Bootstrapping Nature: Non-perturbative Approaches to Critical Phenomena, Training Week
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Lattice Models
Numerical Simulations and Applications

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Outline

I. Introduction: models and experimental motivations

II. Principles of key numerical methods

III. Connecting to RG: scaling dimensions, finite-size scaling

IV. Applications: deconfined quantum criticality and related phenomena
(+ spin glasses if time permits)

Why study lattice quantum models?

1) Materials and device driven studies

- "strongly correlated" electronic materials
- **quantum magnets (spin degrees of freedom of insulators)**
- trapped cold atoms in optical lattices
- quantum emulators: programmable devices (for now mainly spin models)

2) Exploring new physics

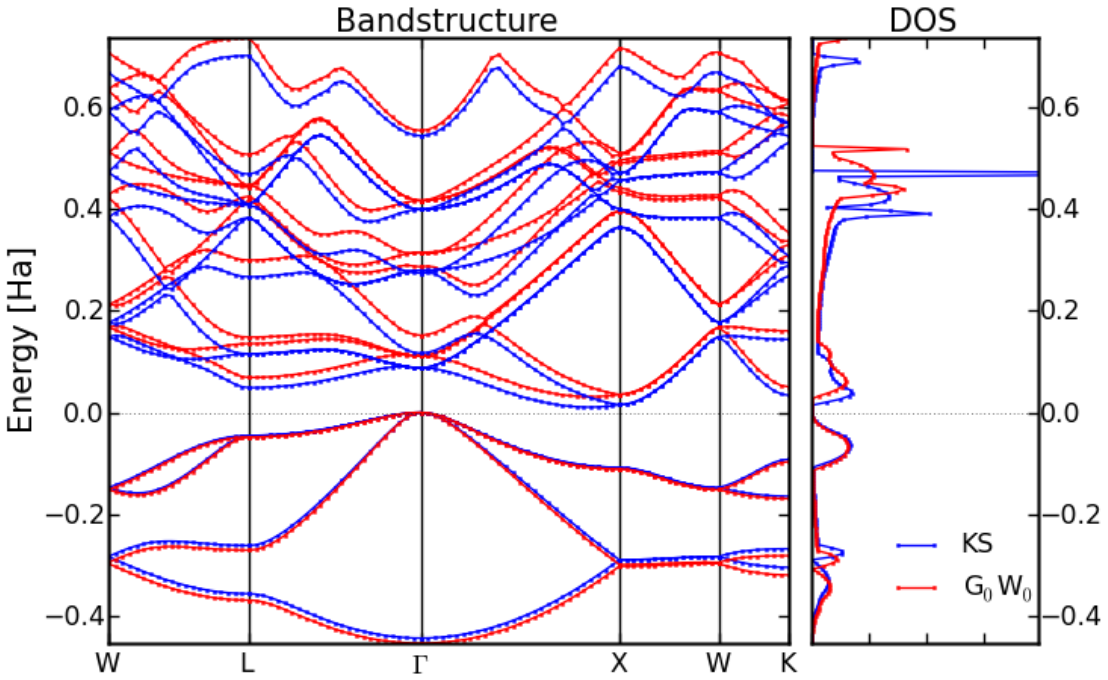
- minimal models to capture known and new phenomena
- study phenomena carefully without "distraction" of details
- characterize new types of ground states
- excitations not described by traditional quasiparticles
- **quantum phase transitions beyond the LGW paradigm**
- finite-T physics like thermalization, many-body localization

3) Connect to quantum field theory

- test existing theories
- stimulate new theories by discovering novel physics

Electron systems; band structure and “ab initio” calculations

- electrons are treated as weakly interacting quasiparticles
- many commercial and free “ab initio” software packages available



Example: Si

http://exciting-code.org

- normally fails for “strongly correlated” systems

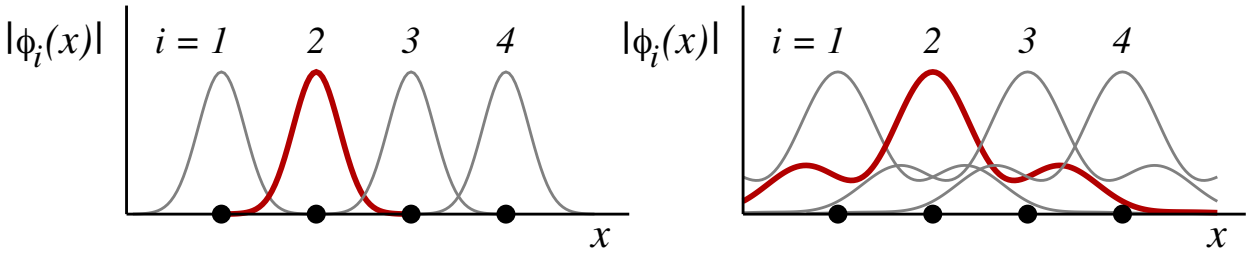
Not a topic of these lectures

Effective low-energy Hamiltonians

Goal: to capture essentially physics of strong correlations/entanglement
(new states, phenomena, beyond “ab initio” methods)

Starting point: Tight-binding model

- electron “hopping” between relevant orbitals (Wannier states)



Include electron-electron interactions

$$H = -\sum_{\sigma}\sum_{i,j} t_{ij}(c^{\dagger}_{\sigma j}c_{\sigma i} + c^{\dagger}_{\sigma i}c_{\sigma j}) + \sum_{ijkl}\sum_{\tau\sigma} V^{\sigma\tau}_{ijkl}c^{\dagger}_{\tau l}c_{\tau k}c^{\dagger}_{\sigma j}c_{\sigma i}$$

Only on-site interactions, one site per unit cell →
one-band Hubbard model

$$H = -t\sum_{\sigma}\sum_{\langle i,j\rangle}(c^{\dagger}_{\sigma i}c_{\sigma j} + c^{\dagger}_{\sigma j}c_{\sigma i}) + U\sum_{i} n_{\uparrow i}n_{\downarrow i}$$

