\[ \mathcal{H} |\psi\rangle = E |\psi\rangle \]

**Studying Continuous Symmetry Breaking with Exact Diagonalization**

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Quantum Materials, Experiment & Theory  
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Outline of the lecture

- Short Overview on Exact Diagonalization
- Introduction to Continuous Symmetry Breaking, Lieb-Mattis Model
- General Formalism
- Many Examples …
- Outlook: other symmetry groups than SO(3), quantum critical points, …
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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!

- Some people will tell you that’s all there is.

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

Quantum Mechanics Toolbox
Hilbert space sizes

- The Hilbert space of a quantum many body system grows exponentially in general.

- For N spin 1/2 particles, the complete Hilbert space has dim=$2^N$ states.
  - 10 spins dim=1,024
  - 20 spins dim=1,048,576
  - 30 spins dim=1,073,741,824
  - 40 spins dim=1,099,511,627,776
  - 50 spins dim=1,125,899,906,842,624 ...

- The quantum mechanical wave function is a vector in this Hilbert (vector) space and we would like to know the ground state and a few other low lying eigenstates.

\[ |↑\rangle \text{ or } |↓\rangle \]
Symmetries

Consider a XXZ spin model on a lattice. What are the symmetries of the problem?

$$H = \sum_{i,j} J_{i,j}^{x,y} (S_i^x S_j^x + S_i^y S_j^y) + J_{i,j}^z S_i^z S_j^z$$

- The Hamiltonian conserves total $S^z$, we can therefore work within a given $S^z$ sector. This easily implemented while constructing the basis, as we discussed before.

- The Hamiltonian is invariant under the space group, typically a few hundred elements. (in many cases = Translations x Pointgroup). Needs some technology to implement...

- At the Heisenberg point, the total spin is also conserved. It is however very difficult to combine the SU(2) symmetry with the lattice symmetries in a computationally useful way (non-sparse and computationally expensive matrices).

- At $S^z=0$ one can use the spin-flip (particle-hole) symmetry which distinguishes even and odd spin sectors at the Heisenberg point. Simple to implement.
Spatial Symmetries

- Spatial symmetries are important for reduction of Hilbert space
- Symmetry resolved eigenstates teach us a lot about the physics at work, dispersion of excitations, symmetry breaking tendencies, topological degeneracy, ... ⇒ more about this in the second lecture

40 sites square lattice
$T \otimes PG = 40 \times 4$ elements

Icosidodecahedron (30 vertices)
$I_h: 120$ elements
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, cluster spectra, etc

- **Fractional Quantum Hall states**: energy gaps, overlap with model states, entanglement spectra

- **Quantum dimer models / constrained models (anyon chains, ...)**

- **Full Configuration Interaction in Quantum Chemistry, Nuclear structure**

- **Quantum Field Theory**
Exact Diagonalization: Present Day Limits

- Spin S=1/2 models:
  - 40 spins square lattice, 39 sites triangular, 42 sites Honeycomb lattice
  - 48 sites kagome lattice, soon 50-52 spins square lattice
  - 64 spins or more in elevated magnetization sectors
  - up to ~500 billion basis states

- Fractional quantum hall effect
  - different filling fractions \( \nu \), up to 16-20 electrons
  - up to 3.5 billion basis states

- Hubbard models (~ Full CI in Quantum Chemistry)
  - 20 sites square lattice at half filling, 21 sites triangular lattice
  - 24 sites honeycomb lattice
  - up to 160 billion basis states
Exact Diagonalization Literature

N. Laflorencie & D. Poilblanc,
“Simulations of pure and doped low-dimensional spin-1/2 gapped systems”

R.M. Noack & S. Manmana,
“Diagonalization- and Numerical Renormalization-Group-Based Methods for Interacting Quantum Systems”,

A. Weisse, H. Fehske
“Exact Diagonalization Techniques”

A. Läuchli
“Numerical Simulations of Frustrated Systems”
available upon e-mail request.
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What are the finite size manifestations of a continuous symmetry breaking? (e.g., in superfluids/superconductors, magnetic order, spin nematic order)

Order parameter is zero on a finite system! (symmetric partition function)

So usually one looks into order parameter correlations \[(\text{order parameter})^2\]
"Tower of States" spectroscopy

- Order parameter is not a conserved quantity
- Order parameter is zero on a finite size sample (Wigner-Eckart)
- How does one get spontaneous symmetry breaking anyway?
- Ground state degeneracy is building up as we approach the thermodynamic limit, which will allow to form a symmetry breaking wave packet at zero energy cost
“Tower of States” spectroscopy

- What are the finite size manifestations of a continuous symmetry breaking? (e.g., in superfluids/superconductors, magnetic order, spin nematic order)

- 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. ED is good at spectra.

