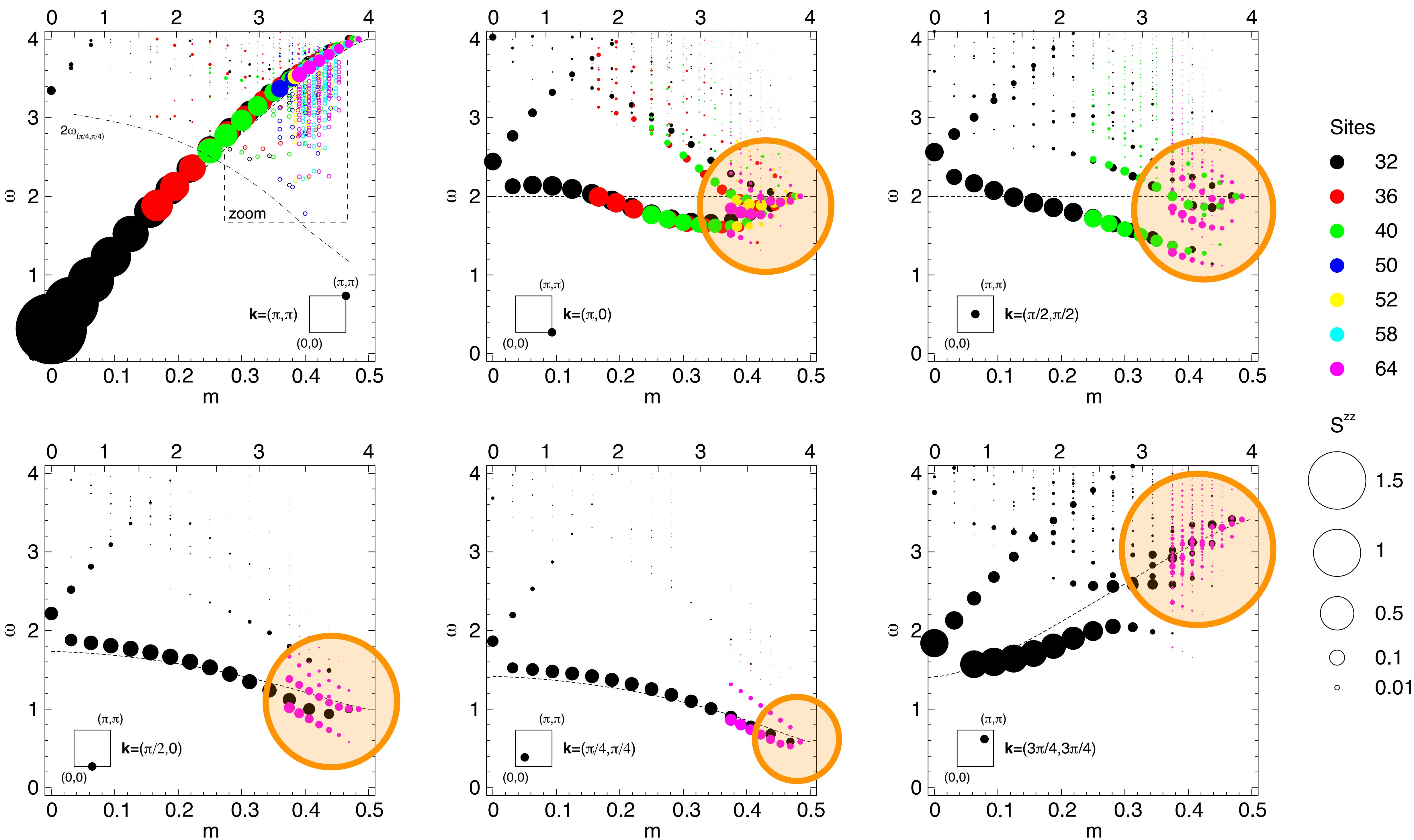
Field dependence:
Finite size pole structure

Longitudinal dynamical structure factors $S^{zz}(\omega,\mathbf{k})$



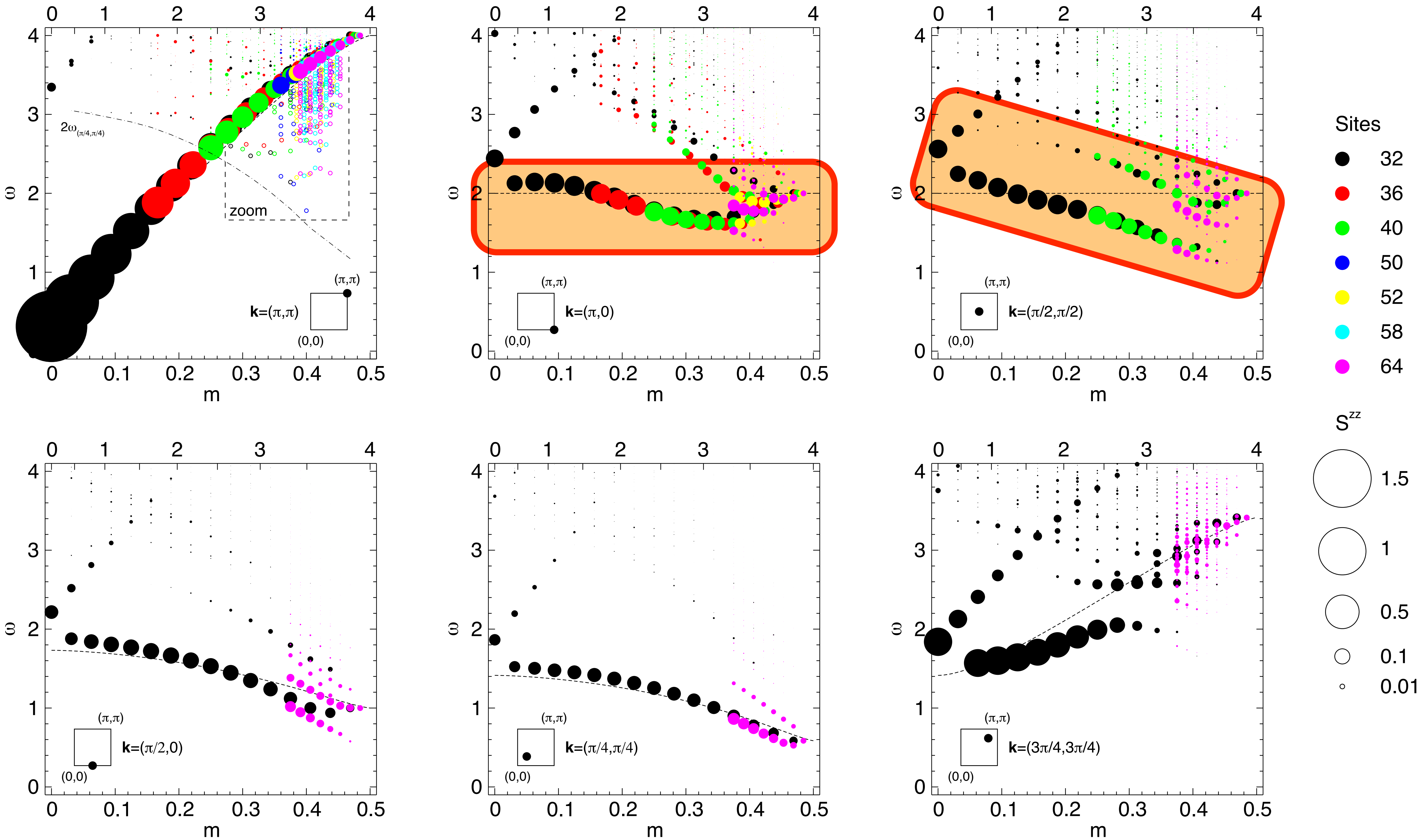
Field dependence:
Finite size pole structure

Longitudinal dynamical structure factors $S^{zz}(\omega,\mathbf{k})$



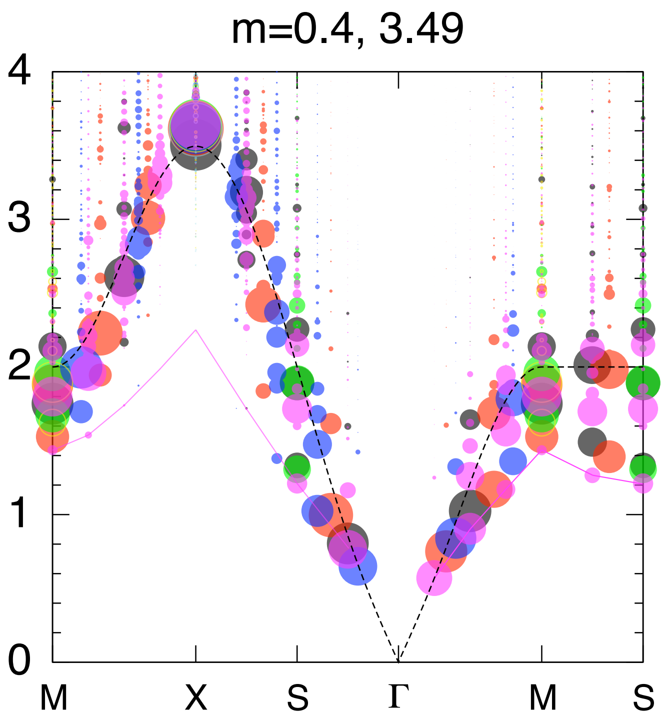
Field dependence:
Finite size pole structure

