MAQUIS

Modern Algorithms for Quantum Interacting Systems

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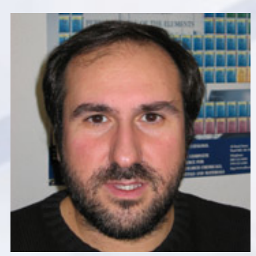
PI		Prof. Thierry Giamarchi	(UniGE)
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Scientific vision – «More is different»

Weakly- versus strongly-correlated systems

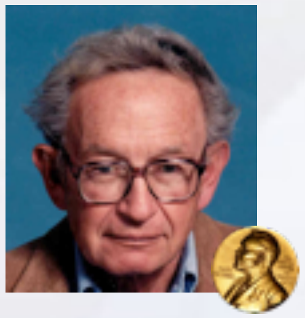
Hilbert space

Good approximations exist for weakly-correlated systems $\mathcal{O}(N)$

- Density Functional Theory / Kohn-Sham equations
- Diagrammatic perturbation theory / Landau Fermi-liquid theory

Strongly-correlated systems are much less understood $\mathcal{O}(e^N)$

- Interaction between a large number of quantum particles leads to new physical phenomena
  - Superconductors – Luttinger liquids – Correlated insulators – Quantum magnets – Quantum Hall systems
- Many open problems
  - Origin of high-T_c superconductivity
  - Ground states of frustrated quantum magnets
  - Quantum phase transitions
  - New types of excitations (collective modes, fractionalization, anyons)



«More is different»
(P. W. Anderson)

Scientific vision – «More is different»

Weakly- versus strongly-correlated systems

- One- and quasi-one dimensional systems
- Frustrated quantum magnets
- Fermions in two dimensions

Scientific vision – (1+ε) dimension

Low dimensionality magnifies the role of interactions

- Long-range order is suppressed by quantum fluctuations
- Mean-field approaches fail
- Particle motion induces collective motion

New paradigm: Luttinger liquid

- Low-energy excitations are collective modes
- Spin and charge degrees of freedom are separated
- Dimensional crossovers with lowering temperature: 1D → 2D → 3D

Good analytical methods exist in strict 1D…

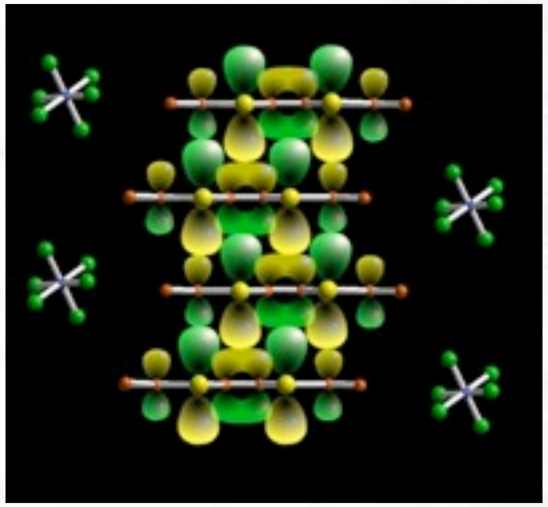
– Exact solutions (Bethe Ansatz) – Effective field theories (bosonization)

- … but they are limited to simple models and/or low energy

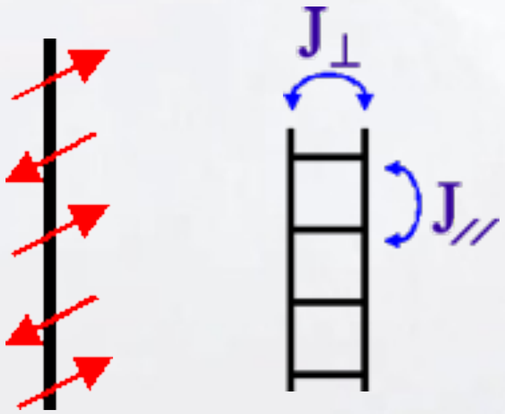
Density Matrix Renormalization Group (DMRG)

- Mature exact and powerful method for 1D and quasi-1D problems
- State-of-the-art: N = 300 in 1D or 8 × 20 in quasi-1D

