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School and Workshop on Highly Frustrated Magnets and Strongly Correlated Systems: From Non-Perturbative Approaches to Experiments

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Strong coupling approaches and effective Hamiltonian

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Strong coupling approaches and effective Hamiltonian

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Scope

- Introduction: why strong coupling?
- Brief review of degenerate perturbation theory
- Frustrated magnets in zero field: coupling triangles, tetrahedra,...
- Ladders and coupled dimers in a field
- Perturbing Ising models
- Alternatives to degenerate perturbation

Heisenberg model

Standard analytical approach: expansion in 1/S

➡ Spin-waves around classical GS

Problem: frustration → highly degenerate GS

→ No natural starting point for 1/S

Alternative?

Strong coupling I

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

1) Suppose $J_{ij}^{\alpha} \gg J_{i'j'}^{\alpha'}$

2) Write $H = H_0 + V$ with

$$H_0 = \sum_{(i,j),\alpha} J_{ij}^{\alpha} \; S_i^{\alpha} S_j^{\alpha} \qquad V = \sum_{(i',j'),\alpha'} J_{i'j'}^{\alpha'} \; S_{i'}^{\alpha'} S_{j'}^{\alpha'}$$

Strong coupling II

3) If GS of H_0 degenerate, treat V with degenerate perturbation theory

⇒ Effective Hamiltonian

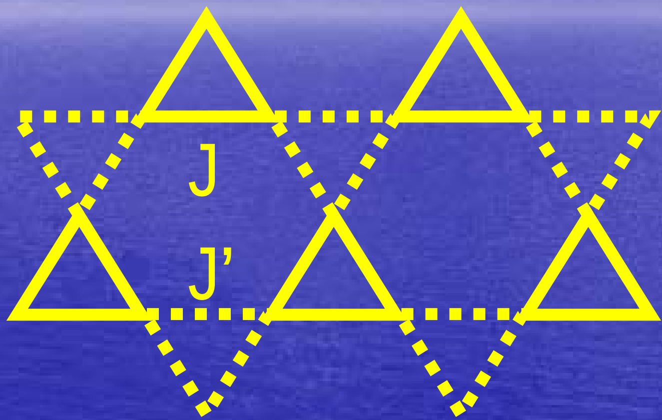
Small parameters: $J^{\alpha'}_{i'j'}/J^{\alpha}_{ij}$

NB: often useful to assume some parameters are small even if they are not (like 1/S for S=1/2!)

Examples

Weakly coupled triangles

$$J'/J \ll 1$$



⟹ Trimerized kagome

Heisenberg model with Ising anisotropy

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

$J^{xy}/J^z \ll 1$ ⟹ Perturbation around Ising limit

Degenerate Perturbation Theory

$$H = H_0 + V, \quad \text{Hilbert space } \mathcal{H}$$

H_0 : degenerate GS manifold, energy E_0, Hilbert space $\mathcal{H}_0$

Goal: Find an effective Hamiltonian H_{eff} acting in $\mathcal{H}_0$ such that:

$$H_{\text{eff}}|\phi\rangle = E|\phi\rangle \Rightarrow H|\psi\rangle = E|\psi\rangle, \quad |\phi\rangle \in \mathcal{H}_0, \quad |\psi\rangle \in \mathcal{H}$$

First order: Standard result of elementary quantum mechanics:

$$\langle\phi|H_{\text{eff}}|\phi'\rangle = \langle\phi|H_0|\phi'\rangle + \langle\phi|V|\phi'\rangle, \quad |\phi\rangle, |\phi'\rangle \in \mathcal{H}_0$$

Second order

Extremely useful, yet not totally standard

Second order: Suppose $H_0|m\rangle = E_m|m\rangle$, $E_m \neq E_0$. Then:

$$\langle\phi|H_{\text{eff}}|\phi'\rangle = \langle\phi|H_0|\phi'\rangle + \langle\phi|V|\phi'\rangle + \sum_{|m\rangle \notin \mathcal{H}_0} \frac{\langle\phi|V|m\rangle\langle m|V|\phi'\rangle}{E_0 - E_m}$$

Alternative: Denote by P the projector on $\mathcal{H}_0$, and define $Q = 1 - P$.

$$PH_{\text{eff}}P = PH_0P + PVP + PVQ\frac{1}{E_0 - QH_0Q}QVP$$

Proof: Suppose $H|\psi\rangle = E|\psi\rangle$. Since $P+Q=1$, this can be written:

$$(P+Q)H(P+Q)|\psi\rangle = E|\psi\rangle$$

Project onto $\mathcal{H}_0$ and $\mathcal{H}-\mathcal{H}_0$:

$$PHP|\psi\rangle + PHQ|\psi\rangle = EP|\psi\rangle \qquad (1)$$
$$QHP|\psi\rangle + QHQ|\psi\rangle = EQ|\psi\rangle \qquad (2)$$

$$(2) \Rightarrow Q|\psi\rangle = (E-QHQ)^{-1}QHP|\psi\rangle$$

$$(1) \Rightarrow PHP|\psi\rangle + PHQ\frac{1}{E-QHQ}QHP|\psi\rangle = EP|\psi\rangle$$

Expand $\frac{1}{E-QHQ}$ using $\frac{1}{A-B} = \frac{1}{A}\sum_{n=0}^{\infty}\left(B\frac{1}{A}\right)^n$ with:

$A = E_0 - QH_0Q$ and $B = QVQ - E + E_0$:

$$H_{eff} = PH_0P + PVP + PVQ\frac{1}{E_0 - QH_0Q}\sum_{n=0}^{\infty}\left((QVQ - E + E_0)\frac{1}{E_0 - QH_0Q}\right)^n QVP$$