Longitudinal dynamical structure factors $S^{zz}(\omega,\mathbf{k})$

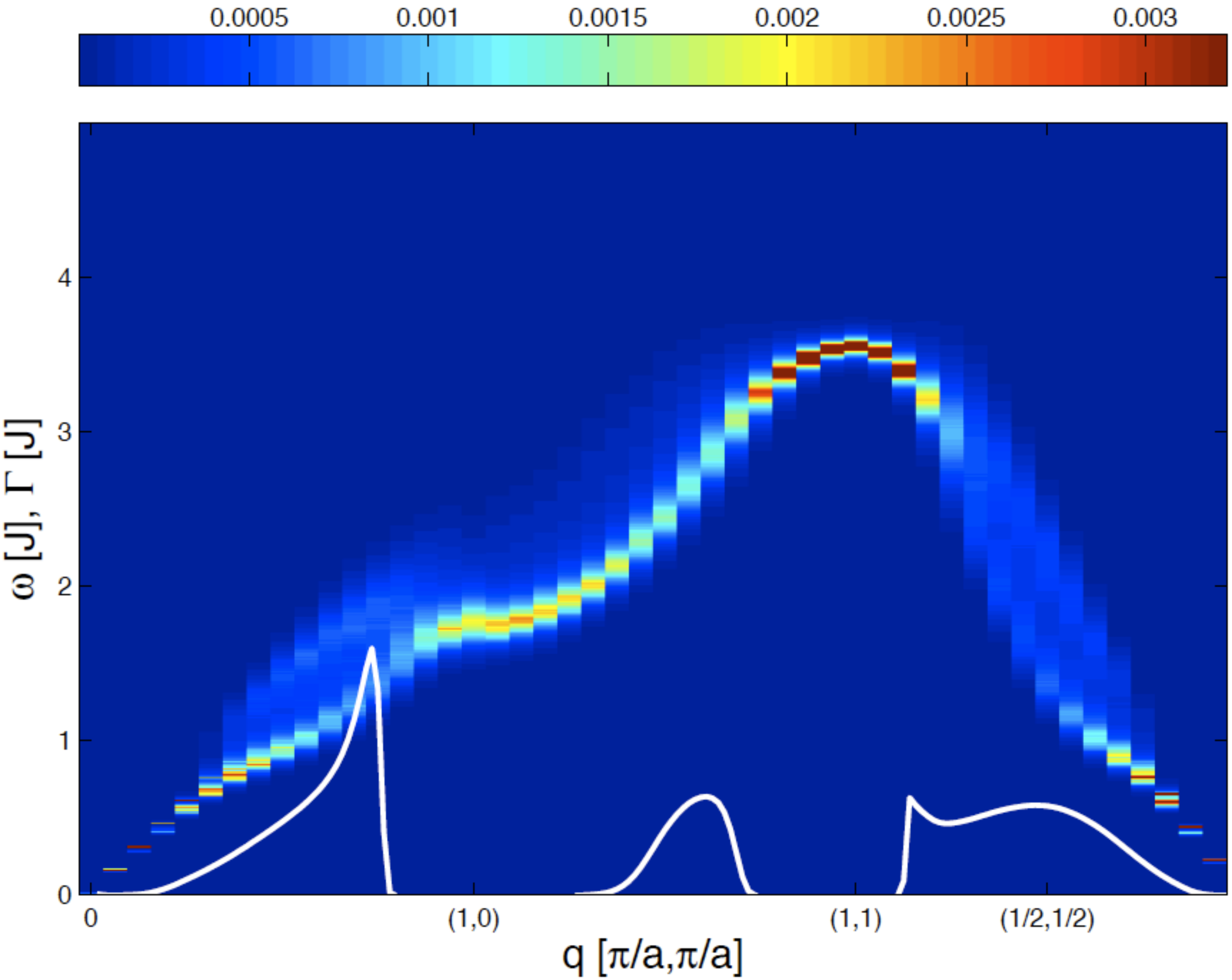


Square Lattice AFM
QMC + Analytical Continuation results

L=32
H/J=3.5



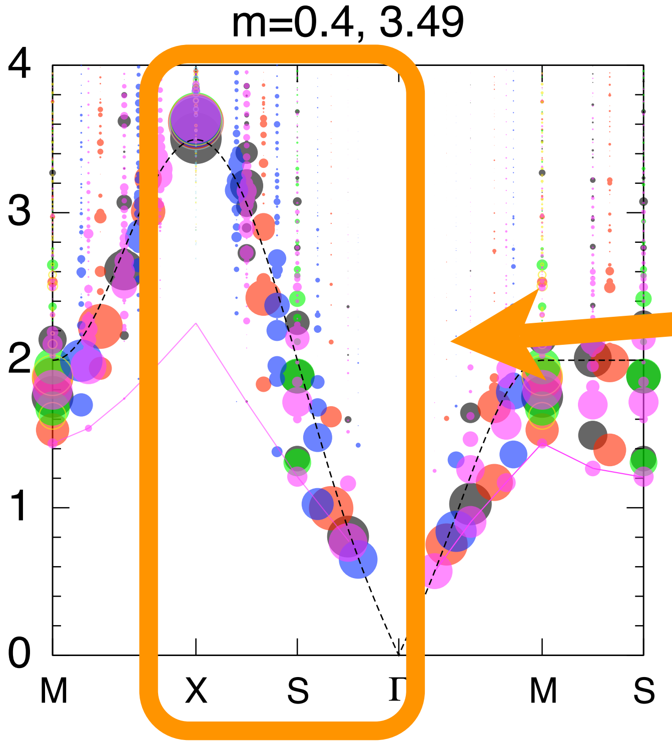
Our ED results



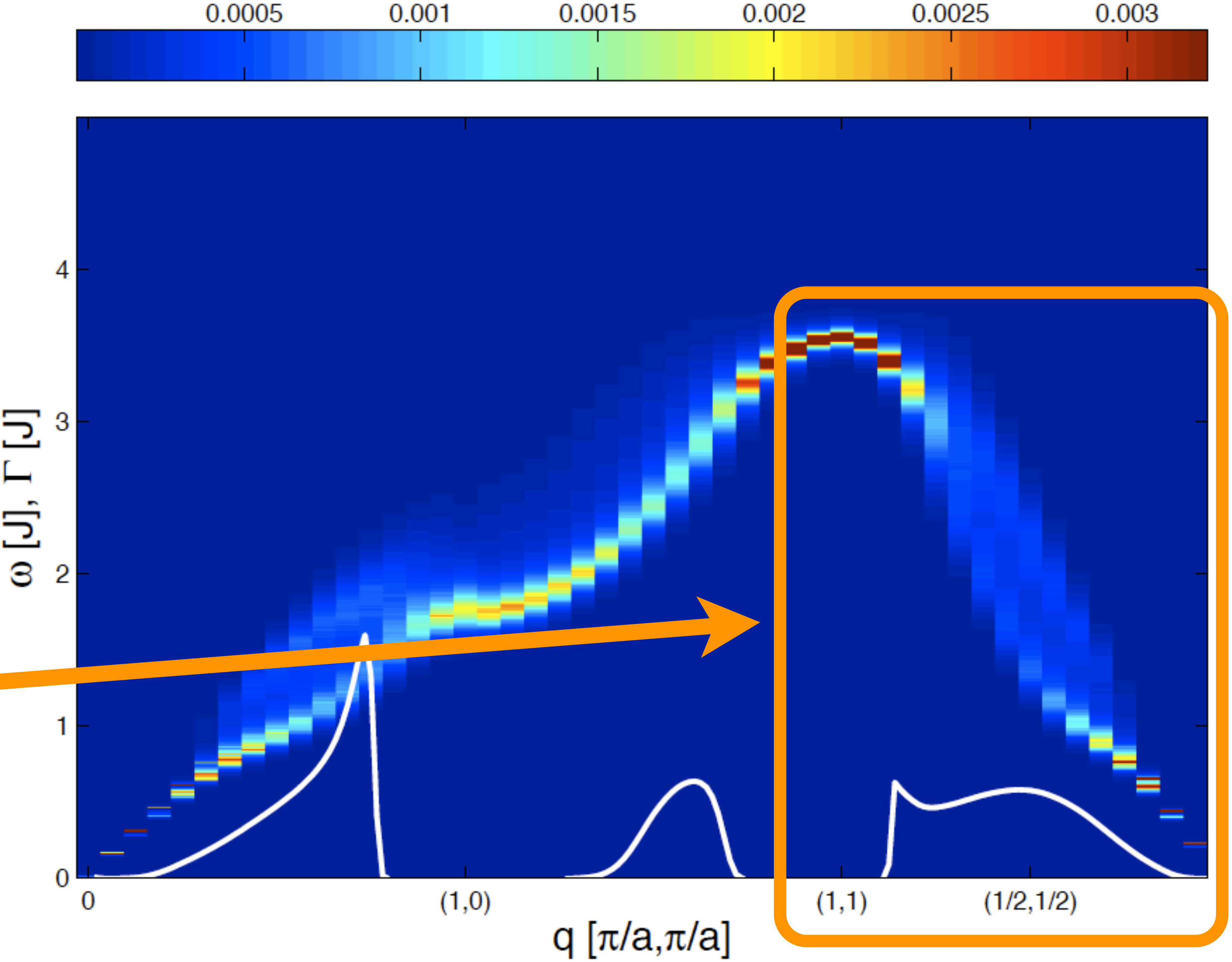
O. Syljuåsen, PRB '08

Square Lattice AFM
QMC + Analytical Continuation results

L=32
H/J=3.5