Heisenberg model

Example: square lattice,
- start from Hubbard model

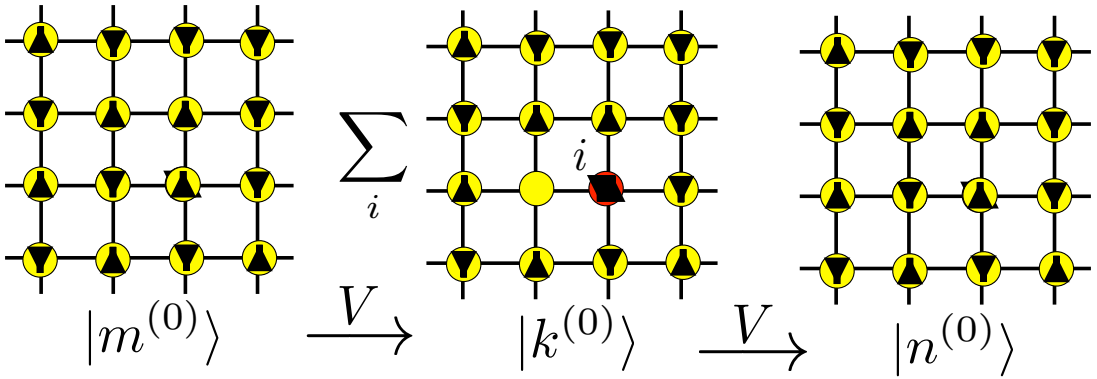
$$H = -t\sum_{\sigma}\sum_{\langle i,j\rangle}(c^{\dagger}_{\sigma i}c_{\sigma j} + c^{\dagger}_{\sigma j}c_{\sigma i}) + U\sum_{i} n_{\uparrow i}n_{\downarrow i} \quad = V + H_0$$

Half-filling → S=1/2 Heisenberg antiferromagnet:

- large U/t in Hubbard model → few doubly-occupied sites, insulator

- treat the kinetic energy as a perturbation of the ground state of the U term (H_0)

- 2^N degenerate groud states in space D, $E_0^{(0)} = 0$. 2nd-order energy shift:



$$\Delta^{(2)}_{nm} = \sum_{k\notin D}\frac{\langle n^{(0)}|V|k^{(0)}\rangle\langle k^{(0)}|V|m^{(0)}\rangle}{E^{(0)}_D - E^{(0)}_k}$$

Think of this as the matrix form of "second-order" operator

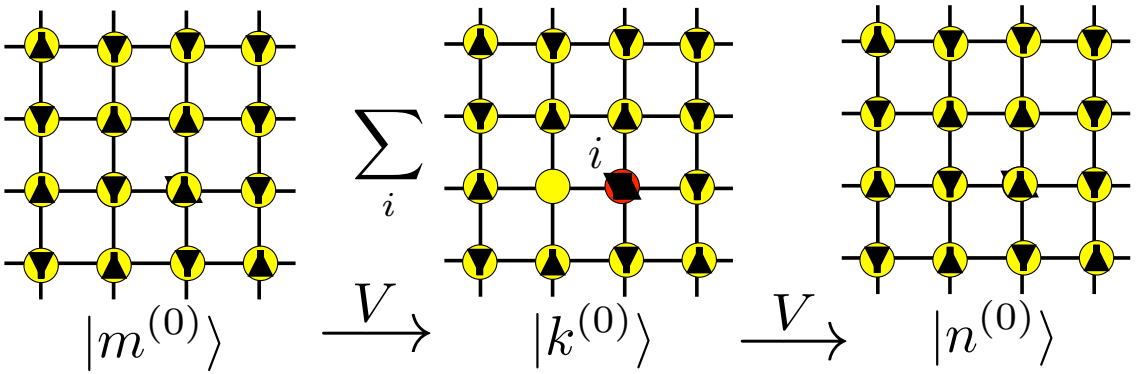
$$V_2 = \frac{V|k^{(0)}\rangle\langle k^{(0)}|V}{E^{(0)}_D - E^{(0)}_k}$$

If we diagonalize this matrix we get shifts including all 2nd order contributions

This matrix is the effective spin Hamiltonian!

$$H^{\text{eff}}_{nm} = -\frac{1}{U}\sum_{k\notin D}\langle n^{(0)}|V|k^{(0)}\rangle\langle k^{(0)}|V|m^{(0)}\rangle$$

$$= -\frac{1}{U}\langle n^{(0)}|V^2|m^{(0)}\rangle$$



Let's calculate the contributions from two nearest neighbors i,j

The spin states are defined by

$$|\sigma_1,\ldots,\sigma_N\rangle = \prod_{k=1}^{N} c^\dagger_{k\sigma_k}|\text{vac}\rangle$$

sum over i includes all states with one doubly-occupied states which can be reached by moving a particle to a neighboring site

- virtual states with one doubly-occupied site are created
- use convention: particles created in order 1,…,N, spin ↓ before ↑
- proceeding with anticommutation rules we get

$$c^\dagger_{i\uparrow}c_{j\uparrow}c^\dagger_{j\uparrow}c_{i\uparrow}|\ldots\uparrow_i\ldots\downarrow_j\ldots\rangle = +|\ldots\uparrow_i\ldots\downarrow_j\ldots\rangle$$

$$c^\dagger_{i\downarrow}c_{j\downarrow}c^\dagger_{j\uparrow}c_{i\uparrow}|\ldots\uparrow_i\ldots\downarrow_j\ldots\rangle = -|\ldots\downarrow_i\ldots\uparrow_j\ldots\rangle$$

$$c^\dagger_{j\downarrow}c_{i\downarrow}c^\dagger_{i\downarrow}c_{j\downarrow}|\ldots\uparrow_i\ldots\downarrow_j\ldots\rangle = +|\ldots\uparrow_i\ldots\downarrow_j\ldots\rangle$$

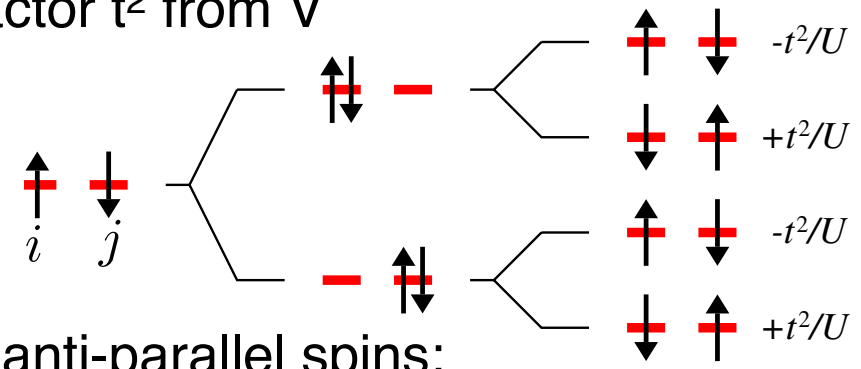
$$c^\dagger_{j\uparrow}c_{i\uparrow}c^\dagger_{i\downarrow}c_{j\downarrow}|\ldots\uparrow_i\ldots\downarrow_j\ldots\rangle = -|\ldots\downarrow_i\ldots\uparrow_j\ldots\rangle$$

the signs will not depend on the location of i,j

We also get a minus sign from -1/U and a factor t^2 from V

$$H^{\text{eff}}_{nm} = -\frac{1}{U}\langle n^{(0)}|V^2|m^{(0)}\rangle = \sum_{\langle ij\rangle} H^{\text{eff}}_{nm}(i,j)$$

$$H^{\text{eff}}_{nm}(i,j) = -\frac{1}{U}\langle n^{(0)}|V(i,j)^2|m^{(0)}\rangle$$