Organic conductors



Spin chains and ladders



Quantum wires

Nanotubes

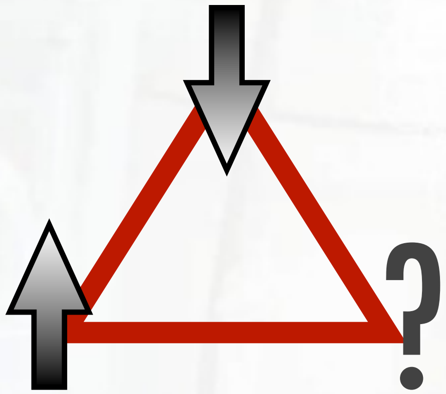
Quantum Hall edge states

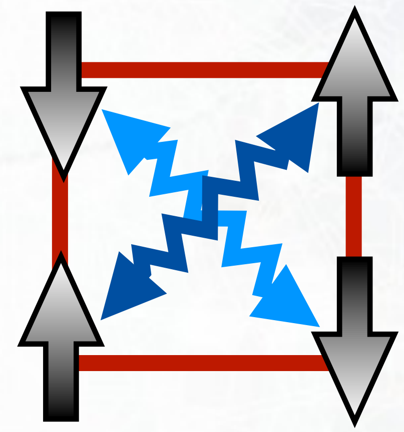
1D cold atoms systems

Scientific vision – Frustrated magnetism

Frustration due to geometry or competing interactions

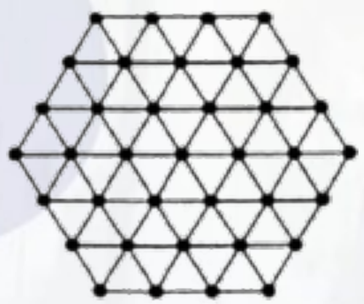
- Large number of nearly degenerate ground states
- Rich excitation spectrum



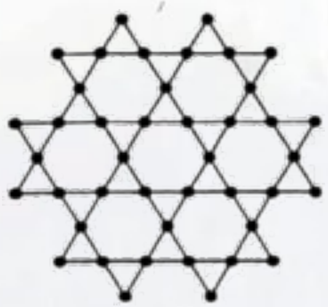


The only reliable information comes from exact diagonalization on small clusters

- Size of Hilbert space: 2^N for N spins 1/2
- Sign problem in quantum Monte Carlo
- State-of-the-art: N<40 (using lattice symmetries)
- Kagome lattice requires at least N = 36
- Pyrochlore lattice requires at least N = 48

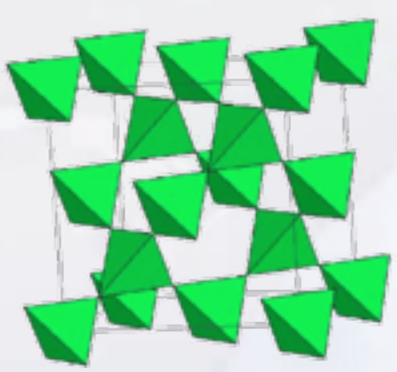


Triangular



Kagome

Face-centered cubic



Pyrochlore

Challenge

- Ground state and low-energy eigenvalues of sparse matrices of dimension 10^{12}

Scientific vision – Fermions in 2 dimensions

Fascinating open questions in 2D

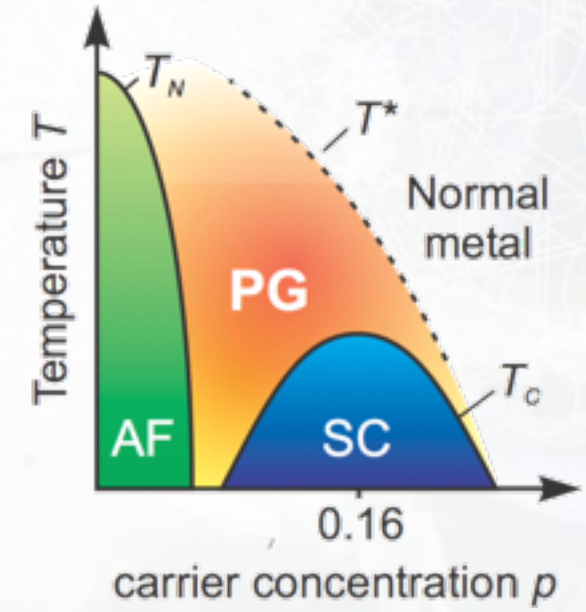
- Competing orders
- Quantum phase transitions
- Correlated insulators
- High-T_c superconductivity
- Quantum Hall effect (anyonic excitations)