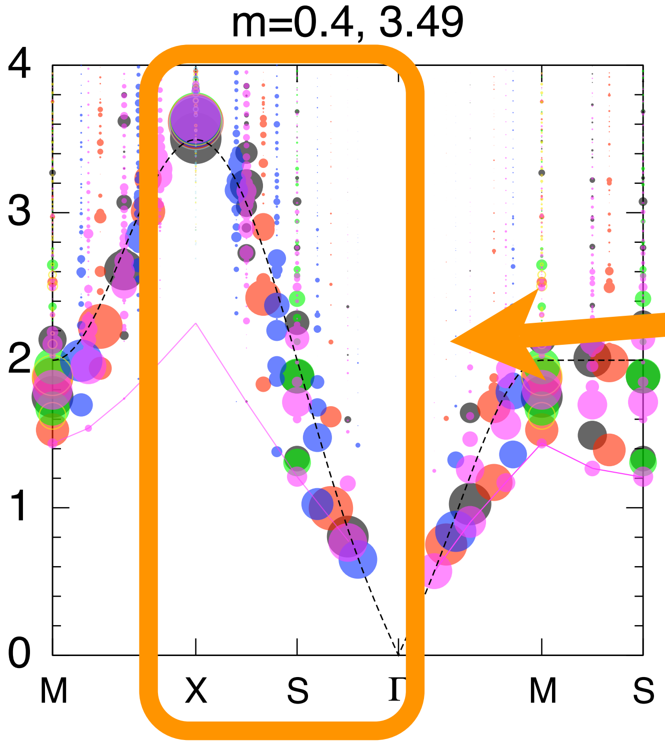
Our ED results



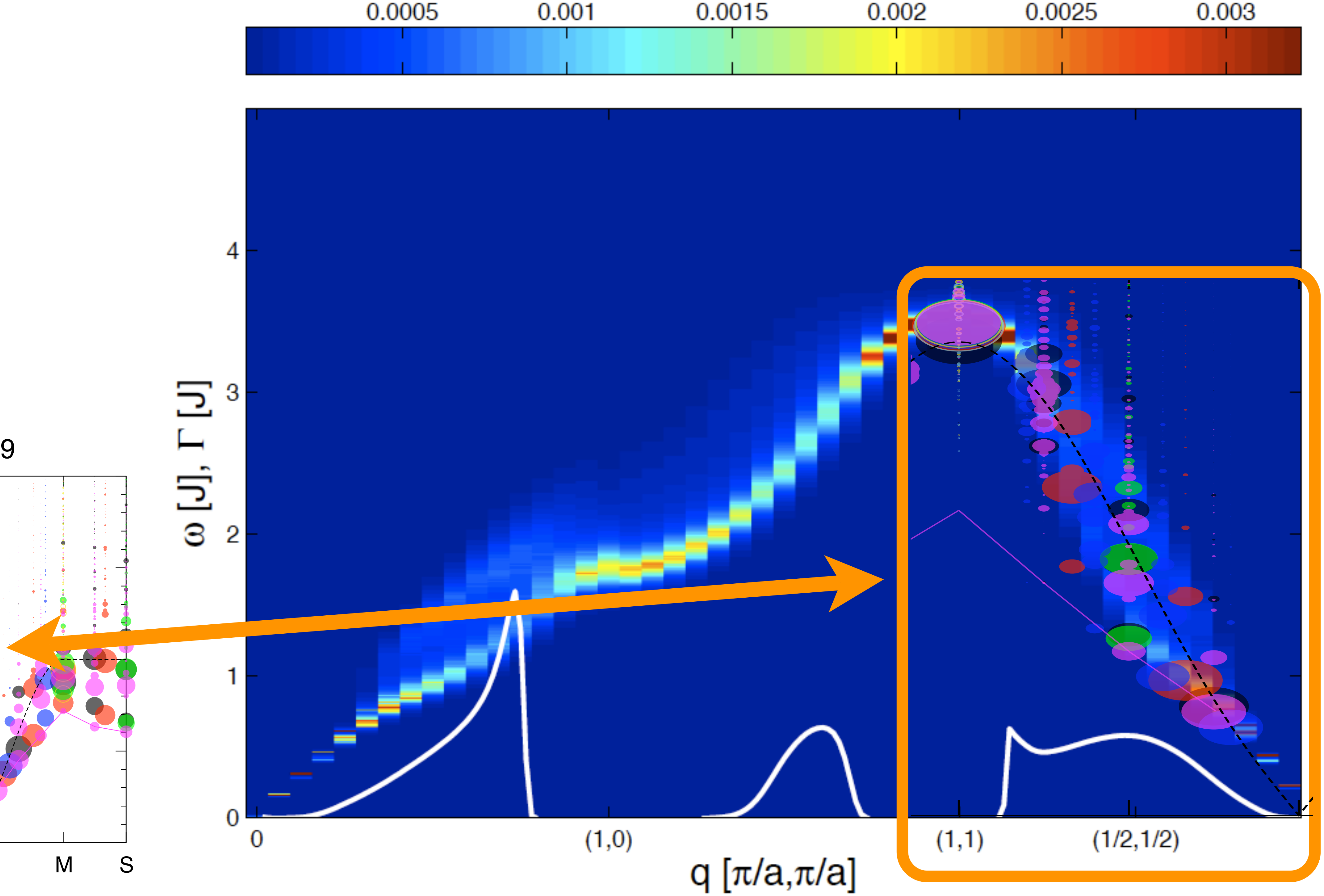
O. Syljuåsen, PRB '08

Square Lattice AFM
QMC + Analytical Continuation results

L=32
H/J=3.5



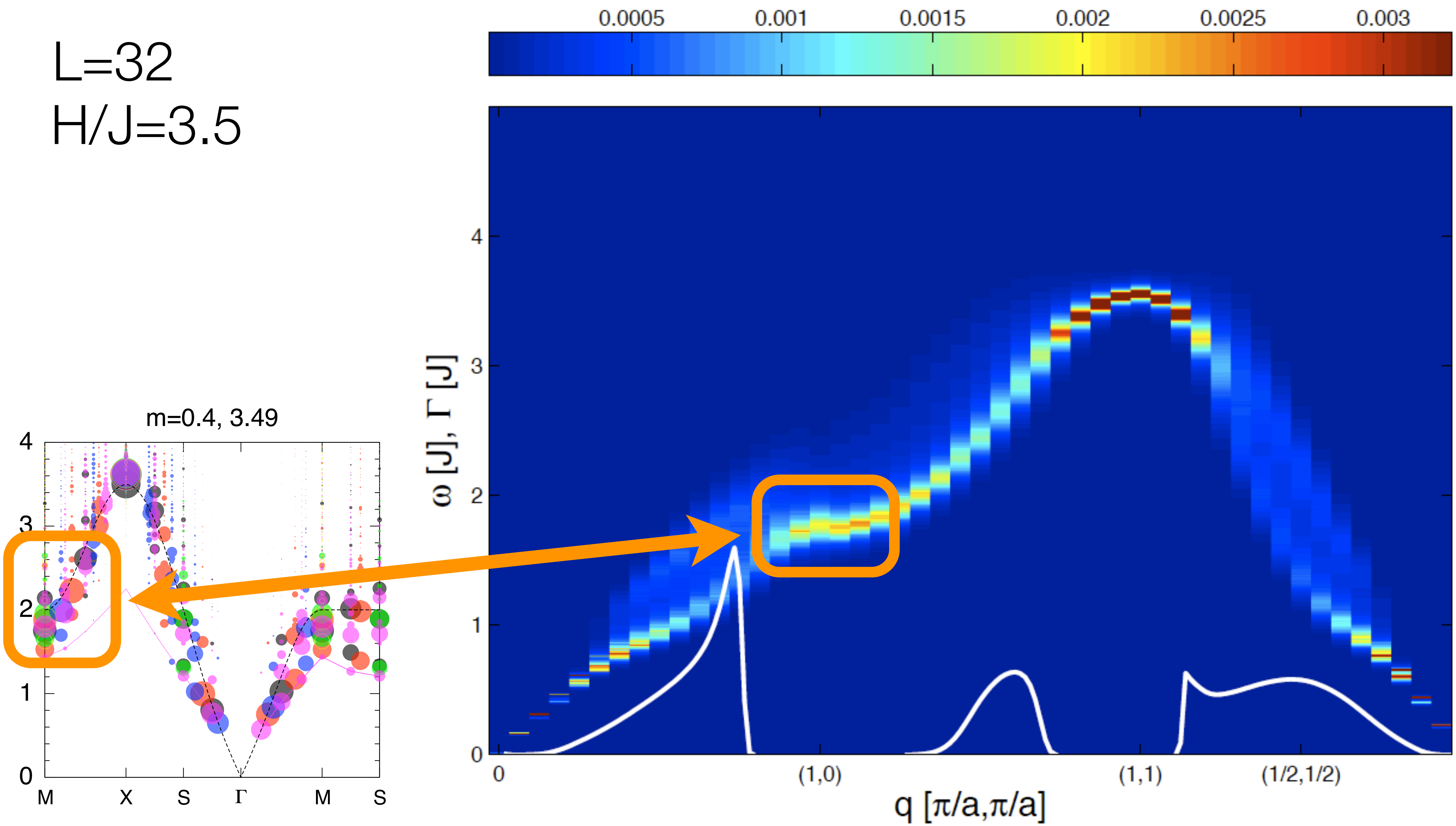
Our ED results



O. Syljuåsen, PRB ‘08

Square Lattice AFM
QMC + Analytical Continuation results

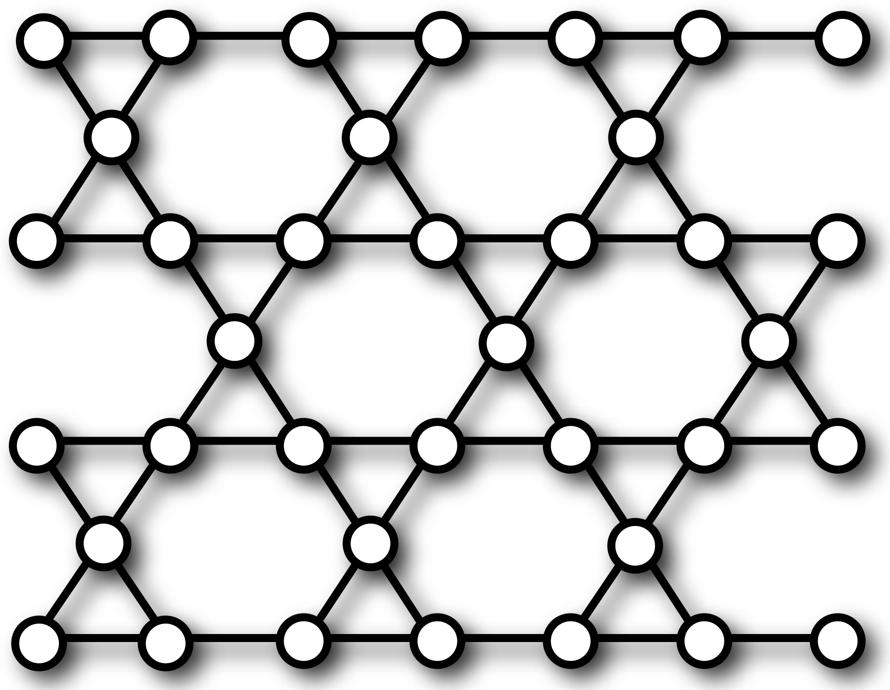
L=32
H/J=3.5