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

- Symmetry properties of levels in the Tower states are crucial and constrain the nature of the broken symmetries.
Toy model: from square lattice Heisenberg antiferromagnet to the Lieb-Mattis model

- Hamiltonian
  \[ H = J \sum_{\langle i, j \rangle} S_i \cdot S_j \]

- Fourier transform
  \[ H = 2J \sum_k \gamma_k S_k \cdot S_{-k} \]

- Keep only the (0,0) and (\pi,\pi) mode

- Lieb Mattis model recovered
  \[ H_0 = \frac{4J}{N} (S_{\text{tot}}^2 - S_A^2 - S_B^2) \]
Symmetry decomposition of order parameter

- Order parameter manifold forms a representation space for the symmetry group of the Hamiltonian (more details later)

- Decompose this (reducible) representation into irreducible representations

1 step translation
bond reflection
plaquette rotation

SU(2) operation
with non-collinear axis
Symmetry decomposition of order parameter

As a result of the group theoretical analysis one obtains

- 1 irrep with $S=0$, $(0,0)$ A1
- 1 irrep with $S=1$, $(\pi,\pi)$ A1
- 1 irrep with $S=2$, $(0,0)$ A1
- 1 irrep with $S=3$, $(\pi,\pi)$ A1
- ...

actual ED results for square lattice Heisenberg model
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General Formalism for Symmetry Decomposition

- Ground state manifold: span of all $|\psi_{GS}\rangle$ a prototypical state (e.g. product state)

$$V_{GS} = \text{span} \{ |\psi_{GS}^i\rangle \}$$

where $|\psi_{GS}^i\rangle$ are the degenerate ground states in the thermodynamic limit. This space is finite dimensional for discrete symmetry breaking and infinite dim. for continuous symmetry breaking.

- The symmetry group acts nontrivially within this subspace (prototypical states “break” symmetries), it forms a (reducible) representation $\Gamma$

$$\Gamma : G \rightarrow \text{Aut}(V_{GS})$$

$$g \mapsto (\langle \psi_{GS}^i | O_g | \psi_{GS}^j \rangle)_{i,j}$$

$$\Gamma = \bigoplus \rho n_{\rho} \rho$$

- The representation can be decomposed into irreducible representations of the symmetry group according to standard group theory formula:

$$n_{\rho} = \frac{1}{|G|} \sum_{g \in G} \chi_{\rho}(g) \text{Tr}(\Gamma(g))$$
General Formalism: Simplification using “stabiliser”

- General action
  \[ \Gamma : \mathcal{G} \rightarrow \text{Aut}(V_{\text{GS}}) \]
  \[ g \mapsto \left( \langle \psi_G | O_g | \psi_G' \rangle \right)_{i,j} \]

- Often we have
  \[ \langle \psi_G | O_g | \psi_G' \rangle = \begin{cases} 1 \text{ if } O_g | \psi_G' \rangle = | \psi_G \rangle \\ 0 \text{ otherwise} \end{cases} \]
  i.e. ~ Permutation matrix

Then we can simplify the representation reduction formula

\[ n_\rho = \frac{1}{| \text{Stab}(| \psi_G \rangle \rangle |} \sum_{g \in \text{Stab}(| \psi_G \rangle \rangle)} \chi_\rho(g) \]

using the “stabiliser” subgroup concept

\[ \text{Stab}(| \psi_G \rangle \rangle) \equiv \{ g \in \mathcal{G} : O_g | \psi_G \rangle = | \psi_G \rangle \} \]

we only need:
- the stabilizer \( \text{Stab}(| \psi_G \rangle \rangle) \) of a prototypical state \( | \psi_G \rangle \) in the groundstate manifold
- the characters of the irreducible representations of the symmetry group \( \mathcal{G} \)
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First a simple example:

Discrete Symmetry Breaking

- Columnar Dimer Valence Bond Crystal (4 different singlet states) occurs in Quantum Dimer models and some frustrated quantum magnets

\[ G = D = T \times PG \]

\[ \chi_k(t) = e^{i k \cdot t} \]

<table>
<thead>
<tr>
<th>Irreps ( C_4 )</th>
<th>( C_4 )</th>
<th>( C_2 )</th>
<th>((C_4)^3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
</tr>
<tr>
<td>B</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>( E_a )</td>
<td>+1</td>
<td>+i</td>
<td>-i</td>
</tr>
<tr>
<td>( E_b )</td>
<td>+1</td>
<td>-i</td>
<td>+1</td>
</tr>
</tbody>
</table>

Table 1: Character table for pointgroup \( C_4 \).

\[ \text{Stab}(\Psi_{cVBS}) = \{1 \times 1\} \cup \{1 \times C_2\} \cup \{t_y \times 1\} \cup \{t_y \times C_2\} \]

where \( C_2 \) denotes the rotation about an angle \( \pi \) around the center of a plaquette.

\[ n_{(\pi,0)A} = \frac{1}{|\text{Stab}(\Psi_{cVBS})|} \sum_{d \in \text{Stab}(\Psi_{cVBS})} \chi_A(d) \chi_{k=(\pi,0)}(d) \]

\[ = \frac{1}{4} \left[ 1 + 1 + 1 + 1 \right] = 1 \]

\[ n_{(\pi,0)B} = \frac{1}{|\text{Stab}(\Psi_{cVBS})|} \sum_{d \in \text{Stab}(\Psi_{cVBS})} \chi_B(d) \chi_{k=(\pi,0)}(d) \]

\[ = \frac{1}{4} \left[ 1 + (-1) + 1 + (-1) \right] = 0 \]
First a simple example:
Discrete Symmetry Breaking

Staggered Valence Bond Crystal, also fourfold degenerate

\[ \text{Irreps} \quad \text{cVBS} \quad \text{sVBS} \]
\[ \begin{array}{ccc}
(0,0) \ A & 1 & 1 \\
(0,0) \ B & 1 & 1 \\
(\pi,0) \ A & 1 & 0 \\
(0,\pi) \ A & 1 & 0 \\
(\pi,\pi)E_a & 0 & 1 \\
(\pi,\pi)E_b & 0 & 1 \\
\end{array} \]

36 sites, \( K/J=0.6, \ \theta=0.17\pi \)

Found in a ring-exchange model:
AML et al., PRL 2005
Continuous Symmetry Breaking

Collinear magnetic order

collinear magnetic order: spins are all (anti)parallel to a common axis in spin space

\[ |\psi\rangle = |\uparrow\uparrow\uparrow\downarrow\cdots\rangle \]

(simplified) square lattice space group, SO(3) spin symmetry group

\[ G = D \times C \]
\[ D = \mathbb{Z}_2 \times \mathbb{Z}_2 = \{1, t_x, t_y, t_{xy}\} \]
\[ C = SO(3) \]

Ground state manifold

\[ V_{GS} = \{O_g |\psi\rangle ; g \in G\} \]

Stabilizer of a single Néel state:

- No translation in real space or a diagonal \( t_{xy} \) translation together with a spin rotation \( R_z(\alpha) \) around the \( z \)-axis with an arbitrary angle \( \alpha \).

- Translation by one site, \( t_x \) or \( t_y \), followed by a rotation \( R_a(\pi) \) of 180° around an axis \( a \perp z \) perpendicular to the \( z \)-axis.

\[ \text{Stab}(|\psi\rangle) = \{1 \times R_z(\alpha)\} \cup \{t_{xy} \times R_z(\alpha)\} \cup \{t_x \times R_a(\pi)\} \cup \{t_y \times R_a(\pi)\} \]
Continuous Symmetry Breaking
Collinear magnetic order