Truncate expansion at $n=0$. QED

Higher order I

$$H_{eff} = \Gamma^{\dagger} H \Gamma$$

$$\Gamma = \bar{P} P (P \bar{P} P)^{-1/2}$$

$$(P\bar{P}P)^{-1/2} = P + \sum_{n=1}^{\infty} \frac{(2n-1)!!}{(2n)!!} [P(P-\bar{P})P]^n$$

$$\bar{P} = P - \sum_{n=1}^{\infty} \sum_{k_1+\ldots+k_{n+1}=n, k_i \geq 0} S^{k_1} V S^{k_2} V \ldots V S^{k_{n+1}}$$

$$S^0 = -P, \quad S^k = \left(\frac{Q}{E_0 - Q H_0 Q} \right)^k$$

Higher order II

$$H_{eff}^{(n)} = \sum_{k_1+...+k_{n-1}=n-1, k_i \geq 0} f(k_1, k_2, ..., k_{n-1}) V S^{k_1} V S^{k_2} V ... S^{k_{n-1}} V$$

The true eigenstates are related to the eigenstates of H_{eff} by:

$$|\psi\rangle = \Gamma|\phi\rangle$$

Likewise, the observables transform according to:

$$O \rightarrow \Gamma^\dagger O \Gamma$$

Standard example: superexchange

Hubbard model

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

$$H_0 = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

½-filling → 1 e^-/ site

$$V = -t \sum_{\langle i,j \rangle,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.$$

2nd order perturbation

Heisenberg model

$$H_{\text{eff}} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j, \qquad J = \frac{4t^2}{U}$$

One triangle

$$H = J(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1) = \frac{J}{2}\left[(\vec{S}_1 + \vec{S}_2 + \vec{S}_3)^2 - \vec{S}_1^2 - \vec{S}_2^2 - \vec{S}_3^2\right]$$

$$\vec{S}_i^2 = 3/4 \quad \Longrightarrow \quad H = \frac{J}{2}\left[(\vec{S}_{\rm tot})^2 - \frac{9}{4}\right]$$

$$\frac{1}{2} \otimes (\frac{1}{2} \otimes \frac{1}{2}) = \frac{1}{2} \otimes (0 \oplus 1) = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{3}{2}$$

$$P|\sigma_1\ \sigma_2\ \sigma_3\ \rangle = |\sigma_3\ \sigma_1\ \sigma_2\ \rangle, \quad [P, H] = 0, \quad P^3 = 1 \rightarrow \text{eigenvalues} : 1,\ e^{\frac{2i\pi}{3}},\ e^{\frac{-2i\pi}{3}}$$

$$|L\uparrow\rangle = \frac{1}{\sqrt{3}}\Big(|\uparrow\uparrow\downarrow\rangle + e^{\frac{2i\pi}{3}}|\uparrow\downarrow\uparrow\rangle + e^{\frac{-2i\pi}{3}}|\downarrow\uparrow\uparrow\rangle\Big)$$

$$|L\downarrow\rangle = \frac{1}{\sqrt{3}}\Big(|\downarrow\downarrow\uparrow\rangle + e^{\frac{2i\pi}{3}}|\downarrow\uparrow\downarrow\rangle + e^{\frac{-2i\pi}{3}}|\uparrow\downarrow\downarrow\rangle\Big)$$

$$|R\uparrow\rangle = \frac{1}{\sqrt{3}}\Big(|\uparrow\uparrow\downarrow\rangle + e^{\frac{-2i\pi}{3}}|\uparrow\downarrow\uparrow\rangle + e^{\frac{2i\pi}{3}}|\downarrow\uparrow\uparrow\rangle\Big)$$

$$|R\downarrow\rangle = \frac{1}{\sqrt{3}}\Big(|\downarrow\downarrow\uparrow\rangle + e^{\frac{-2i\pi}{3}}|\downarrow\uparrow\downarrow\rangle + e^{\frac{2i\pi}{3}}|\uparrow\downarrow\downarrow\rangle\Big)$$

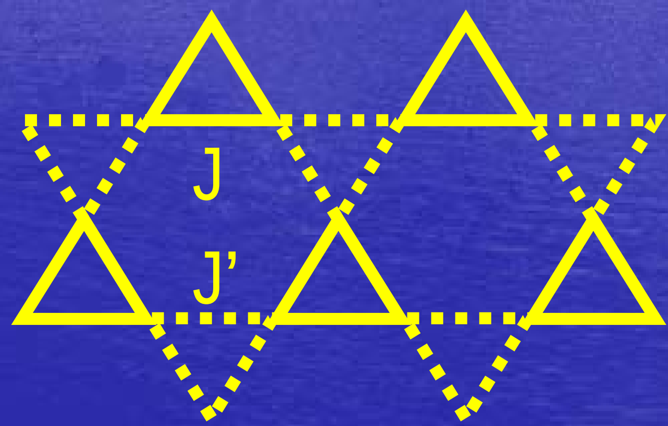
Coupled triangles

Pseudo-spin
'chirality'

$$\tau^z|L\sigma\rangle = -\frac{1}{2}|L\sigma\rangle, \quad \tau^z|R\sigma\rangle = \frac{1}{2}|R\sigma\rangle, \quad \tau^+|L\sigma\rangle = |R\sigma\rangle, \ldots$$

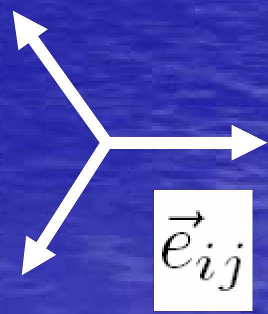
Spin

$\vec{\sigma}$: acts on the spin



First-order perturbation in J'

$$H_{\text{eff}} = \frac{J'}{9}\sum_{\langle ij\rangle}{}' \vec{\sigma}_i \cdot \vec{\sigma}_j (1 - 4\vec{e}_{ij}\cdot\vec{\tau}_i)(1 - 4\vec{e}_{ij}\cdot\vec{\tau}_j)$$