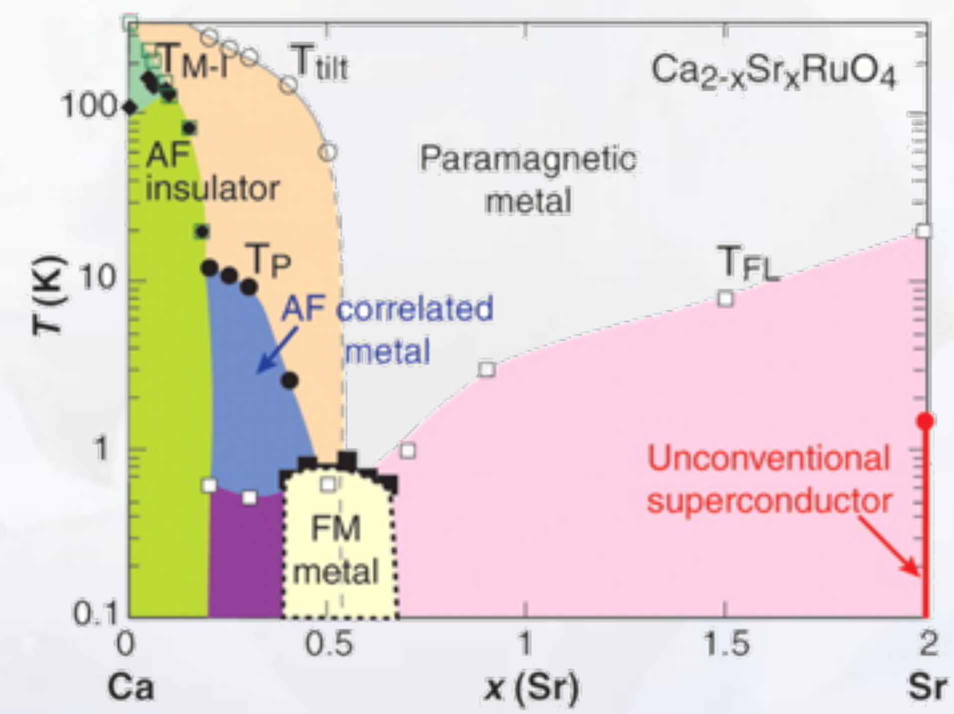
Tremendous potential for applications

Two is exactly between one and infinity

- Analytical methods work in 1D but fail in 2D
- Mean-field approaches are exact in ∞D, good in 3D, but dubious in 2D
- Numerical methods suffer from severe limitations
  - Sign problem in quantum Monte Carlo
  - Bad scaling and finite-size effects in exact diagonalization

Cuprates
Manganites
Ruthenates





2D organic conductors / Ferroelectrics / Multiferroics / 2D cold atomic gases

Models

Spin-1/2 Heisenberg model

$$\mathcal{H} = \frac{1}{2}\sum_{ij} J_{ij}\,\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \mu_{\mathrm{B}}\boldsymbol{H} \cdot \sum_i g_i \boldsymbol{S}_i$$

- Coupled quantum spins on a lattice
- Model for quantum magnets, quantum phase transitions

One-band Hubbard model

$$\mathcal{H} = \sum_{ij\sigma} t_{ij}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + \mathrm{h.c.}\right) + U\sum_i n_{i\uparrow}n_{i\downarrow}$$

- Fermions on a lattice, with local electron-electron interaction
- Model for high-T_c superconductors, correlated insulators, quantum phase transitions

$$n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$$

Solution methods

Analytical

- Diagrammatic theory
- Bosonization
- Slave particles
- Bethe Ansatz
- Renormalization group

} Powerful, but not sufficient

Numerical

- Exact diagonalization (ED)
- Density-Matrix Renormalization Group (DMRG)
- Quantum Monte Carlo (QMC)

} Needed for
- Quantitative results
- Intractable problems

Algorithms – Exact diagonalization

Advantages

- Can be used for any model
- Similar to configuration-interaction in quantum chemistry

Goal

- Obtain low-lying eigenstates of a sparse matrix
- Matrix size increases exponentially with problem size
  - Heisenberg model: 2^N – Hubbard model: 4^N
  - Only order-N non-zero elements per row, but irregularly distributed

Implementation

- Lanczos algorithm

$$\beta_{n+1} \boldsymbol{v}_{n+1} = \mathcal{H} \boldsymbol{v}_n - \alpha_n \boldsymbol{v}_n - \beta_n \boldsymbol{v}_{n-1}$$