Irreducible representations of the symmetry group

\[ \chi_k(t) = e^{i k \cdot t} \quad k \in \{(0, 0), (0, \pi), (\pi, 0), (\pi, \pi)\} \]

\[ \chi_S(R) = \frac{\sin \left[(S + \frac{1}{2})\phi\right]}{\sin \frac{\phi}{2}} \]

Multiplicity of irreducible representations (general formula)

\[
n_{(k,S)} = e^{ik_0} \frac{1}{4|R_z(\alpha)|} \int_0^{2\pi} d\alpha \chi_S(R_z(\alpha)) + e^{i(k_0 + e_y)} \frac{1}{4|R_z(\alpha)|} \int_0^{2\pi} d\alpha \chi_S(R_z(\alpha))
\]

\[
+ e^{ik_0} e_x \frac{1}{4|R_x(\pi)|} \int_0^{2\pi} d\alpha \chi_S(R_x(\pi)) + e^{i(k_0 + e_y)} \frac{1}{4|R_x(\pi)|} \int_0^{2\pi} d\alpha \chi_S(R_x(\pi))
\]

evaluated for the present case (details in lecture notes)

<table>
<thead>
<tr>
<th>S</th>
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<th>( M.A1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
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<tr>
<td>1</td>
<td>0</td>
<td>1</td>
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<td>2</td>
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<td>0</td>
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<tr>
<td>3</td>
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<td>1</td>
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Continuous Symmetry Breaking
Collinear magnetic order

- Exact Diagonalization for a N=32 site square lattice Heisenberg model

![Graph showing energy levels vs. angular momentum for a N=32 site square lattice Heisenberg model.](image)

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<td>0</td>
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<td>3</td>
<td>0</td>
<td>1</td>
</tr>
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</table>

- $\Delta/J$ vs. $S_{tot}(S_{tot}+1)$
- $N = 32$

The graph illustrates the energy levels for different angular momenta ($S_{tot}$) and their scaling with $\Delta/J$. The symbols represent different quantum numbers for the excited states.
Beyond the collinear Neel state

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 $\Rightarrow$ nontrivial momenta must appear in TOS
- non-collinear magnetic structure $\Rightarrow$ SU(2) is completely broken, number of levels in TOS increases with S
- Quantum numbers are identical to the S=1/2 case
Spin Quadrupolar Order

Order parameter is not a vector as usual, but instead a tensor of rank two.

Belongs to the class of spin nematic states, i.e. $\langle S_i \rangle = 0$, but SU(2) is broken nevertheless.

Single site example: $|S^y = 0\rangle$, $S=1$

and isotropic fluctuations break SU(2) symmetry

$$\langle S^\alpha \rangle = 0$$

anisotropic fluctuations break SU(2) symmetry

$$\langle (S^y)^2 \rangle = 0 \quad \langle (S^x)^2 \rangle \neq 0$$
Tower of States
S=1 on triangular lattice: Ferroquadrupolar phase

- $\theta = -\pi/2$ : ferroquadrupolar phase, finite quadrupolar moment, no spin order
- No spatial symmetry breaking.
  $\Rightarrow$ only trivial spatial irrep appears in TOS
- Ferroquadrupolar order parameter, only even $S$
- All directors are collinear
  $\Rightarrow$ SU(2) is broken down to U(1),
  number of states in TOS is independent of $S$. 

$S(S+1)$
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.

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Continuous symmetry breaking with other groups

- SU(N) quantum magnetism in ultracold atomic gases

- Here an SU(3) example on the triangular lattice:

- S(S+1) scaling gets replaced by quadratic Casimir of irreducible representations of symmetry group.

AML, F. Mila, K. Penc
PRL (2006)
Quantum Critical Points

Universal spectrum of the critical field theory at the quantum critical point

Spectrum scales as $1/L$. Here an example for the Ising CFT in 2+1D:

$$\tau = i - \text{Square}$$

$$\tau = \frac{1}{2} + \frac{\sqrt{3}}{2}i - \text{Triangular}$$

Conclusions

- Exact Diagonalization based spectroscopy of quantum many body Hamiltonians is a very powerful technique.

- Well developed framework to diagnose and characterise (continuous) symmetry breaking on finite size systems. Recent extensions to quantum critical points

- More details in lecture notes written together with M. Schuler and A. Wietek
Thank you for your attention!