The fluctuation process is only possible for anti-parallel spins:

$$H^{\text{eff}}(i,j)|\ldots\uparrow_i\ldots\downarrow_j\ldots\rangle = 2(t^2/U)\,(-|\ldots\uparrow_i\ldots\downarrow_j\ldots\rangle + |\ldots\downarrow_i\ldots\uparrow_j\ldots\rangle)$$

$$H^{\text{eff}}(i,j)|\ldots\downarrow_i\ldots\uparrow_j\ldots\rangle = 2(t^2/U)\,(-|\ldots\downarrow_i\ldots\uparrow_j\ldots\rangle + |\ldots\uparrow_i\ldots\downarrow_j\ldots\rangle)$$

$$H^{\text{eff}}(i,j)|\ldots\uparrow_i\ldots\uparrow_j\ldots\rangle = 0$$

$$H^{\text{eff}}(i,j)|\ldots\downarrow_i\ldots\downarrow_j\ldots\rangle = 0$$

We can identify these outcomes with a spin-spin interaction.

Standard spin operators defined in the subspace with singly-occupied sites:

$$S^z_i|\ldots\uparrow_i\ldots\rangle = \tfrac{1}{2}|\uparrow_i\rangle, \qquad S^z_i|\ldots\downarrow_i\ldots\rangle = -\tfrac{1}{2}|\ldots\downarrow_i\ldots\rangle$$

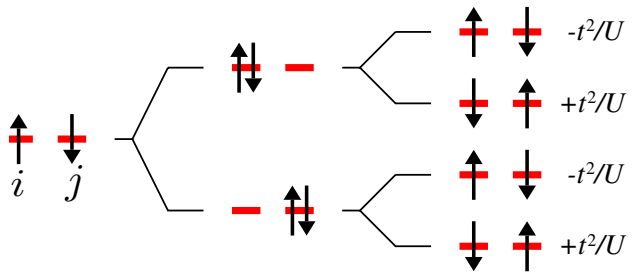
$$S^+_i|\ldots\uparrow_i\ldots\rangle = 0, \qquad S^+_i|\ldots\downarrow_i\ldots\rangle = |\ldots\uparrow_i\ldots\rangle$$

$$S^-_i|\ldots\uparrow_i\ldots\rangle = |\ldots\downarrow_i\ldots\rangle, \qquad S^-_i|\ldots\downarrow_i\ldots\rangle = 0,$$

$$H^{\text{eff}}(i,j) = \frac{2t^2}{U}(2S_i^z S_j^z - 1/2 + S_i^+ S_j^- + S_i^- S_j^+)$$

$$= J(S_i^z S_j^z - 1/4 + [S_i^+ S_j^- + S_i^- S_j^+]/2)$$

$$J = 4t^2/U$$ exchange constant



We can rewrite the interaction using:

$$S^x = (1/2)(S^+ + S^-), \quad S^x = (i/2)(S^+ - S^-)$$

$$S_i^x S_j^x = (1/4)(S_i^+ S_j^+ + S_i^+ S_j^- + S_i^- S_j^+ + S_i^- S_j^-)$$

$$S_i^y S_j^y = -(1/4)(S_i^+ S_j^+ - S_i^+ S_j^- - S_i^- S_j^+ + S_i^- S_j^-)$$

$$S_i^x S_j^x + S_i^y S_j^y = (1/2)(S_i^+ S_j^- + S_i^- S_j^+)$$ Note: sign came from anti-commutation

$$H^{\text{eff}}(i,j) = J(S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y) - J/4$$

The constant is normally unimportant and we have the Heisenberg Hamiltonian

$$H_{\text{Heisenberg}} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

Now we have an effective
low-energy Hamiltonian

But we still need to 'solve it'!

- it's not possible to exactly diagonalize the Hamiltonian for large N

1D: Exact Bethe Ansatz solution
- "quasi-ordered state"

$$H_{\text{Heisenberg}} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

2D: Spin wave theory can
account for low-energy physics (but not interesting effects at energy ~ J)
- T=0 states has antiferromagnetic order

3D: Spin-wave theory
- T > 0 antiferromagnetic ordering transition

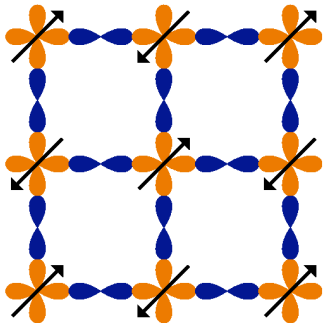
Some times the effective interactions are anisotropic. **XXZ model:**

$$H = \sum_{\langle ij \rangle} J_{xy}(S_i^x S_j^x + S_i^y S_j^y) + J_z S_i^z S_j^z$$

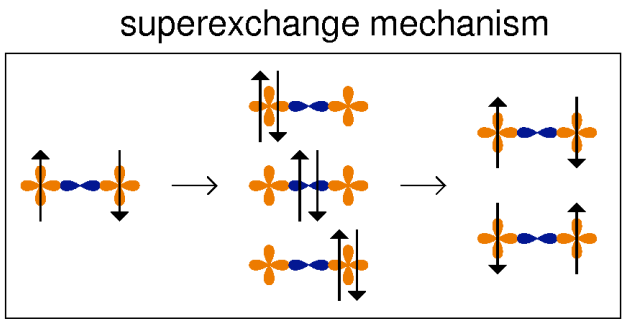
J_z=0 : XY model (or XX model)
J_{xy} = 0 : Ising model