Our ED results

O. Syljuåsen, PRB '08

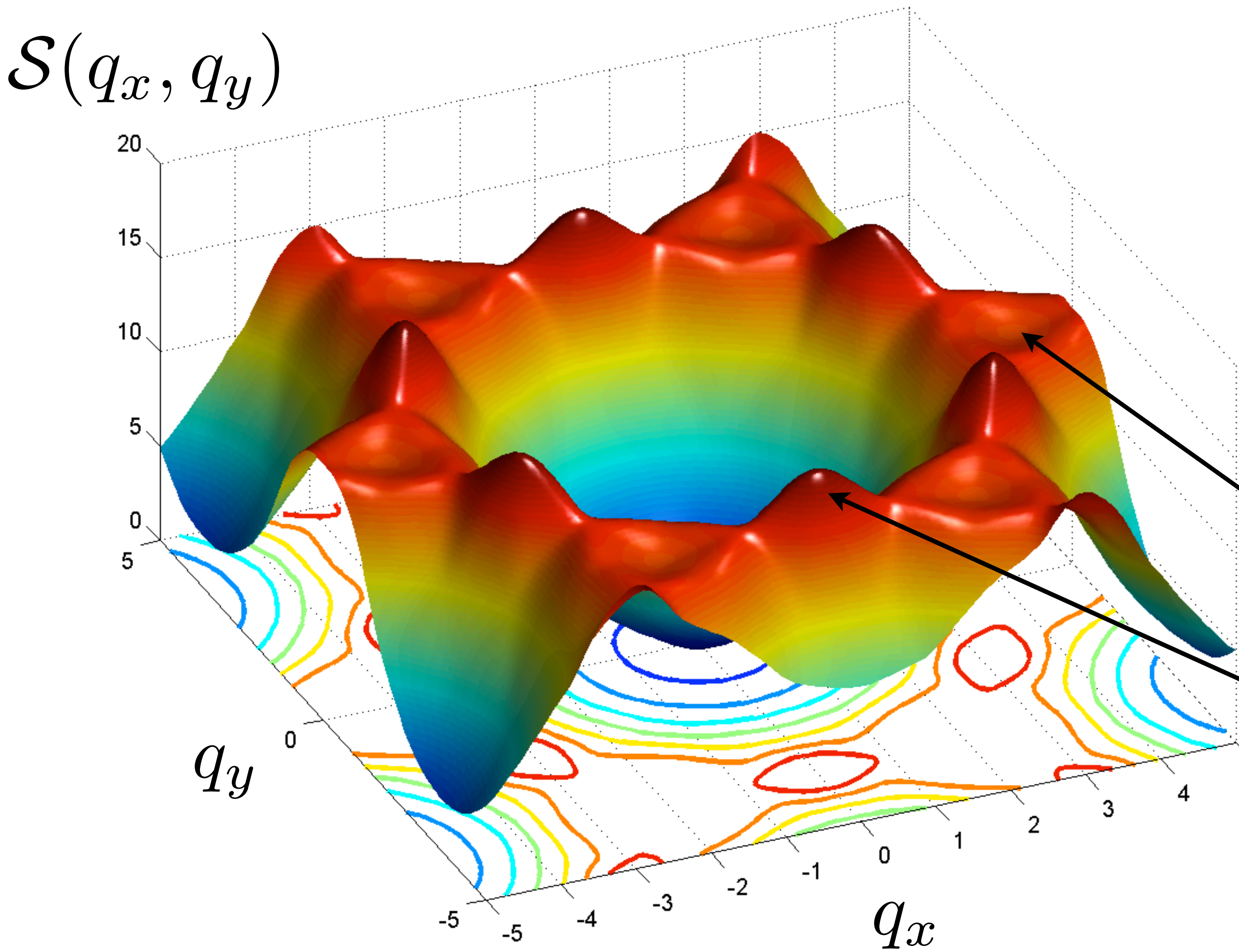
Kagome Antiferromagnet



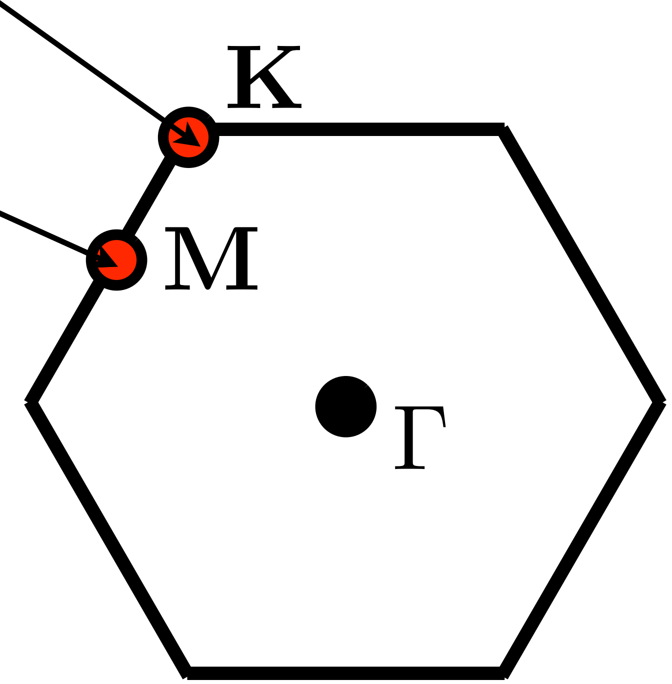
$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

AML & C. Lhuillier, arXiv:0901.1065

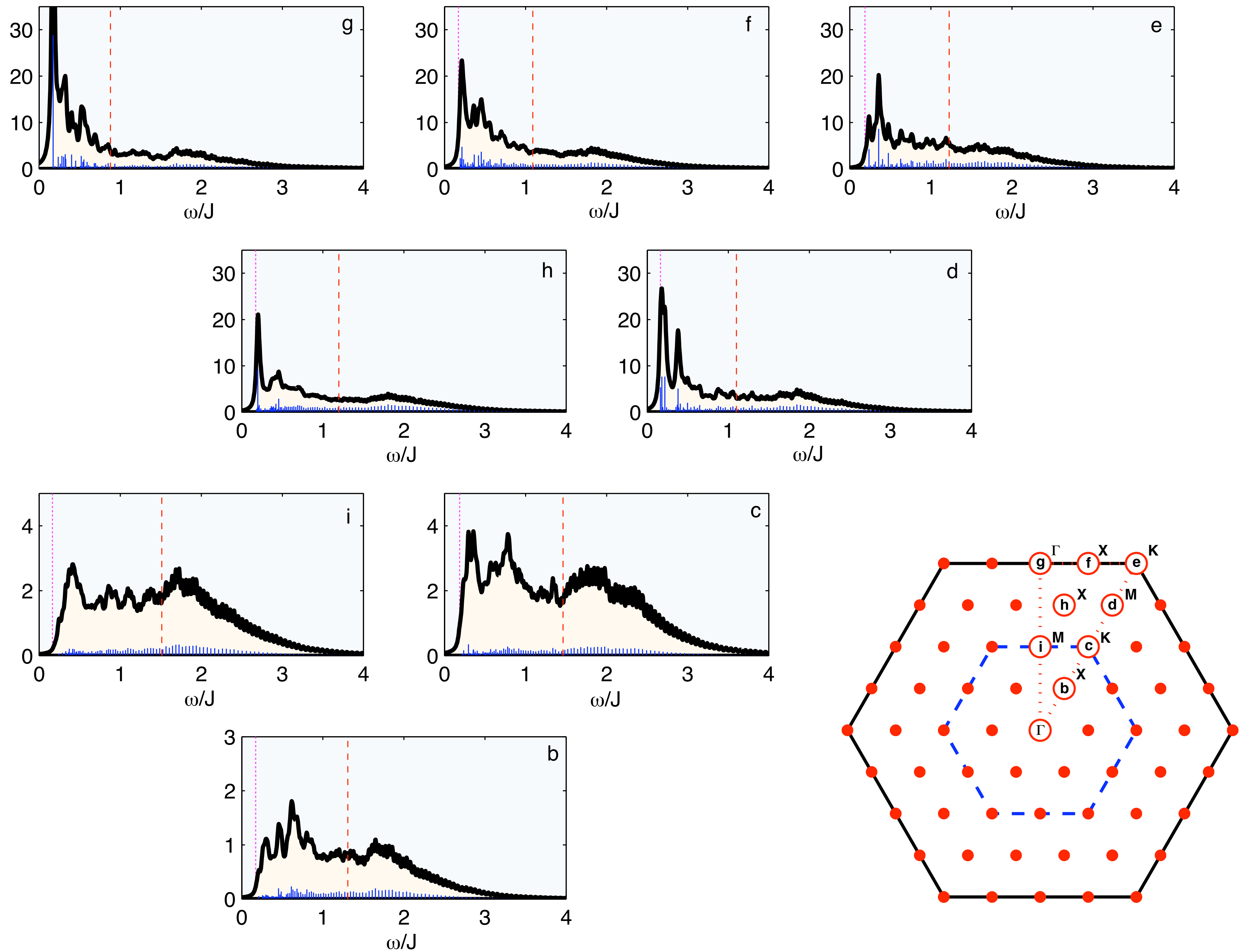
Kagome AFM
Static Structure Factor



- Ring of enhanced scattering at the extended BZ boundary
- No magnetic order!