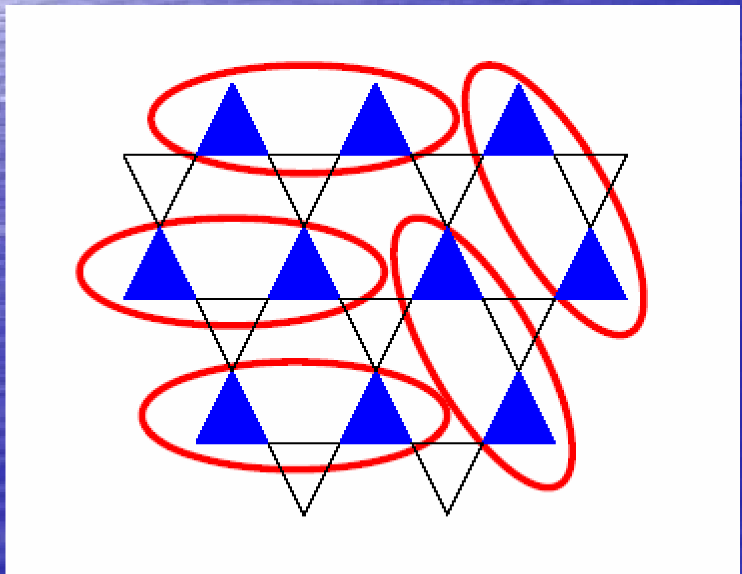


Triangular lattice

Spin-chirality mean-field decoupling

Relevant degrees of freedom selected

⇒ Reasonable to use mean-field



Degenerate GS

⇕

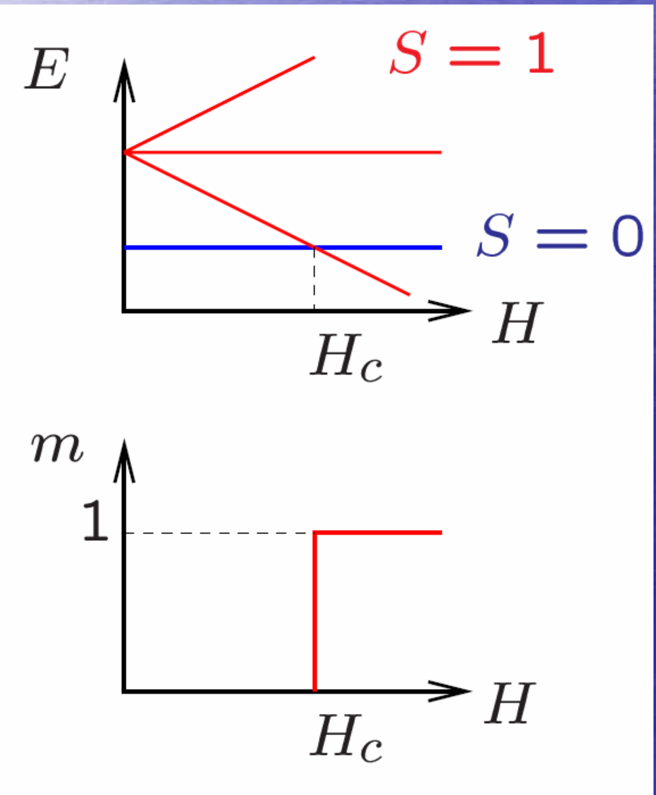
Dimer coverings of triangular lattice

Other examples

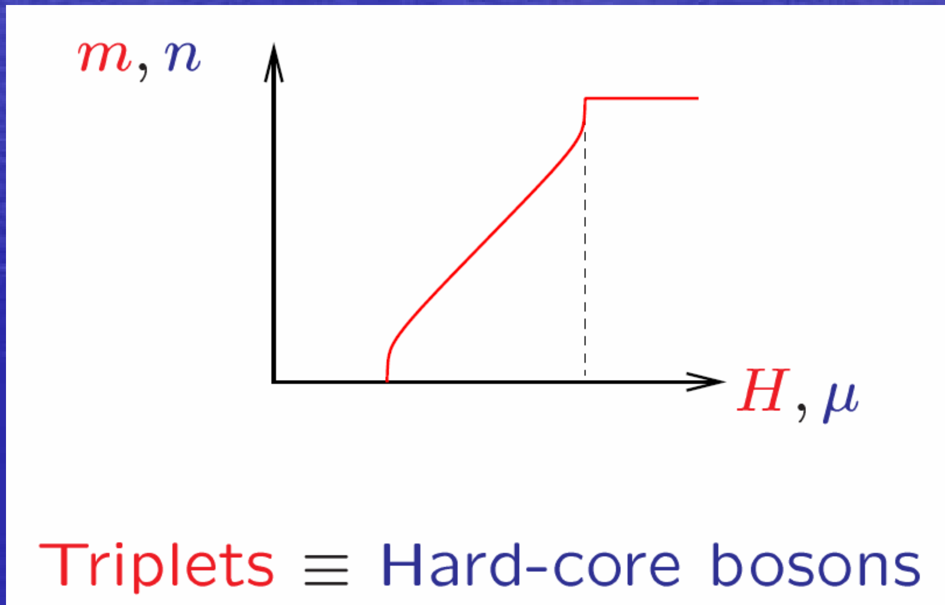
- Tetrahedra: GS is a two-fold degenerate singlet → pure ‘chirality’ effective model
- Odd rings: like for a triangle, GS consists of two doublets → spin-chirality model
- Units with non-degenerate singlet GS in a magnetic field → singlet degenerate with lowest triplet at critical field

