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

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

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  Quantum Mechanics Toolbox
Exact Diagonalization: Applications
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low-lying eigenvalues, not full diagonalization
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  - different filling fractions $\nu$, up to 16-20 electrons
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- 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
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- 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
**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} \text{Im} \langle GS| S(Q)^\dagger \frac{1}{\omega - H + E_{GS} + i\eta} S(Q)|GS\rangle
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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
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AML, Capponi, Assaad, JSTAT 08
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Square Lattice Heisenberg Antiferromagnet

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

weak (zero) field  finite field

A. Lüscher, AML, arXiv:0812.3420
Excitation Spectrum of a Square Lattice
S=1/2 Antiferromagnet in a Field
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\(S=1/2\) Antiferromagnet in a Field

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Numerical simulation can help to settle this issue
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 \((\pi, \pi)\).
Predicted INS Spectra as a function of field
Field dependence:
Finite size pole structure

Longitudinal dynamical structure factors $S^{zz}(\omega, k)$
Field dependence:
Finite size pole structure

Longitudinal dynamical structure factors

\[ S^{zz}(\omega, k) \]
Field dependence: Finite size pole structure

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

Sites
- $32$
- $36$
- $40$
- $50$
- $52$
- $58$
- $64$

$S^{zz}$
- $1.5$
- $1$
- $0.5$
- $0.1$
- $0.01$
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

O. Syljuåsen, PRB '08

FIG. 10: Synthetic superposition of the longitudinal dynamical structure factors along a path of highly symmetric points in the Brillouin zone. Different colors represent data from different clusters and the area of the symbols is proportional to $S_{zz}(\omega, q)$. Dashed lines show the dispersions obtained within linear spin-wave theory [Eq. (B5)] and the solid line represents spin-wave results with first order corrections.

For magnetizations around $m \approx 0.15$, quantum fluctuations are almost negligible and the spin-wave dispersion is in good agreement with numerical results. At higher fields, $m \gtrsim 0.3$, fluctuations are again important and lead to the spontaneous decay of magnons. This instability is reflected in a reduction of weight in main peak accompanied by the appearance of small poles at lower energies. This process starts around $q = X$ and spreads over almost the whole Brillouin zone.

Our ED results

O. Syljuåsen, PRB '08
Square Lattice AFM
QMC + Analytical Continuation results

L = 32
H/J = 3.5

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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

$S(q_x, q_y)$

- Ring of enhanced scattering at the extended BZ boundary
- No magnetic order!
Kagome AFM
Dynamical Spin Structure Factor (~ INS)

Each panel displays the broadened 1\( S(\omega) \) and its label referring to specific points in the extended BZ: energy cut at the wave vector indicated by the panel position in the left part of Fig. Feature appropriate regimes reveal spinon continua with a rich structure. In extensively ordered systems we expect to see dispersive long-lived spin waves. Experiments and therefore a quantity of central interest: In magnetic directly relevant for inelastic neutron scattering (INS) experiments and therefore a quantity of central interest: In magnetic directly relevant for inelastic neutron scattering (INS) experiments.

The energy and moment dependence of the dynamical structure factor: model on the kagome lattice is shown, as an intensity plot (2 and along the path labeled wavevectors of the first frequency moment.) while one dimensional systems in approximated model on the kagome lattice is shown, as an intensity plot (2 and along the path labeled wavevectors. The characteristic width in energy of the spectral weight is carried by the reverse and forward scattering channel. The static structure factor (6 the dynamical spin response function concentrates essentially in the extended BZ (points g, f, e, h, d of Fig.): The main specificity of this system is the stretching of the magnetic response in the sector associated to the Bragg peak \( Q \sim 90\% \). This is quite different from the spectrum of a \( N \) site spinel ordered system on the same system size \( e \). The reverse and forward scattering channel begins immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately beginning immediately begin. 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Kagome AFM
Local Dimer Autocorrelations (~ Raman)

N=36, Kagome

N=32, Checkerboard

N=26, Square

ED, 36 sites

AML, C. Lhuillier, arXiv:0901.1065
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"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 NiGaS₄).

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

- $\theta=0$: 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

\[ \theta = -\pi/2 : \text{ferroquadrupolar phase, finite quadrupolar moment, no spin order} \]

- No translation symmetry breaking.
  \[ \Rightarrow \text{only trivial momentum appears in TOS} \]

- Ferroquadrupolar order parameter, only even S

- all directors are collinear
  \[ \Rightarrow \text{SU(2) is broken down to U(1),} \]
  number of states in TOS is independent of S.
Tower of States

S=1 on triangular lattice: Antiferroquadrupolar phase

- $\theta = 3\pi/8$ : antiferroquadrupolar phase, finite quadrupolar moment, no spin order, three sublattice structure.

- Breaks translation symmetry. Tree site unit cell $\Rightarrow$ nontrivial momenta must appear in TOS

- Antiferroquadrupolar order parameter, complicated $S$ dependence. Can be calculated using group theoretical methods.
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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)

\[
\rho_{AB}^c = \rho_{AB} - \rho_A \otimes \rho_B
\]

- Contains all information on any connect correlation function between A and B:
  \[
  \text{Tr}(\rho_{AB}^c \hat{O}_A \hat{O}_B) = \langle \hat{O}_A \hat{O}_B \rangle - \langle \hat{O}_A \rangle \langle \hat{O}_B \rangle
  \]
- The key step is to perform a singular value decomposition
  \[
  \rho_{AB}^c = \sum_{i=1} \sigma_i X_i^{\prime} Y_i^{\prime \dagger}
  \]

where the \( \sigma_i \) 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.

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

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 !