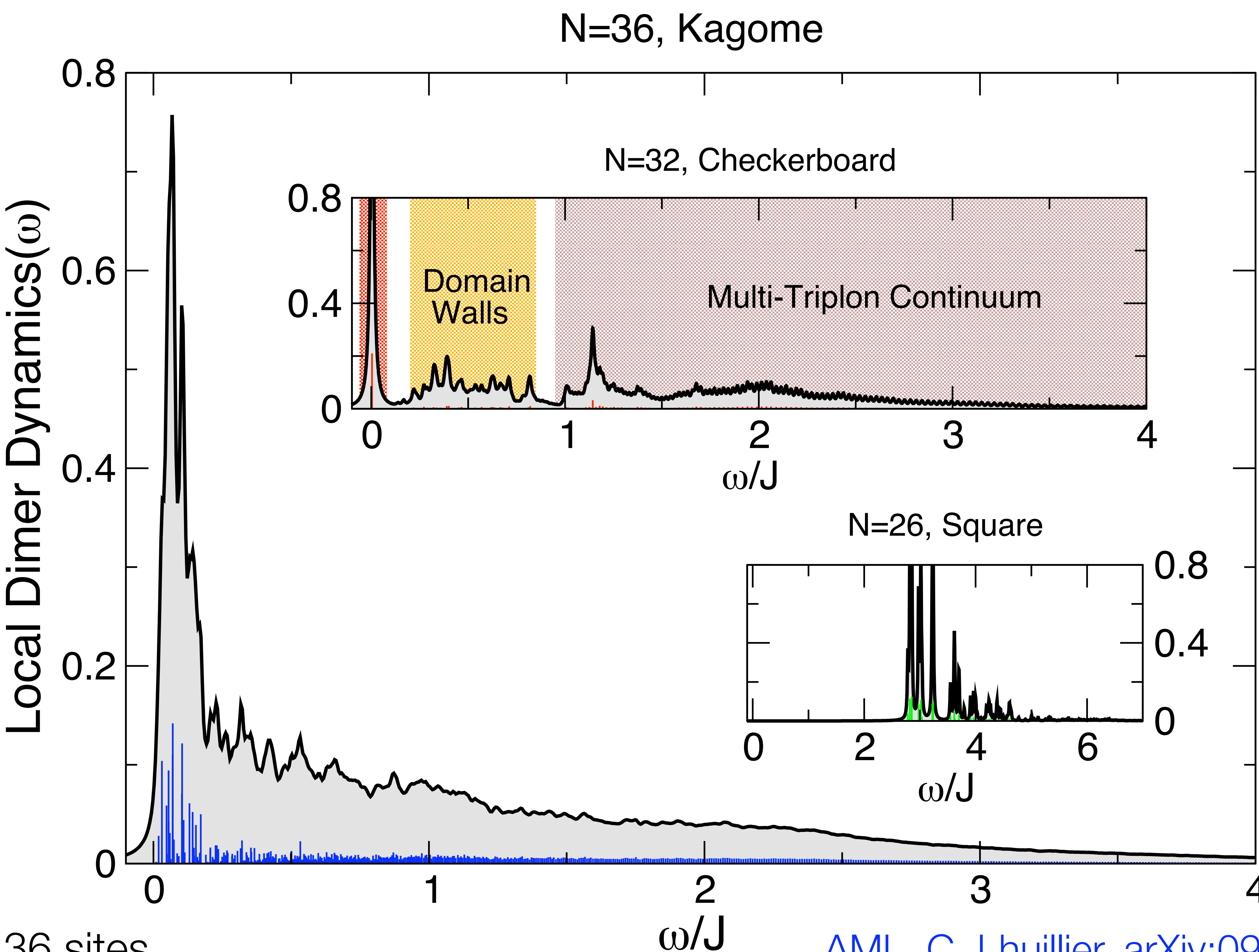
Kagome AFM
Dynamical Spin Structure Factor (~ INS)



ED, 36 sites

AML, C. Lhuillier, arXiv:0901.1065

Kagome AFM
Local Dimer Autocorrelations (~ Raman)



ED, 36 sites

AML, C. Lhuillier, arXiv:0901.1065

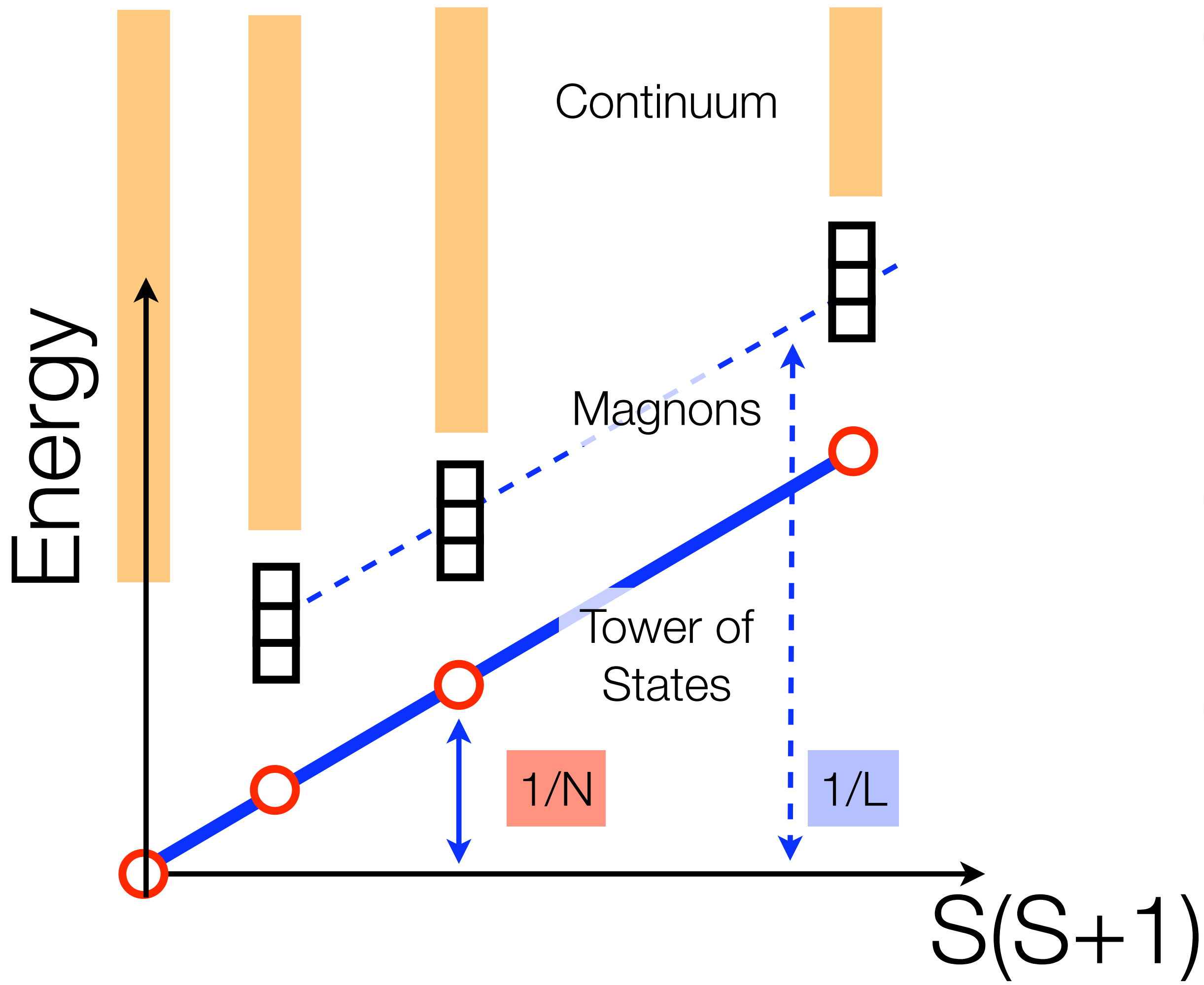
Outline

- Dynamical Spin Correlations
  - Square Lattice AFM in a field
  - Kagome AFM
- “Tower of States” spectroscopy (continuous symmetry breaking)
  - Conventional magnetic vs spin nematic order
- Correlation Density Matrices
  - Concept
  - Applications to spin chains and the Kagome AFM

“Tower of States” spectroscopy

- What are the finite size manifestations of a continuous symmetry breaking ?

- Low-energy dynamics of the order parameter
  Theory: P.W. Anderson 1952, Numerical tool: Bernu, Lhuillier and others, 1992 -



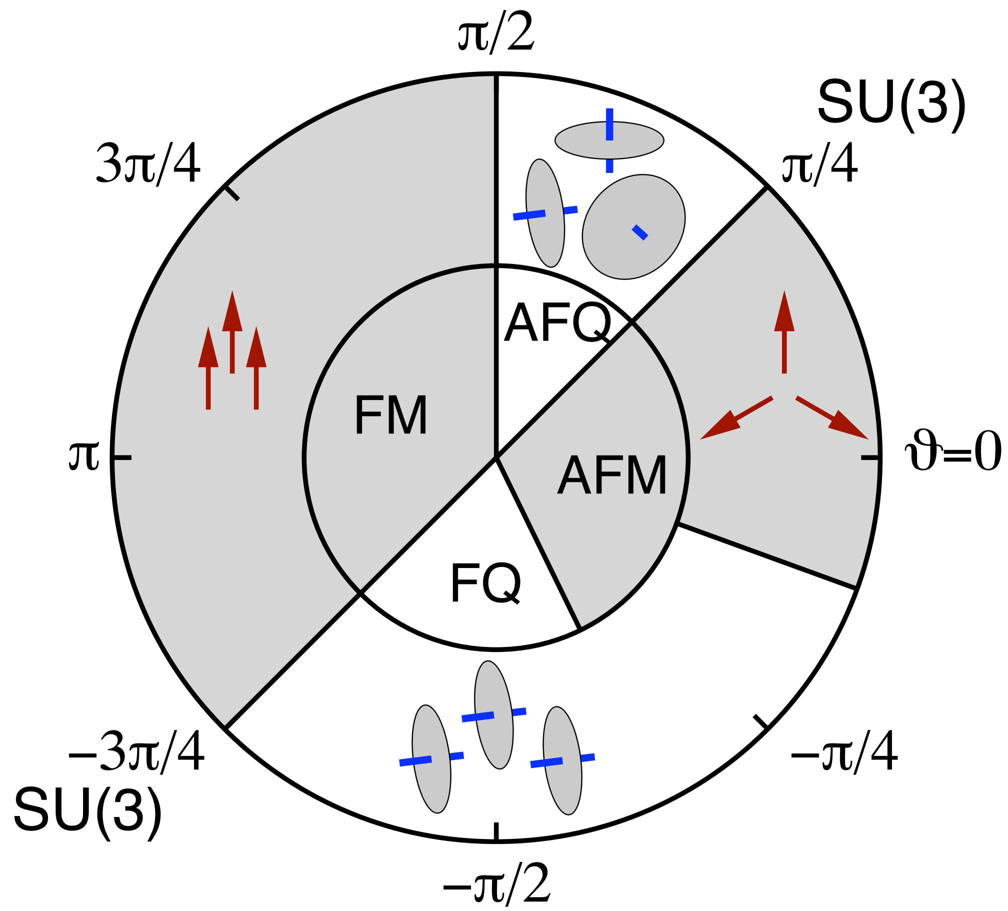
- Dynamics of the free order parameter is visible in the finite size spectrum. Depends on the continuous symmetry group.