Dimers in a magnetic field

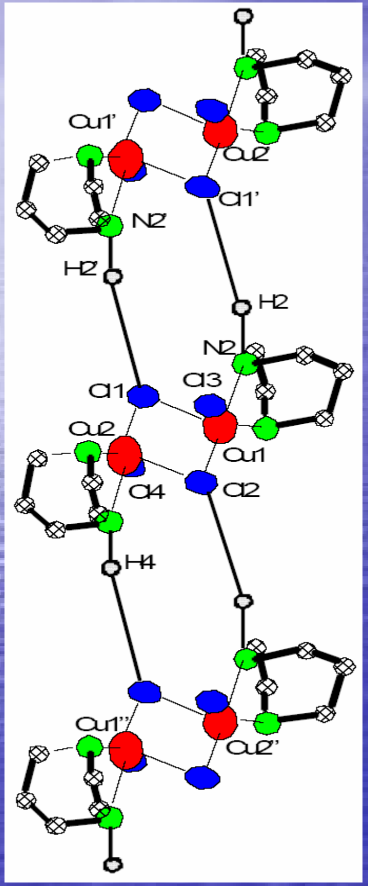
Isolated dimers



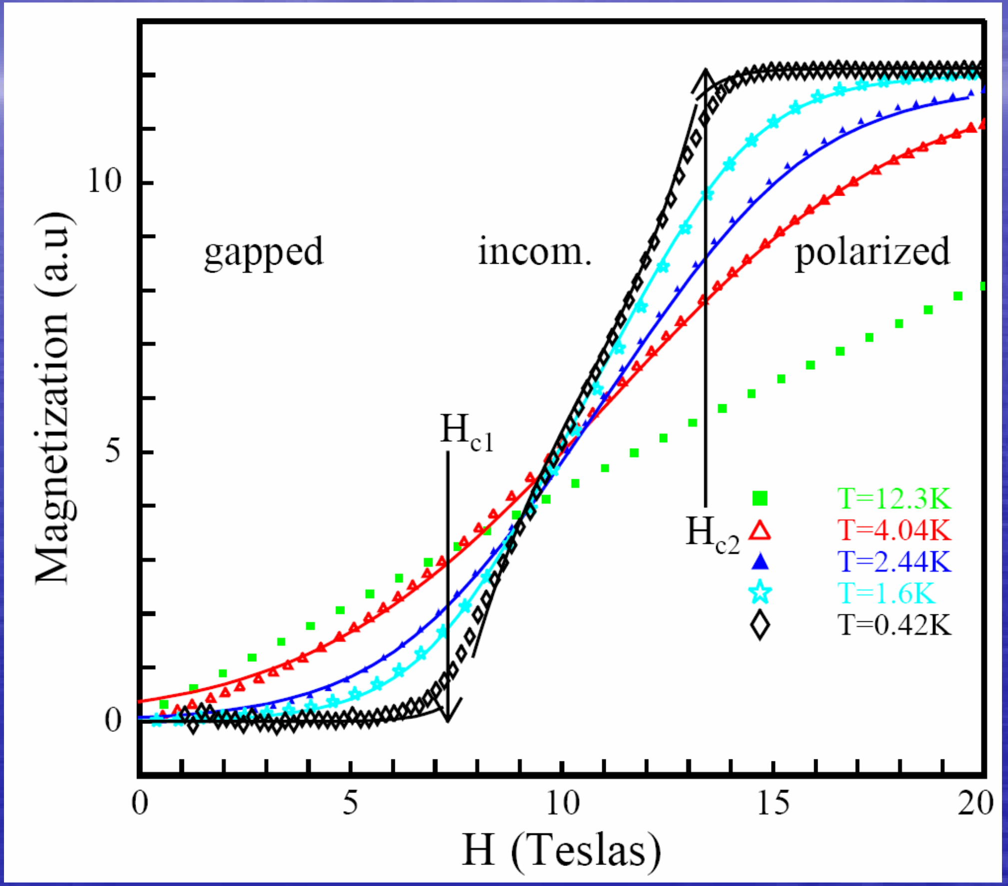
Coupled dimers



Magnetization of spin ladders



CuHpCl

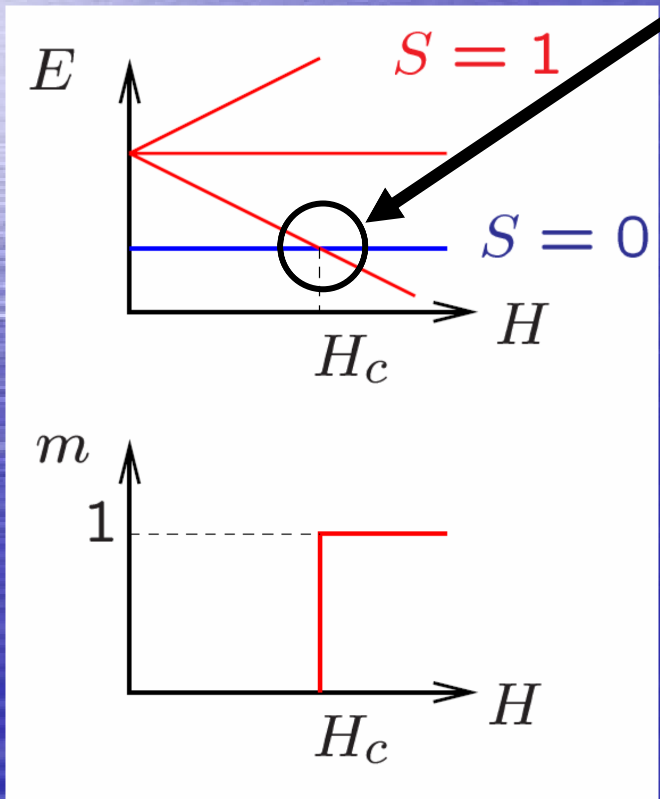


Chaboussant et al, EPJB '98

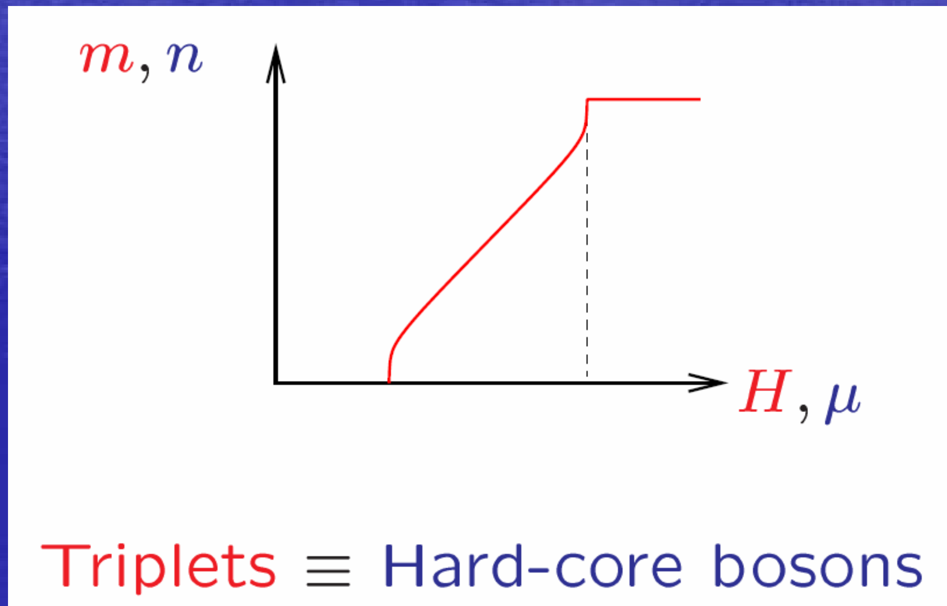
Dimers in a magnetic field

2 states/rung → degenerate GS

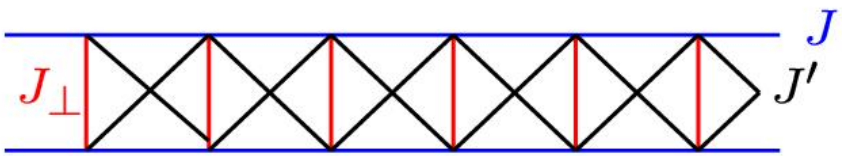
Isolated dimers



Coupled dimers



Frustrated ladders



Close to H_c, $J_\perp \gg J, J'$

Two states/rung: $S=0 \leftrightarrow \sigma^z = |\uparrow\rangle$ $\quad S_z = 1 \leftrightarrow \sigma^z = |\downarrow\rangle$