The Heisenberg model can also apply in more complicated crystals

Some variants of Heisenberg model motivated by CuO_2 based hmaterials

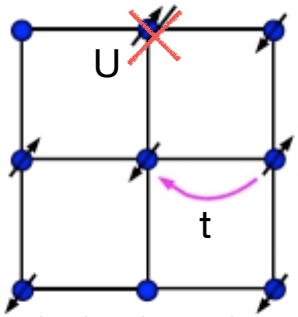


CuO_2 layer



$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

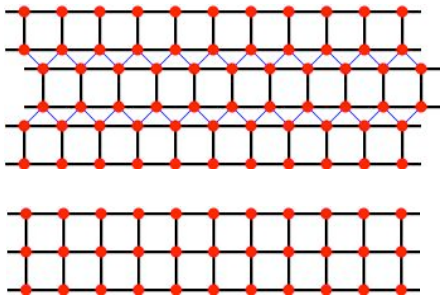
$$J \approx 1500 \text{ K}$$



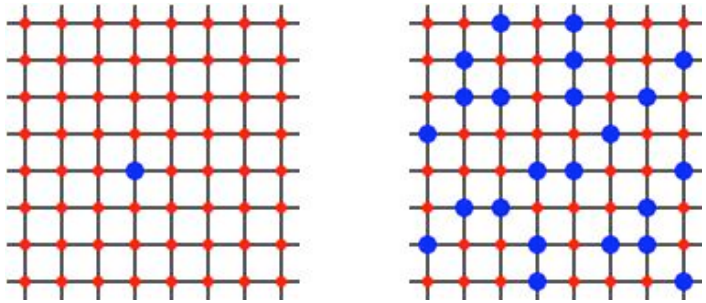
hole doped

Doping charge carriers: superconductivity
- Hubbard & t-J models

Variants of cuprates that are still insulating
- Heisenberg models on other lattices



Ladder systems
- even/odd effects

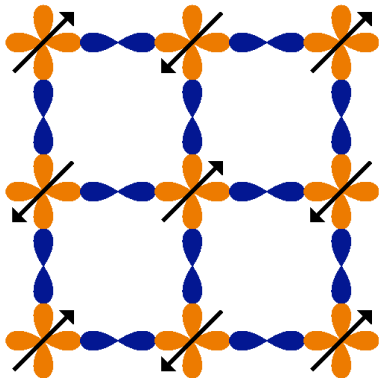


non-magnetic impurities/dilution
- dilution-driven phase transition

- Cu $(S = 1/2)$
- Zn $(S = 0)$

Nature of ground state (ordered vs disordered), excitations, quantum phase transitions…

Quantum versus classical antiferromagnets



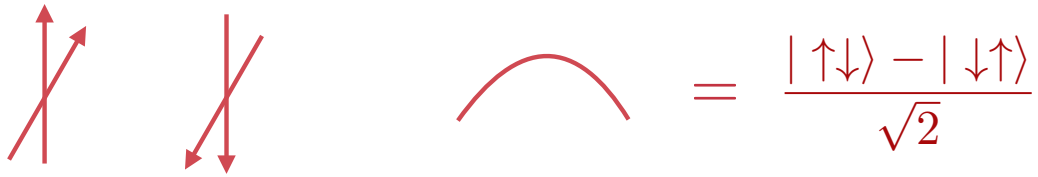
Starting point: S=1/2 Heisenberg model

$$\mathbf{H} = \mathbf{J}\sum_{\langle \mathbf{i},\mathbf{j}\rangle} \mathbf{S_i}\cdot\mathbf{S_j} \quad + \quad \mathbf{g}\times\cdots$$

- nearest-neighbor interactions (J>0)
- extend by longer-range or multi-spin couplings
- maintain spin-rotation invariance (or not)

Consider 2 spins:

- classical (S=∞) ground state is any anti-parallel configuration
- S=1/2 (extreme quantum) is a singlet (singlet-triplet gap = J)



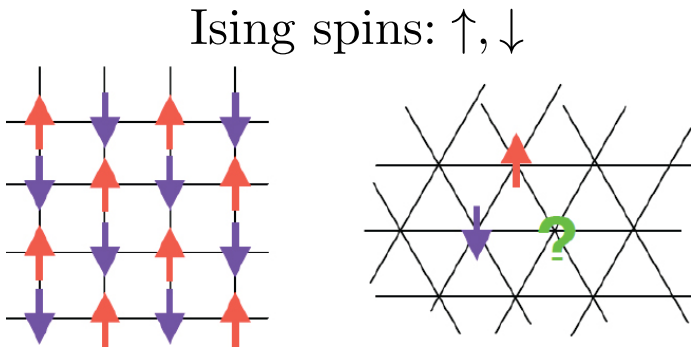
Extended quantum magnets (N→∞) can have aspects of

- classical-like antiferromagnetic order
- non-classical effects can some times be understood using singlets

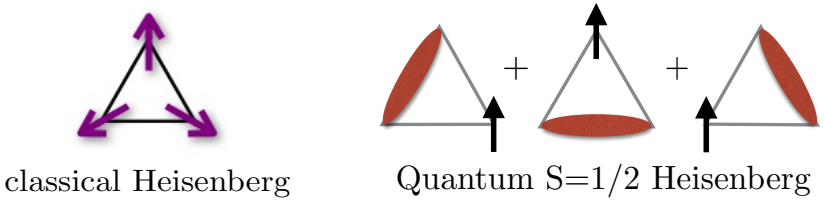
Frustrated quantum spins

Competing antiferromagnetic interactions
- structure of ground state can be highly non-trivial

Even classical spin models (Ising, XY, Heisenberg) can be highly non-trivial when the interactions are frustrated

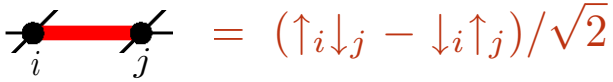


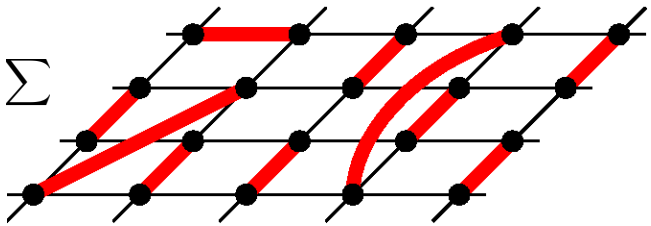
Be careful with classical pictures and intuition:



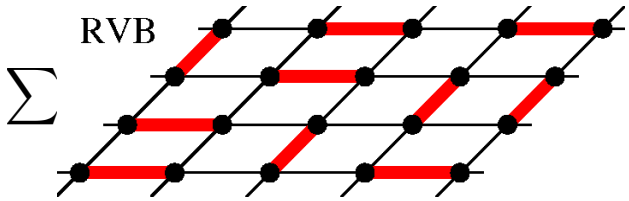
non-magnetic states dominated by short bonds