- U(1): $(S^z)^2$ SU(2): $S(S+1)$

- Symmetry properties of levels in the Tower states are crucial and constrain the nature of the broken symmetries.

Tower of States
S=1 on triangular lattice

- Bilinear-biquadratic S=1 model on the triangular lattice (model for $NiGaS_4$).

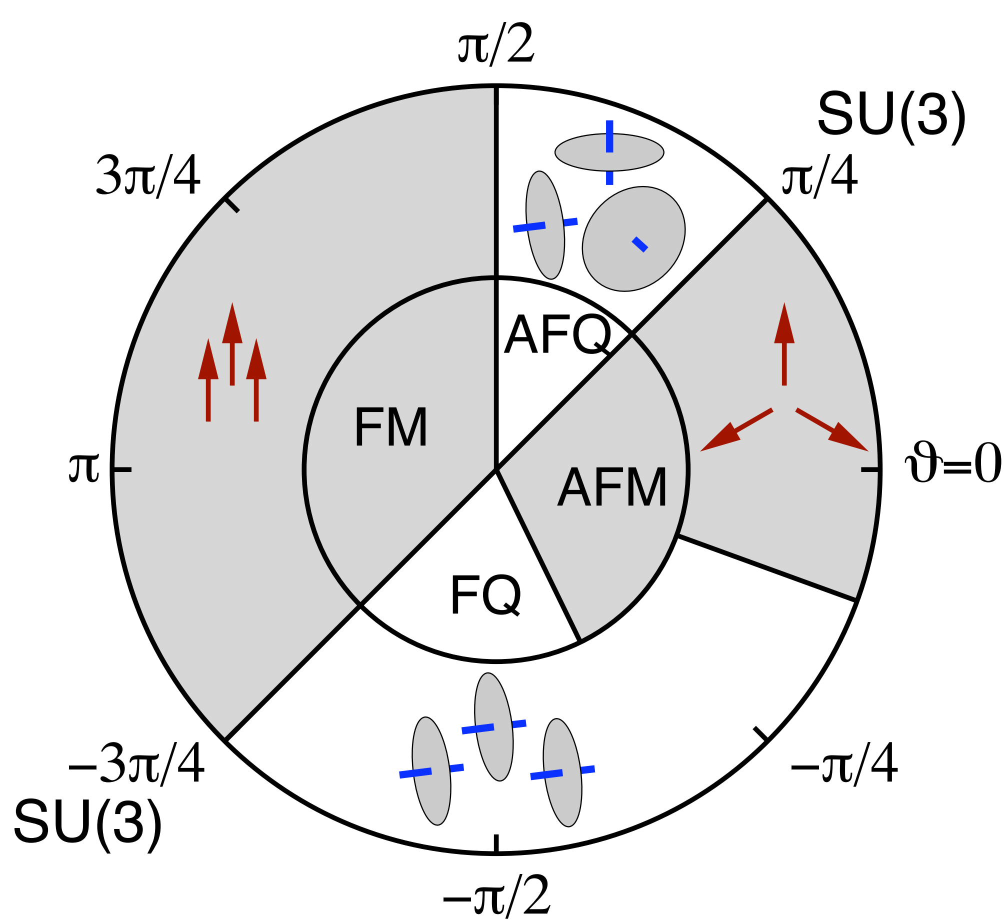


AML, F. Mila, K. Penc, PRL ‘06

Tower of States
S=1 on triangular lattice

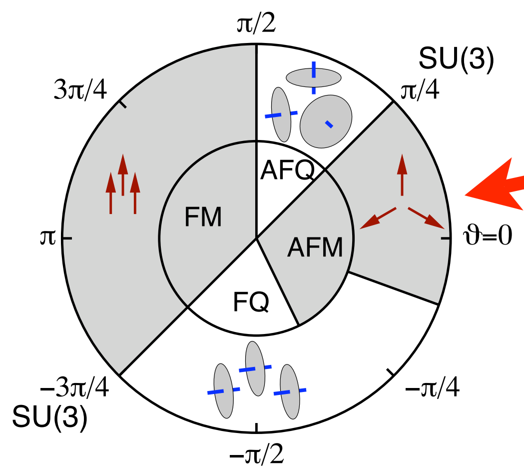
- Bilinear-biquadratic S=1 model on the triangular lattice (model for $NiGaS_4$).

$$H = \sum_{\langle i,j \rangle} \cos(\theta)\ \mathbf{S}_i \cdot \mathbf{S}_j + \sin(\theta)\ \ (\mathbf{S}_i \cdot \mathbf{S}_j)^2$$

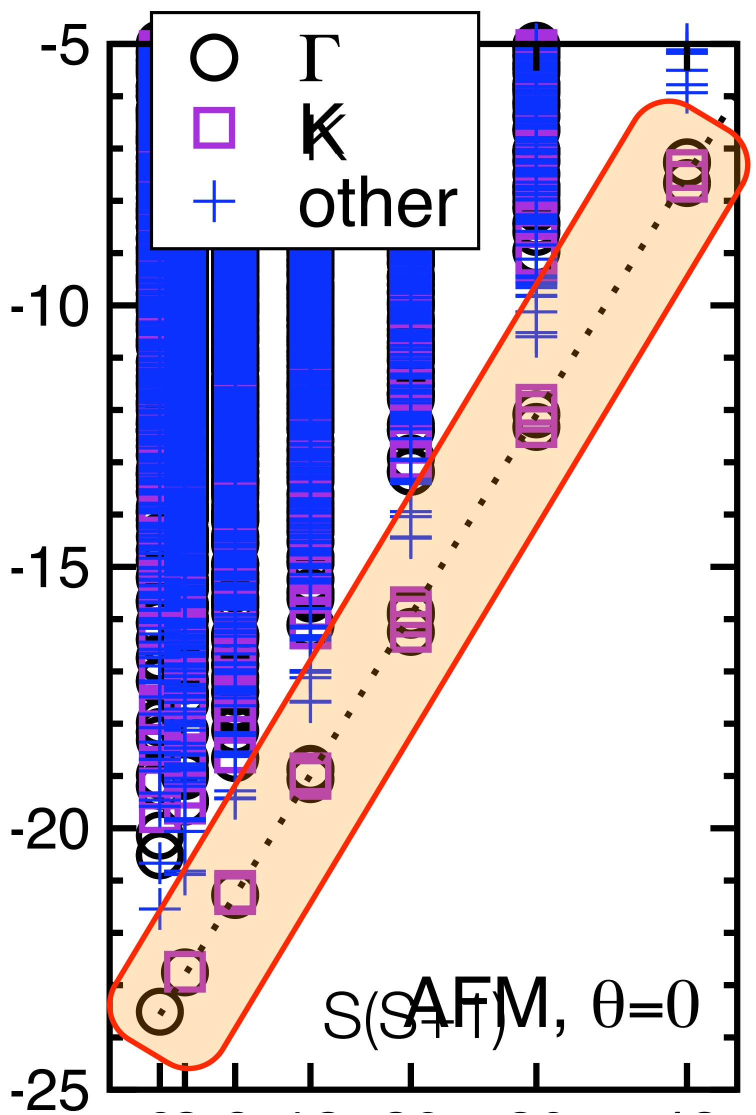


AML, F. Mila, K. Penc, PRL '06

Tower of States
S=1 on triangular lattice: Antiferromagnetic phase



- ϑ=0 : coplanar magnetic order,
  120 degree structure

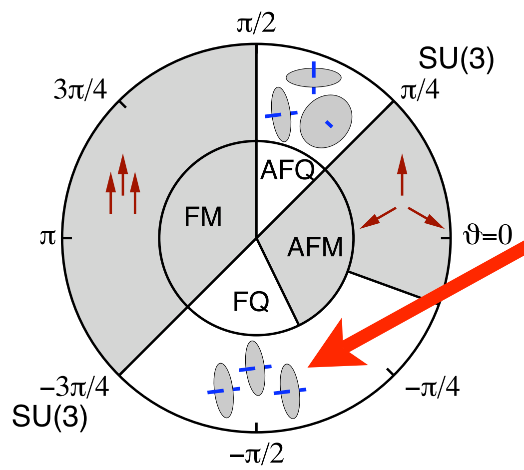


- Breaks translation symmetry. Tree site unit cell
  ⇒ nontrivial momenta must appear in TOS
- non-collinear magnetic structure
  ⇒ SU(2) is completely broken,

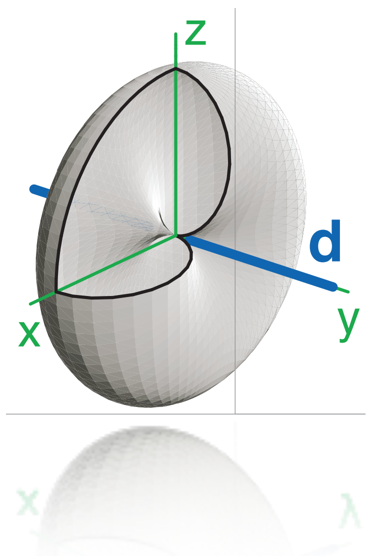
  number of levels in TOS increases with S
- Quantum number are identical to the S=1/2 case