$$\mathcal{H}_{\text{eff}} = J^{xy}_{\text{eff}} \sum_i (\sigma^x_i \sigma^x_{i+1} + \sigma^y_i \sigma^y_{i+1}) + J^z_{\text{eff}} \sum_i \sigma^z_i \sigma^z_{i+1} - H^{\text{eff}} \sum_i \sigma^z_i$$

$$J^{xy}_{\text{eff}} = J - J' \qquad J^z_{\text{eff}} = \frac{J+J'}{2} \qquad H^{\text{eff}} = H - H_c - \frac{J+J'}{2}$$

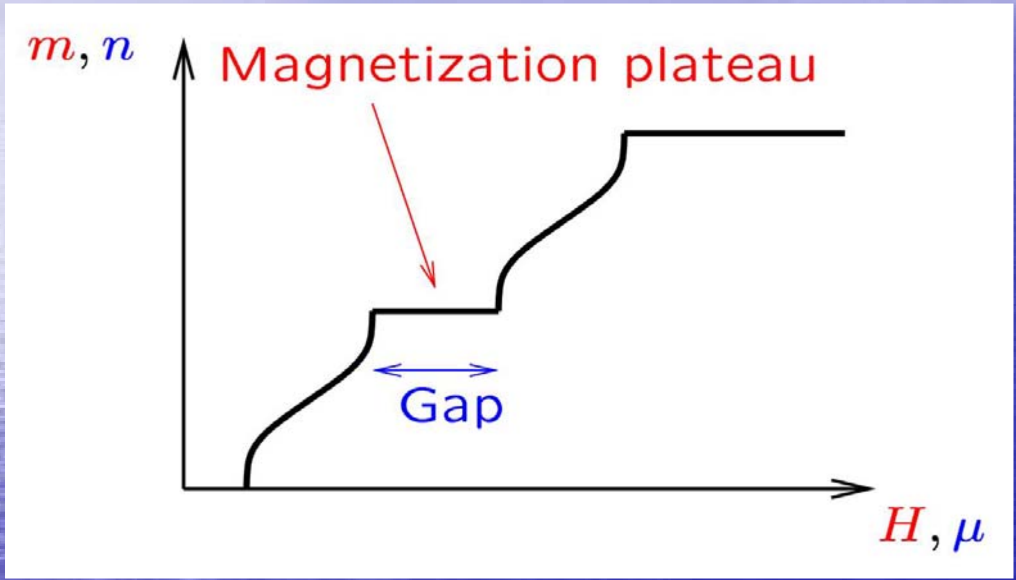
Jordan-Wigner transformation

$$\mathcal{H}_{\text{eff}} = t \sum_i (c^\dagger_i c_{i+1} + \text{h.c.}) + V \sum_i n_i n_{i+1} - \mu \sum_i n_i$$

$$t = \frac{J-J'}{2} \qquad V = \frac{J+J'}{2} \qquad \mu = H - H_c$$

Metal-insulator transition for V=2t (J'=J/3)