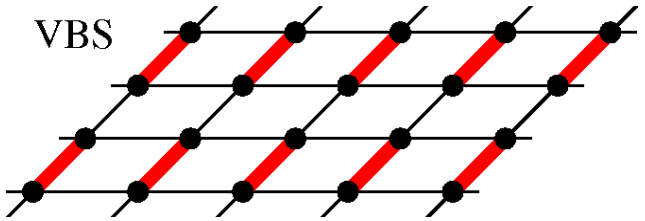
valence bond description (basis)





over-complete basis for the singlet sector





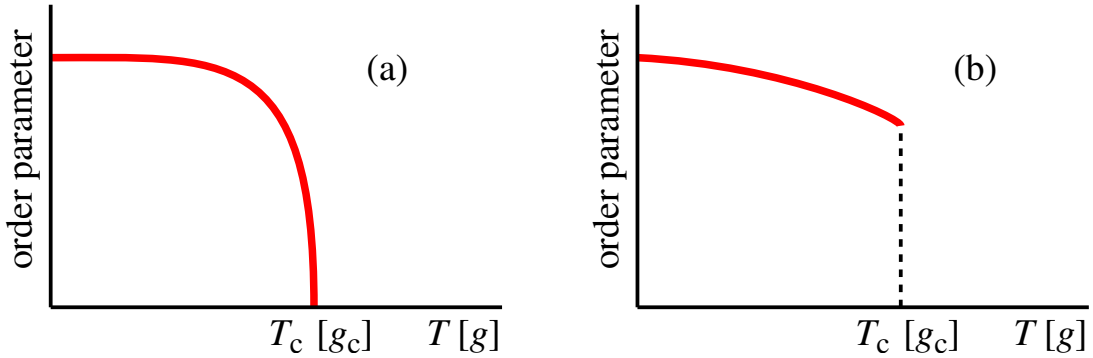
Classical and quantum phase transitions

Classical (thermal) phase transition

- Fluctuations regulated by temperature T>0

Quantum (ground state, T=0) phase transition

- Fluctuations regulated by parameter g in Hamiltonian



In both cases phase transitions can be

- first-order (discontinuous): finite correlation length ξ as $g \to g_c$ or $g \to g_c$
- continuous: correlation length diverges, $\xi \sim |g-g_c|^{-\nu}$ or $\xi \sim |T-T_c|^{-\nu}$

There are many similarities between classical and quantum transitions

- and also important differences

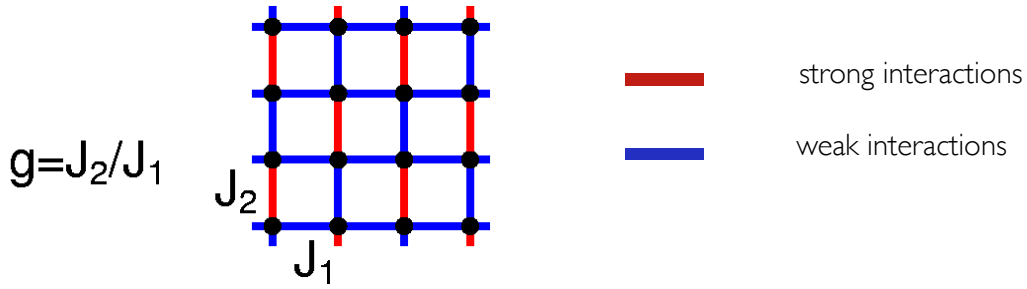
The quantum phases (ground states) can also be highly non-trivial

- even with rather simple lattice models

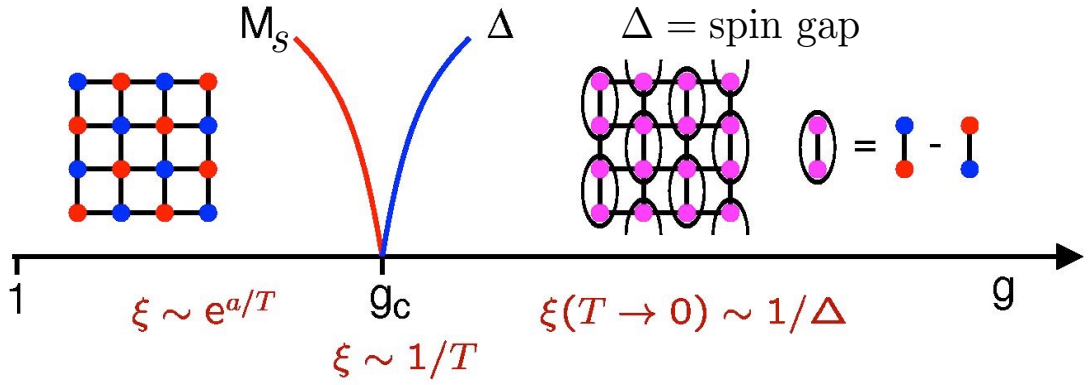
Example: Néel-paramagnetic quantum phase transition

Dimerized S=1/2 Heisenberg models

- **every spin belongs to a dimer (strongly-coupled pair)**
- many possibilities, e.g., bilayer, dimerized single layer



Singlet formation on strong bonds ➙ Néel - quantum-paramagnetic transition



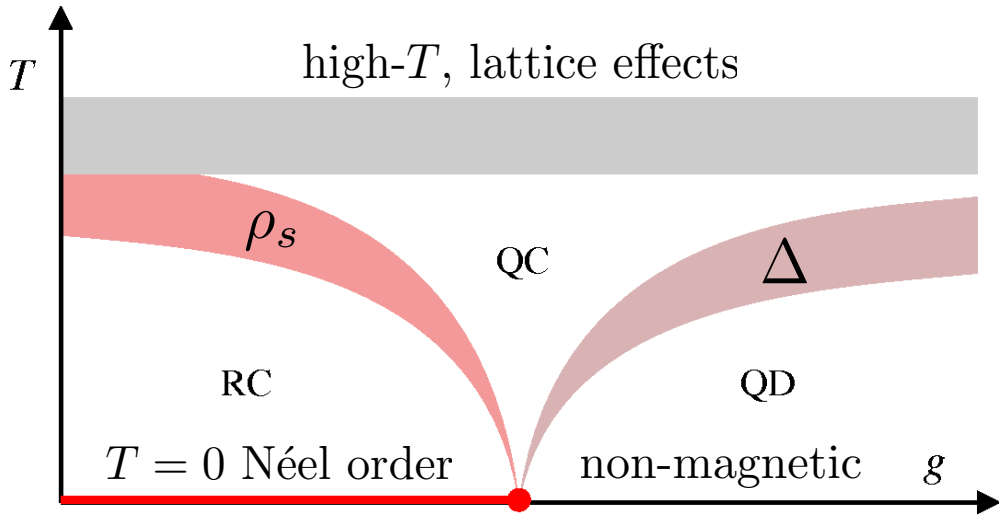
ground state (T=0) phases

Experimental realization (3D coupled-dimer system): $TlCuCl_3$

⇒ 3D classical Heisenberg (O3) universality class; QMC confirmed

What's so special about quantum-criticality?