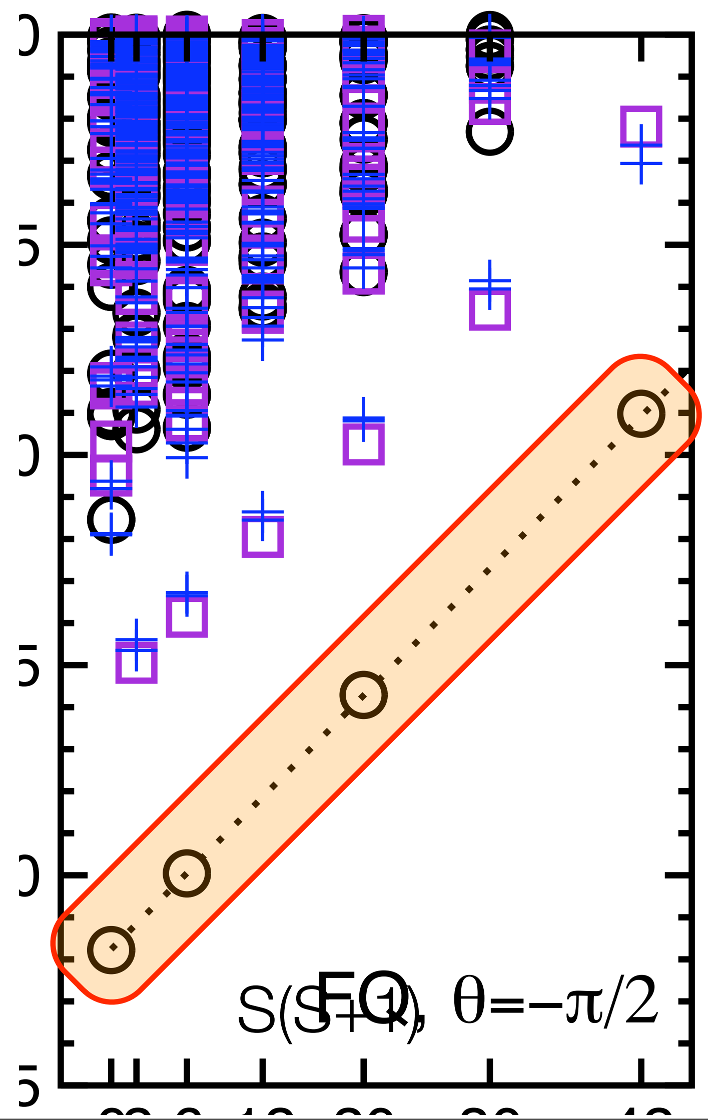
Tower of States

S=1 on triangular lattice: Ferroquadrupolar phase



- ϑ=-π/2 : ferroquadrupolar phase, finite quadrupolar moment, no spin order

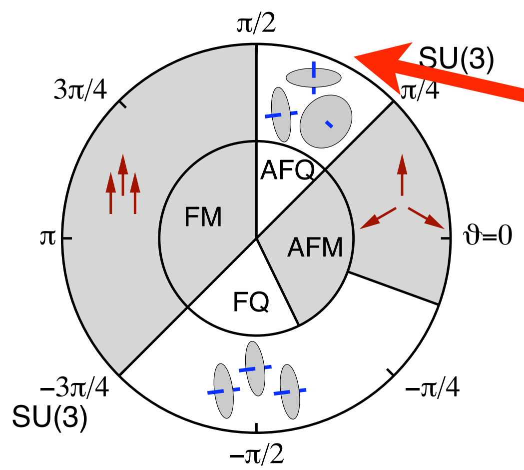




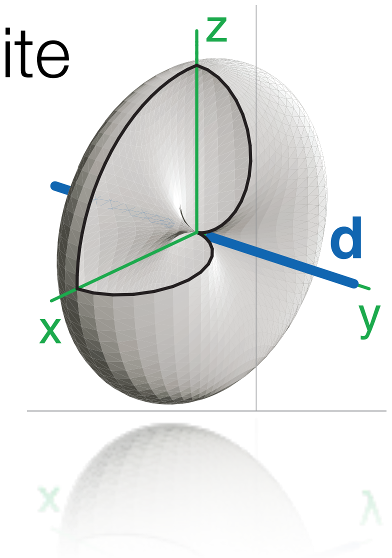
- No translation symmetry breaking.
  ⇒ only trivial momentum appears in TOS
- Ferroquadrupolar order parameter, only even S
- all directors are collinear
  ⇒ SU(2) is broken down to U(1),

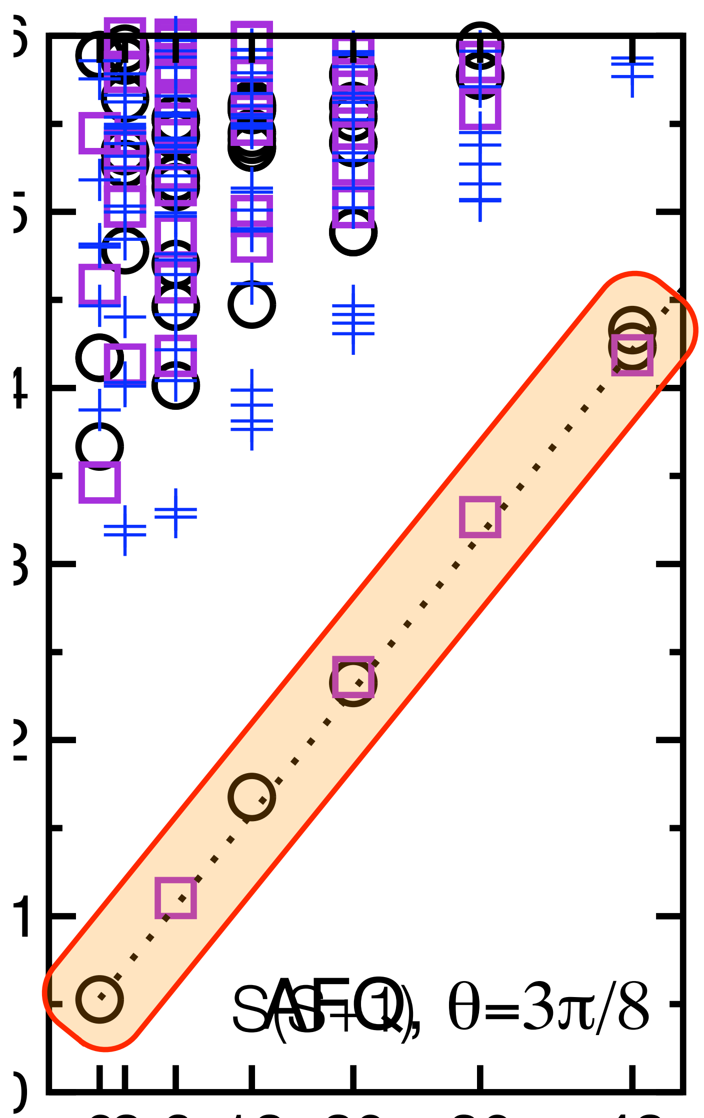
  number of states in TOS is independent of S.

Tower of States
S=1 on triangular lattice: Antiferroquadrupolar phase



- ϑ=3π/8 : antiferroquadrupolar phase, finite quadrupolar moment, no spin order, three sublattice structure.



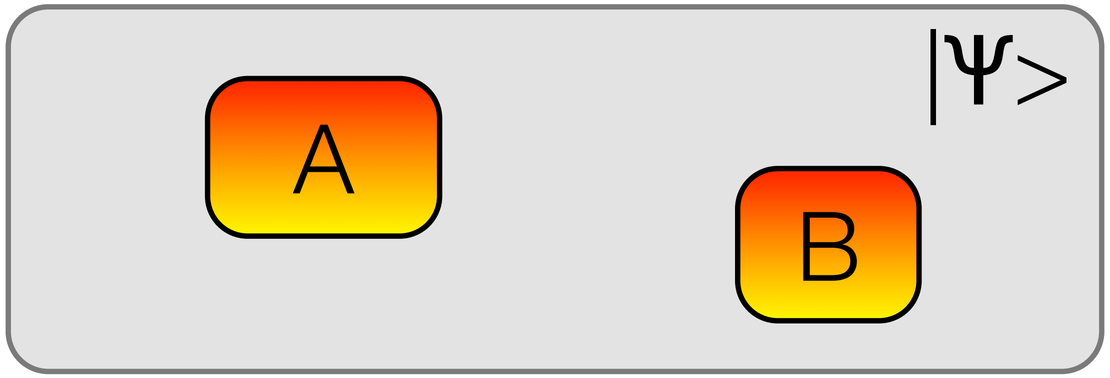


- Breaks translation symmetry. Tree site unit cell ⇒ nontrivial momenta must appear in TOS
- Antiferroquadrupolar order parameter, complicated S dependence. Can be calculated using group theoretical methods.

Outline

- Dynamical Spin Correlations
  - Square Lattice AFM in a field
  - Kagome AFM
- “Tower of States” spectroscopy (continuous symmetry breaking)
  - Conventional magnetic vs spin nematic order
- Correlation Density Matrices
  - Concept
  - Applications to spin chains and the Kagome AFM

The correlation density matrix (CDM)



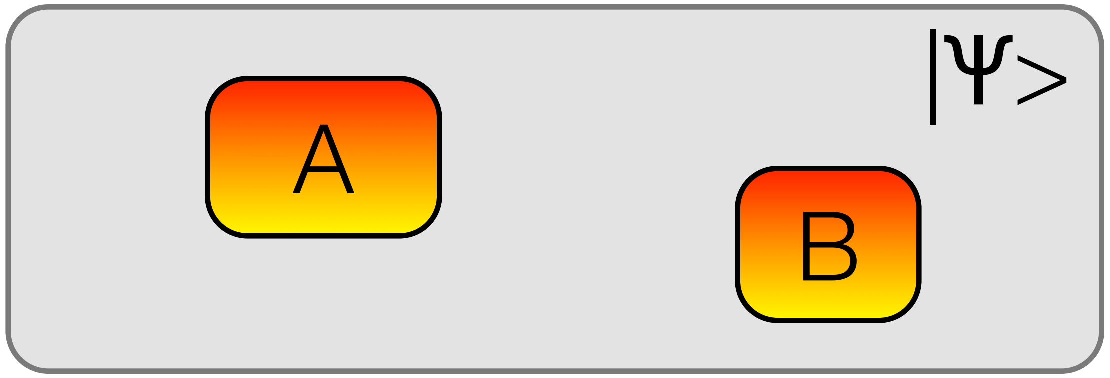
- Is there a systematic way to detect important correlations between parts A and B of a larger system ?
- The correlation density matrix:

$$\rho^c_{AB} = \rho_{AB} - \rho_A \otimes \rho_B$$

contains all the required information

The correlation density matrix (CDM)

$$\rho^c_{AB} = \rho_{AB} - \rho_A \otimes \rho_B$$



- Contains all information on any connect correlation function between A and B:

$$\mathrm{Tr}(\rho^c_{AB}\widehat{O}_A\widehat{O}_B) = \langle\widehat{O}_A\widehat{O}_B\rangle - \langle\widehat{O}_A\rangle\langle\widehat{O}_B\rangle$$