Magnetization Plateau



D. Cabra et al, PRL '97
K. Totsuka, PRB '98
T. Tonegawa et al, PRB '99
F. Mila, EPJB '98

Kinetic energy

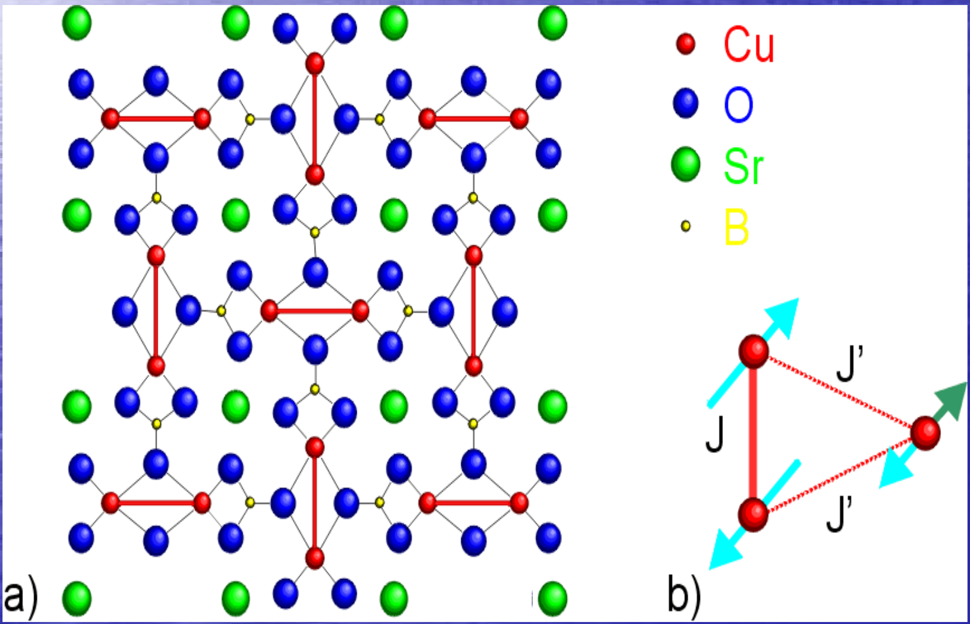
Frustration → Repulsion →

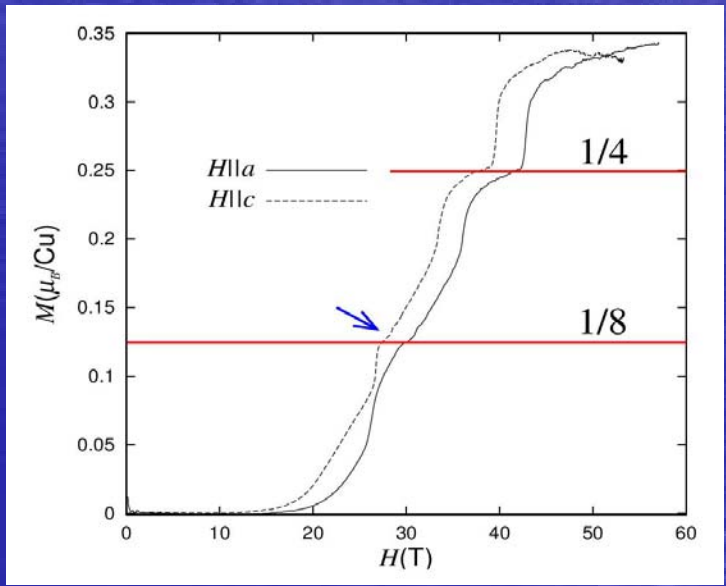
Metal-insulator transition

Magnetization plateau

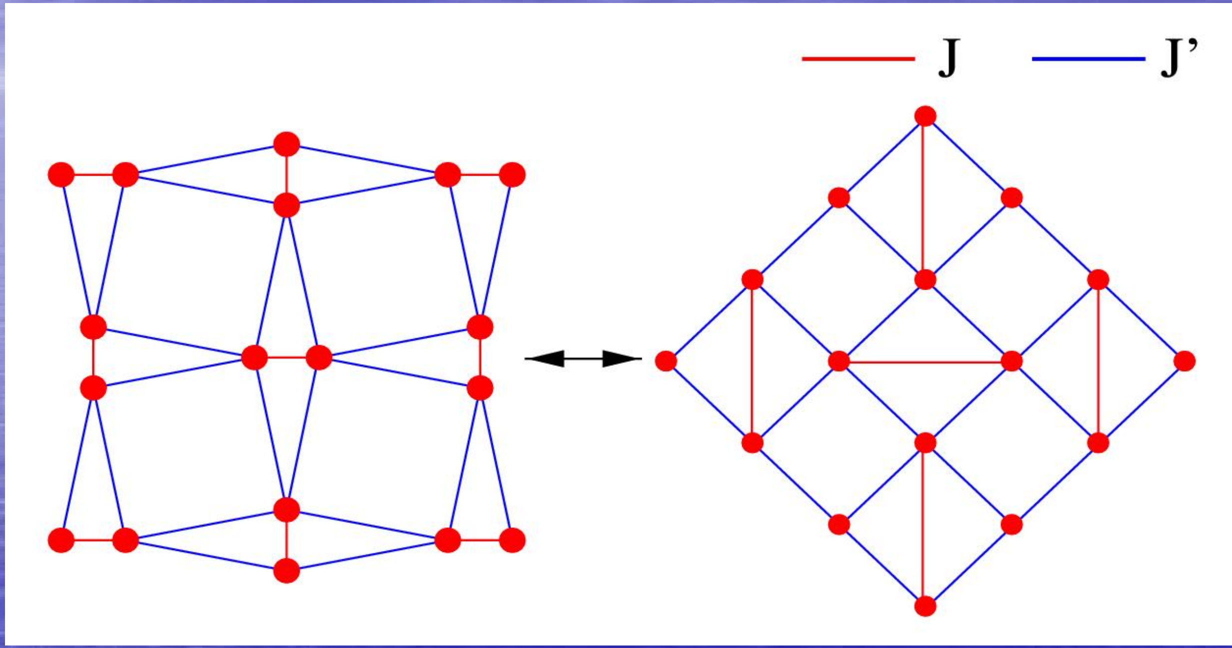
Magnetization of $SrCu_2(BO_3)_2$

Kageyama et al, PRL '99





Shastry-Sutherland model



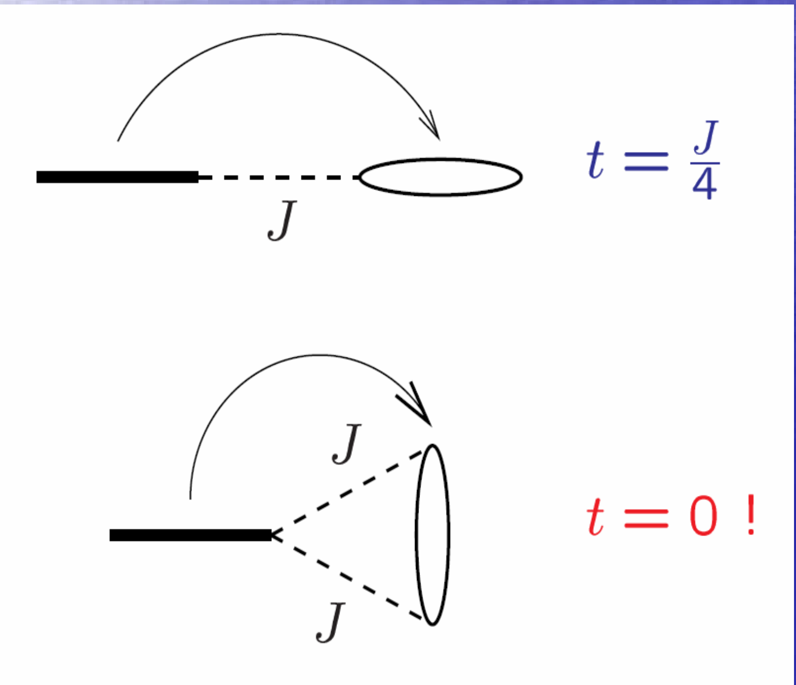
Ground-state Product of singlets on J-bonds (Shastry, Sutherland, '81)