- large T>0 quantum-critical "fan" where T is the only relevant energy scale
- physical quantities show power laws governed by the T=0 critical point



Example: 2D Neel-paramagnet "cross-over diagram" [Chakravarty, Halperin, Nelson 1988]

RC: Renormalized classical
- exponentially divergent correlation length

QC: Quantum critical
- scaling behavior in T

QD: Quantum disordered (paramagnetic)
- finite correlation length at T=0

Changing T changes the imaginary-time size L_τ:

- Finite-size scaling at g_c leads to power laws

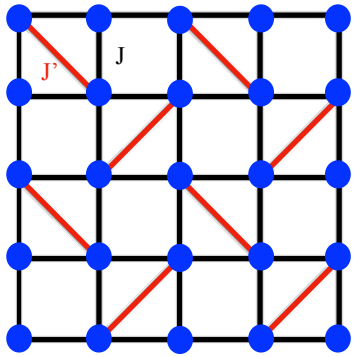
$\xi \sim T^{-1}$ (correlation length)

$C \sim T^2$ (specific heat)

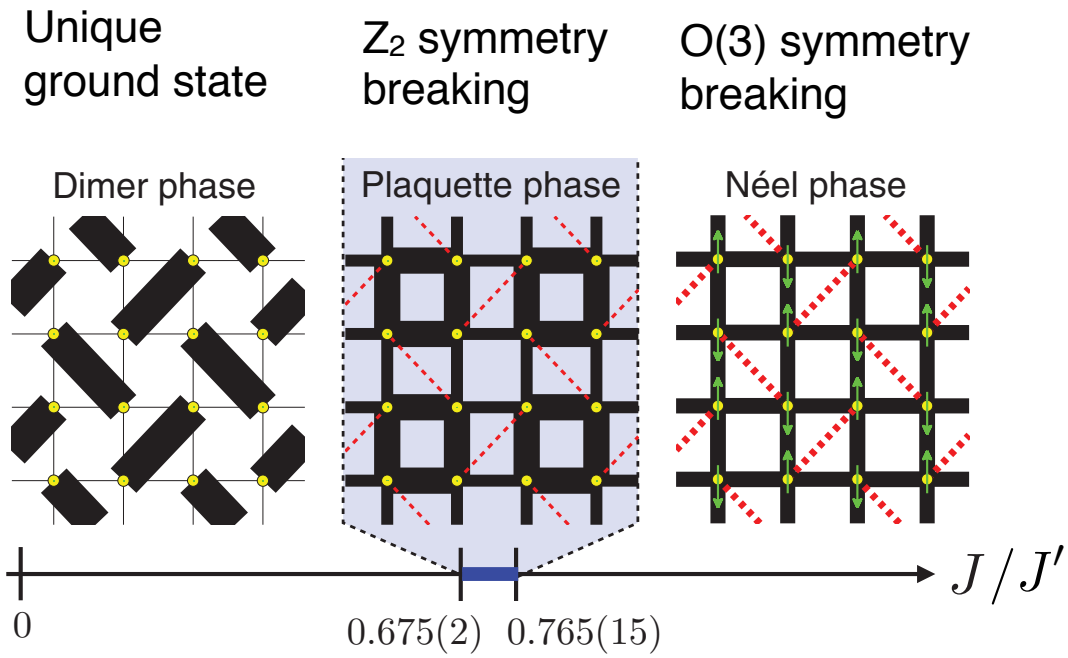
$\chi(0) \sim T$ (uniform magnetic susceptibility)

Experimentally important
- QC effects can extend to relatively high T

Example: Shastry-Sutherland model



$$H_{SS} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle ij \rangle'} \mathbf{S}_i \cdot \mathbf{S}_j$$



J' dimer-singlet state is exact eigenstate
- ground state up to for $J/J_1 \sim 0.68$

Recent work

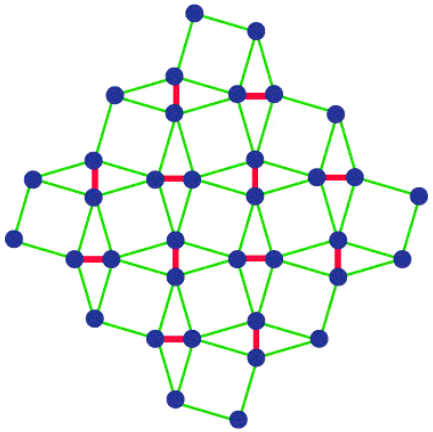
Yang, Sandvik, Wang, PRB 2022
Wang, Zhang, Sandvik, CPL 2022
- gaples spin liquid phase between PS and AFM phases; g ~ (0.79,0.83)

Corboz & Mila, PRB 2013 (tensors)
- Weak first-order Neel to PS transition (caveat: small tensor dimension)

Lee, You, Sachdev, Vishwanath, PRX 2019 (DMRG)
- deconfined quantum critical PS-AFM point

Shastry-Sutherland material

Quasi-2D (layered) quantum magnet $SrCu_2(BO_3)_2$



$$H_{SS} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle ij \rangle'} \mathbf{S}_i \cdot \mathbf{S}_j$$