α_n: $\boldsymbol{v}_n^\dagger \mathcal{H} \boldsymbol{v}_n$

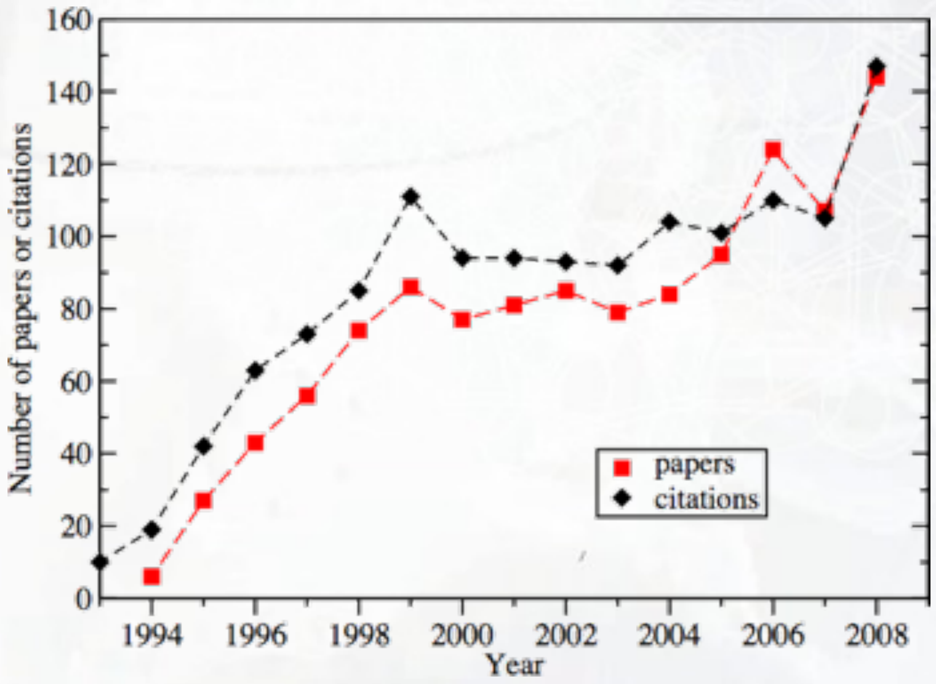
β_n: $|\boldsymbol{v}_n^\dagger \mathcal{H} \boldsymbol{v}_{n-1}|$

Challenges

- Large sparse and block-sparse linear algebra operations
  - Distributed sparse matrix-vector multiplications for matrices of size 10^{12} (state-of-the-art is 10^9)
  - Robust sparse matrix eigensolvers (treatment of roundoff errors requires MPI message ordering)
  - Generation of sparse matrices (distributed search in huge tables)

Algorithms – Density-Matrix Renormalization Group

A new and promising technique



Advantages

- The best numerical method so far for 1D
- Allows to compute equilibrium as well as out-of-equilibrium and time-dependent response

Goal

- N matrices of size m $\times$ m. m grown as a low-order polynomial in N
- Operations on block-sparse matrix with large dense blocks
  - Block generation (outer products) – Singular value decomposition – Eigenvalues, eigenvectors

Challenges

- Extend method to 2D by coupling chains
  - m increases exponentially with number of chains W
- State-of-the-art
  - With m = 10^3 to 10^4, 4 to 8 coupled chains of length 20 can be treated, depending on the model
- Target
  - 15 to 20 coupled chains,equivalent to a 20 $\times$ 20 2D lattice...

$$2^{20\times 20} = 10^{120}$$

Algorithms – Others

Tensor network algorithms

These avoid the exponential scaling when extending DMRG to 2D

- $m \times m$ matrices are replaced by rank-4 tensors
- Projected Entangled Pair States (PEPS)
- Multi-scale Entanglement Renormalization Ansatz (MERA)

Main difficulty

- Contraction of rank-4 tensors (memory requirement $M \sim m^4$, time $T \sim m^{12} \Rightarrow T \sim M^3$)
- $m = 5$ possible on workstations, $m = 10$ needed for useful applications

Refactoring of perfectly parallel applications

Quantum Monte Carlo (QMC)

Stochastic Series Expansion (SSE)

- Importance sampling of terms in a Taylor expansion in coupling strength or inverse temperature

Team – UniGE

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Principal investigator

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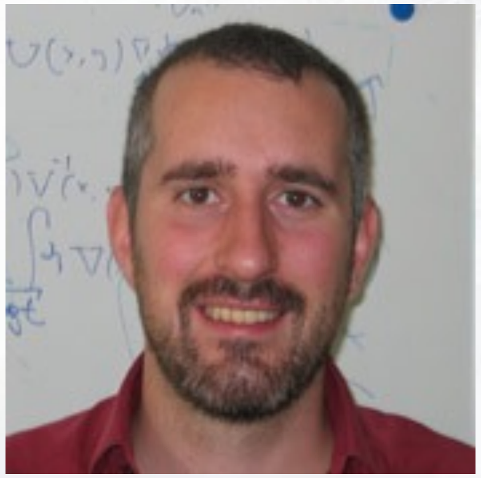
QMC/DMFT

Adrian Kantian
DMRG / t-DMRG



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Team – 4 Developers

As soon as possible:

Module 1
Exact diagonalization

Module 2
DMRG

Module 3
Tensor algorithms

Module 4
Refactoring of existing codes