Triplets Almost immobile and repulsive (Miyahara et al, '99)

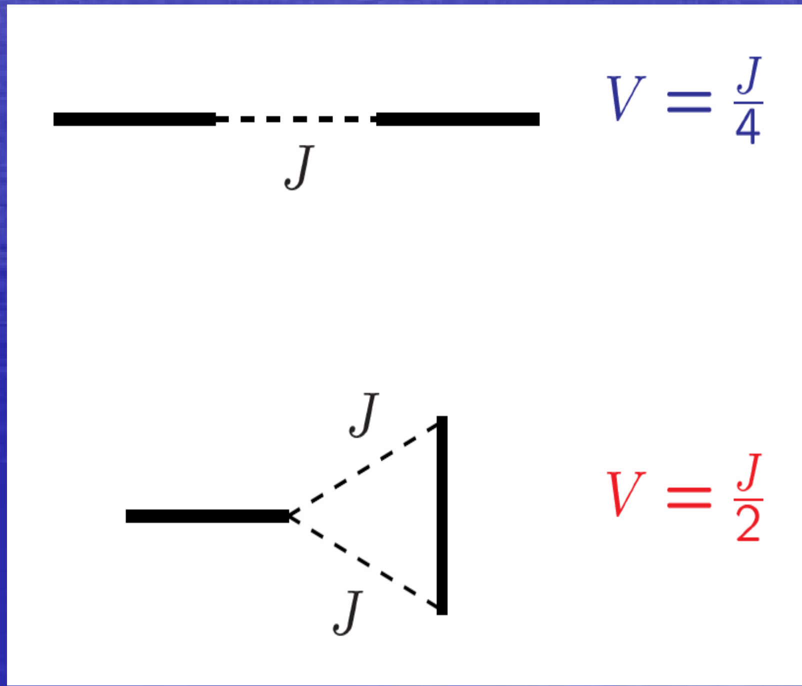
→ **Plateaux** (Miyahara et al, '00)

Frustrated Coupled Dimers

Triplet Hopping



Triplet Repulsion

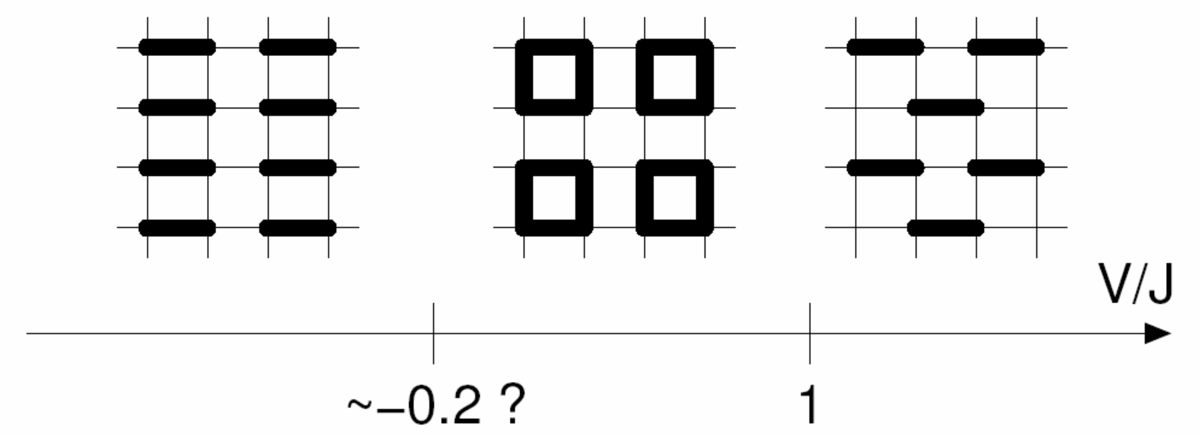


Quantum Dimer Models

Square lattice (Rokhsar-Kivelson, ’88)

$$\mathcal{H} = \sum_{\text{Plaquette}} \left[-J \left(\left|\, \|\,\| \,\right\rangle \left\langle \,=\, \right| + \text{H.c.} \right) + V \left(\left|\, \|\,\| \,\right\rangle \left\langle \, \|\,\| \,\right| + \left|\, = \,\right\rangle \left\langle \, = \,\right| \right) \right]$$