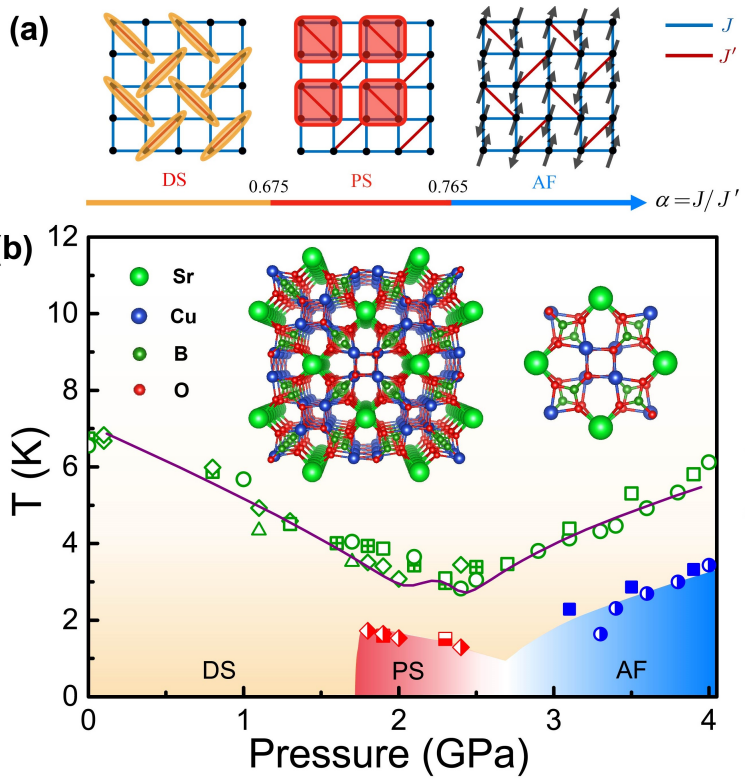
$\alpha = J/J' \approx 0.6$ at $P = 0$

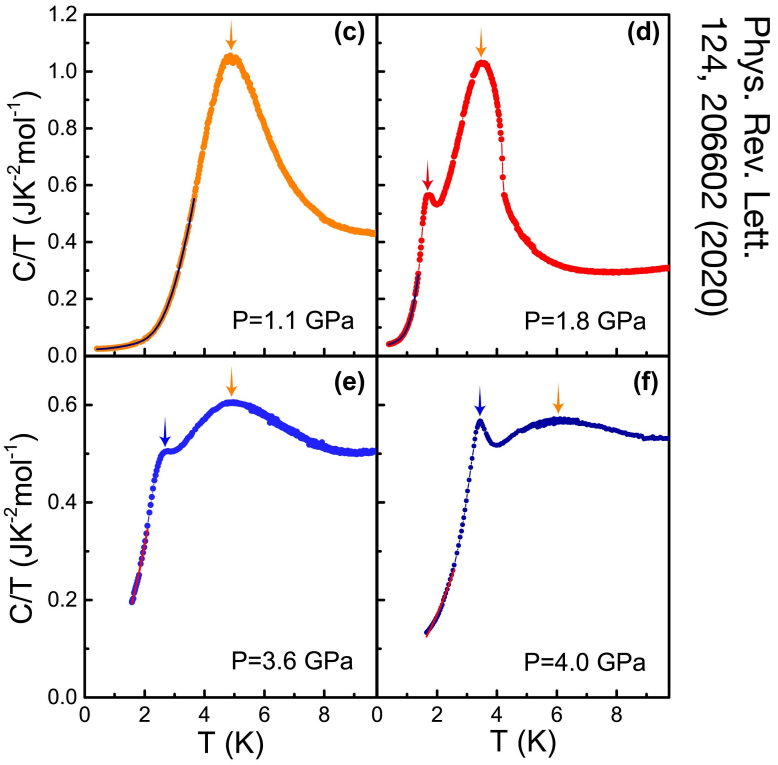
α increases with pressure

Recent work

NMR experiments, high pressure, high magnetic field (arXiv:2204.08133)

proximate deconfined critical point



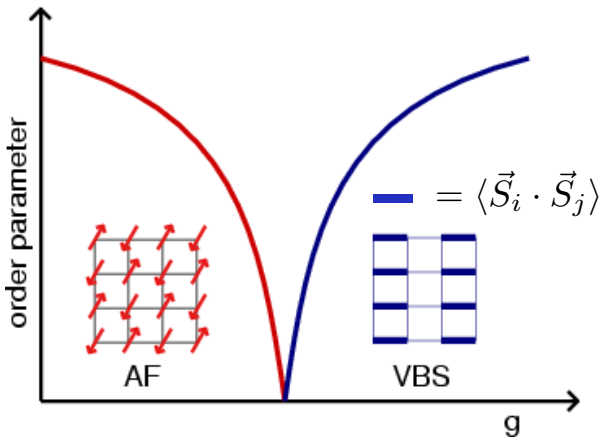


Phys. Rev. Lett. 124, 206602 (2020)

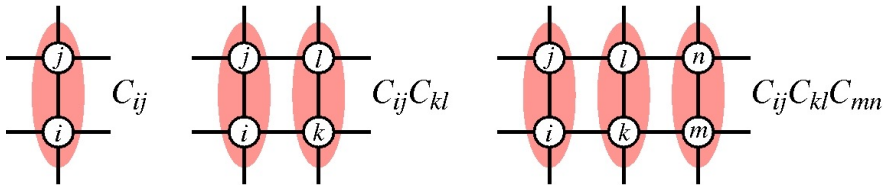
Deconfined quantum criticality

Senthil, Vishwanath, Balents, Sachdev, Fisher (Science 2004)
(+ many previous works; Read & Sachdev, Sachdev & Murthy, Motrunich & Vishwanath….)

Continuous AF - VBS transition at T=0
- would be violation of Landau rule
- first-order would normally be expected
- role of topological defects



Numerical (QMC) tests using J-Q models



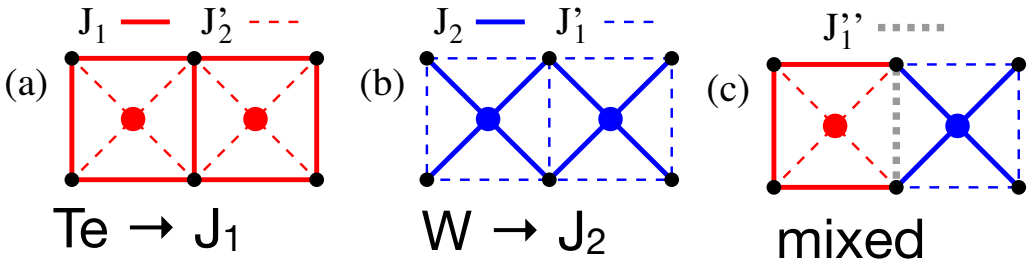
$$C_{ij} = \frac{1}{4} - \vec{S}_i \cdot \vec{S}_j$$