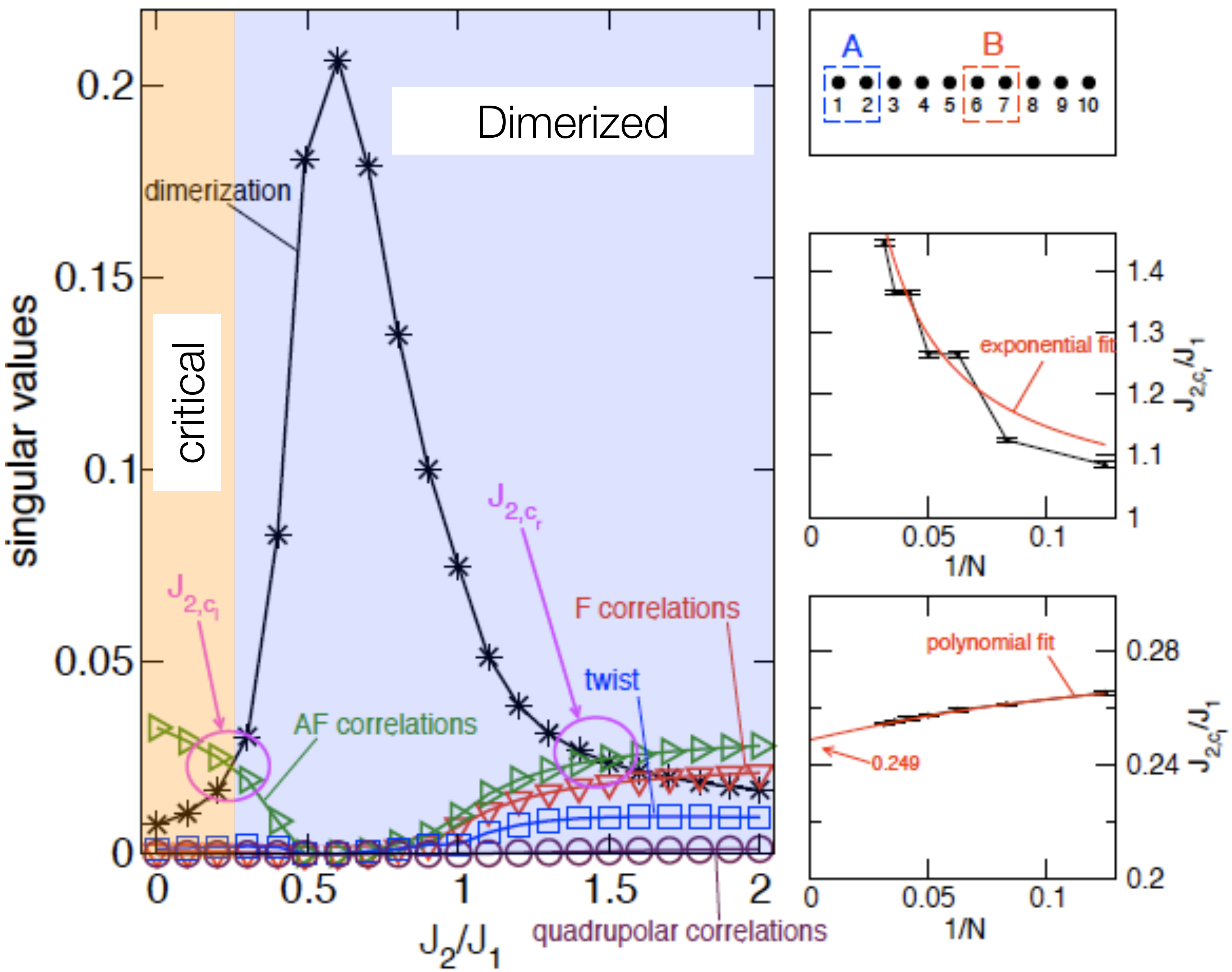
- The key step is to perform a singular value decomposition

$$\rho^c_{AB} = \sum_{i=1} \sigma_i X'_i Y'^{\dagger}_i$$

where the σ_i give the strength of the correlation i and the X_i and Y_i are the operators of the correlator acting in A and B.

S.-A. Cheong, C. Henley, arXiv:0809.0075

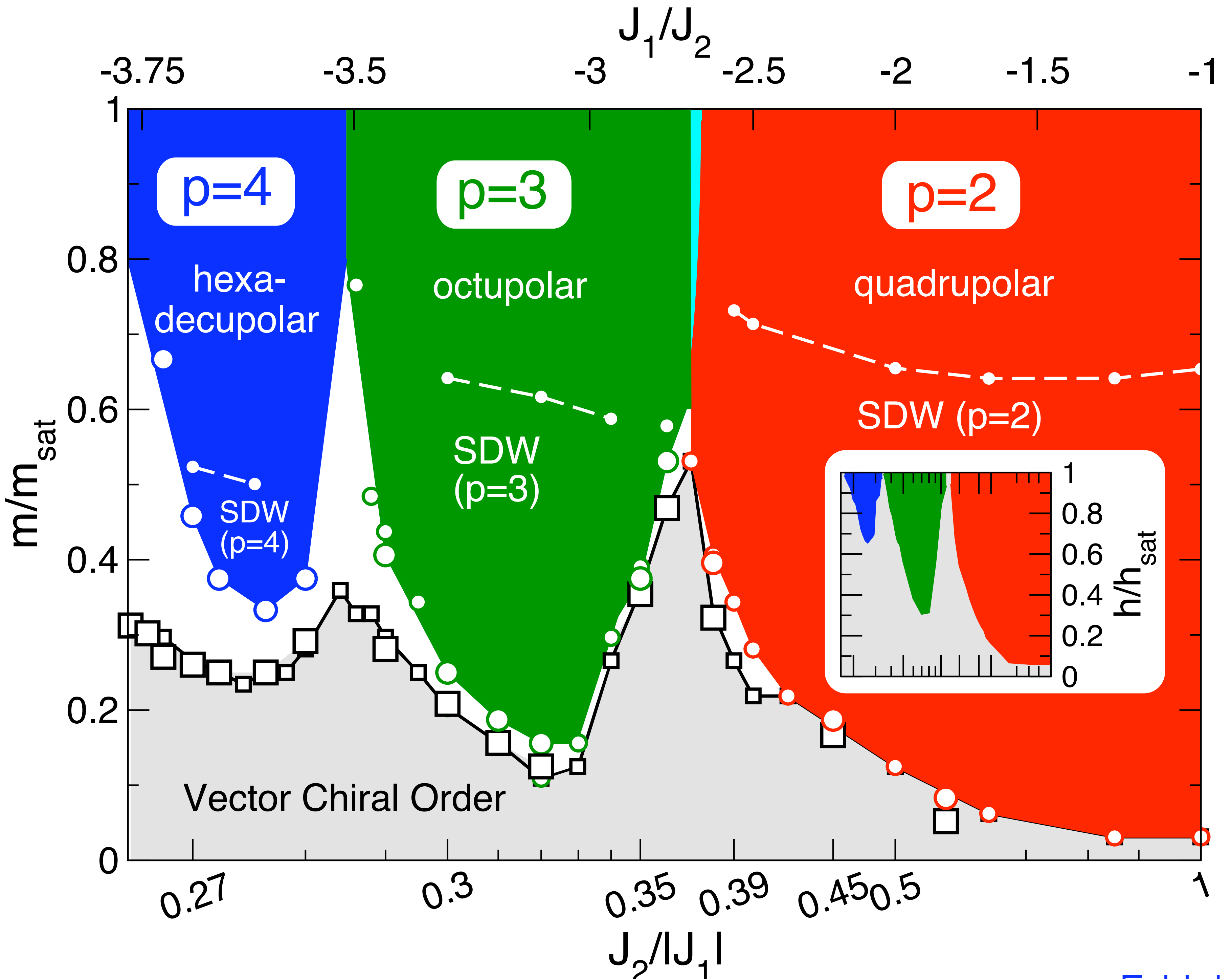
CDM
J_1-J_2 frustrated Heisenberg Chain (all AF)



- Benchmark on existing phase diagrams.
- singular values respect SU(2) symmetry in S=0 GS (multiplicities).
- works very well for the well understood Majumdar-Ghosh chain.

Sudan & AML, unpublished

CDM
J_1-J_2 frustrated Heisenberg Chain (F-AF)



- vector chiral phase at low m
- spin multipolar liquids at high m
- CDM helped us understand that spin multipolar phases are generically imprinted in close-by magnetically ordered states

J. Sudan, A. Lüscher, AML, arXiv:0807.1923 ED/DMRG

F. Heidrich-Meisner et al. PRB ‘06
T. Hikihara et al., PRB ‘08

Conclusions

- Exact Diagonalization has an obvious disadvantage (finite size limitation), but when combined with physical concepts and ideas the method becomes a powerful Quantum Mechanics Toolbox, and can access systems which are difficult or impossible to solve otherwise.
- Dynamical correlation functions gave evidence for decay of spin waves in the square lattice antiferromagnet in a field, while the dynamical spin response of the kagome lattice is very incoherent, with possibly some VBC-triplon remnants at low energy.
- Tower of states spectroscopy is powerful tool to study continuous symmetry breaking.
- Correlation Density Matrices are a novel tool to study correlations (or the absence thereof) in unified framework. First applications to frustrated spin chains revealed new mechanisms for the appearance of spin nematic phases.

Collaborators

- Dynamical Correlation Functions:
  - A. Lüscher (Lausanne), C. Lhuillier (Paris)
- Tower of states spectroscopy
  - K. Penc (Budapest), F. Mila (Lausanne)
- Correlation density matrices
  - J. Sudan, A. Lüscher (Lausanne), C. Henley (Cornell)

Thank you !