The "J-Q" model with two projectors (J-Q_2 model)

$$H = -J \sum_{\langle ij \rangle} C_{ij} - Q \sum_{\langle ijkl \rangle} C_{ij} C_{kl}$$

- **Néel-VBS transition appears to be continuous**
- **Possibly very weakly first-order**
- **Ongoing studies (will be discussed), also J-Q_3 and 'larger' Q_n terms**

Randomly frustrated quantum antiferromagnet: $SrCuTe_{1-x}W_xO_6$



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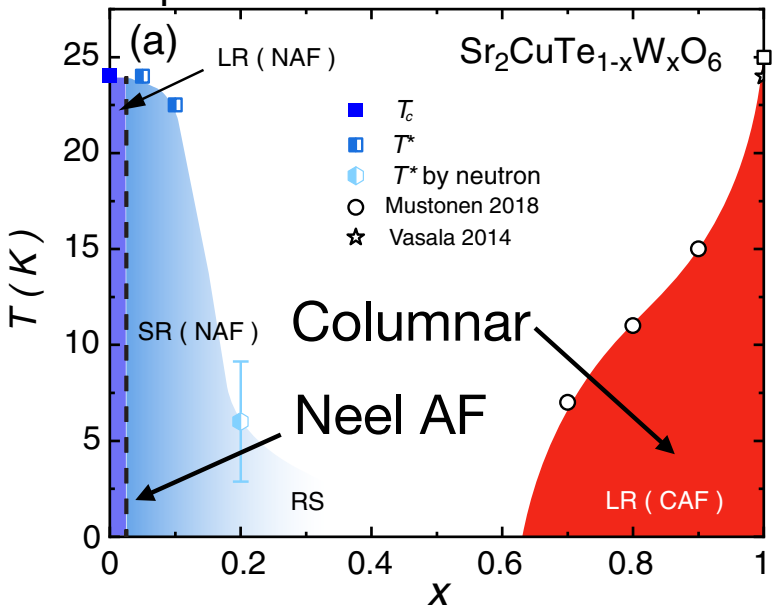
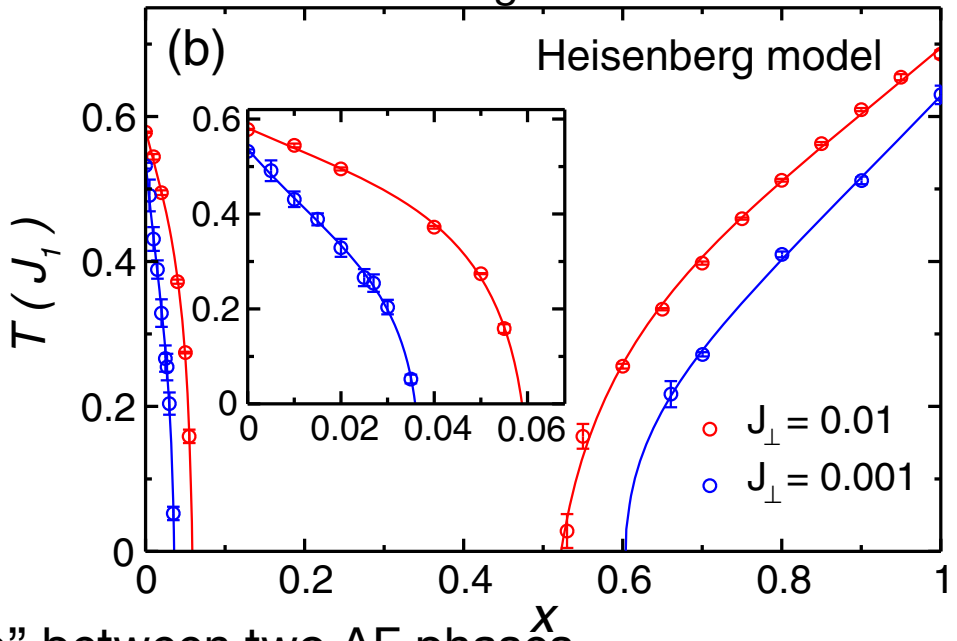
Dominant interaction depends on ion inside Cu plaquette

W fraction x, random mixing

Experiments



Classical modeling



Highly non-trivial "random singlet state" between two AF phases

- can be realized and studied in detail with random J-Q models

Quantum emulation

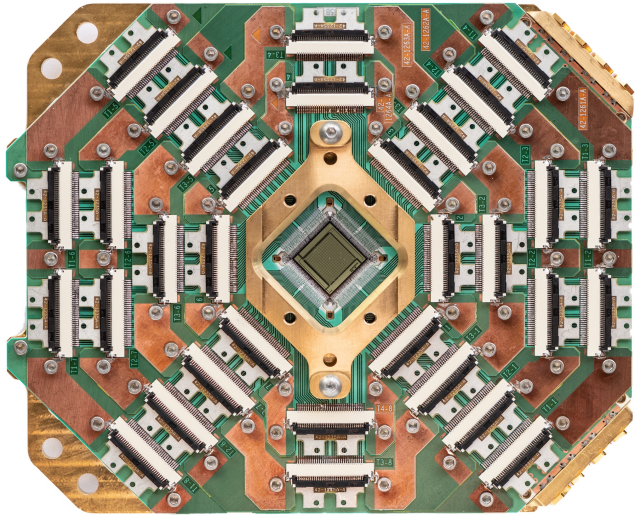
Physical devices with interacting 2-level systems (qubits)

Examples: Arrays of Rydberg atoms, coupled supercondicting qubits

D-Wave Systems

Advantage “computer”

- > 5000 superconducting qubits with programmable couplings



Quantum annealing

$$H(s) = sH_{\text{classical}} + (1-s)H_{\text{quantum}}$$

D-wave device: Programmable classical Ising model

$$H_{\text{classical}} = \sum_{i=1}^{N}\sum_{j=1}^{N} J_{ij}\sigma_i^z\sigma_j^z, \quad \sigma_i^z \in \{-1,+1\}$$

Couplings restricted restricted to “Pegasus lattice”

Quantum fluctuations; transverse field

$$H_{\text{quantum}} = -\sum_{i=1}^{N}\sigma_i^x = -\sum_{i=1}^{N}(\sigma_i^+ + \sigma_i^-)$$

$$[H_{\text{classical}}, H_{\text{quantum}}] \neq 0$$

$$H(t) = A(s[t])H_{\text{quantum}} + B(s[t])H_{\text{classical}}$$

Motivates numerical studies of transverse-field Ising models (uniform, random interactions)

- Annealing dynamics (generalized finite-size scaling)