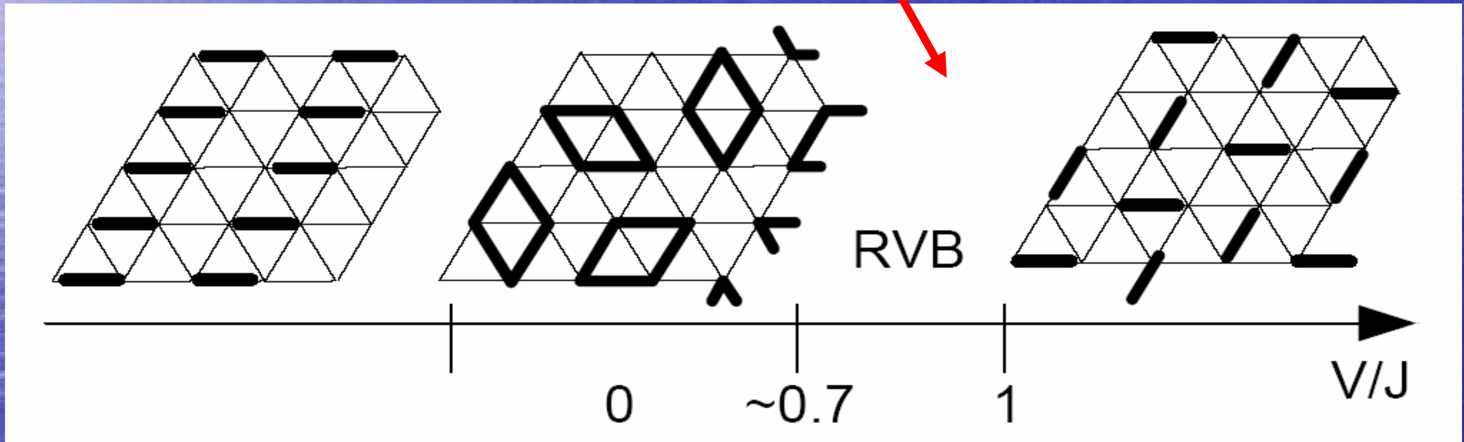
Assume dimer configurations are orthogonal



RK ’88
Leung et al, ‘96

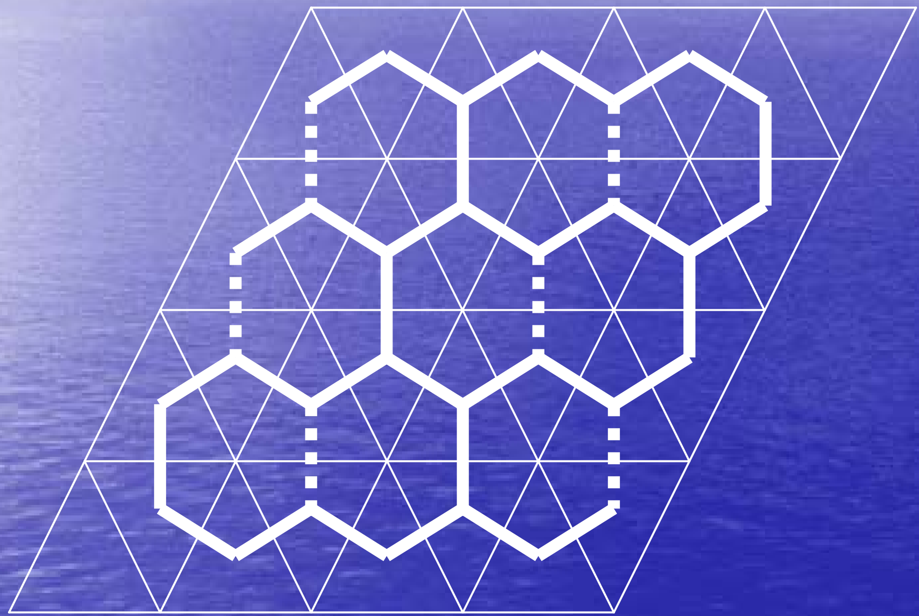
QDM on triangular lattice

Spin liquid with gapped spectrum and topological degeneracy



Equivalent spin model? Yes! The QDM is the effective model of an Ising model in transverse field

Fully Frustrated Ising model

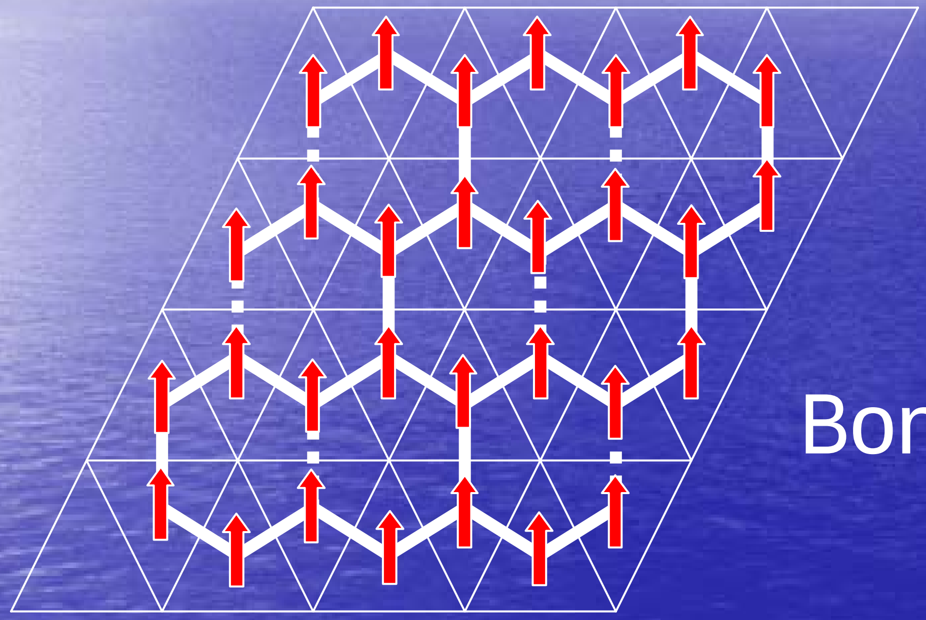


$$H = \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j$$

$J_{ij} = J > 0$ on dashed lines, $J_{ij} = -J < 0$ on solid lines

Ground states: 1 unsatisfied bond/hexagon

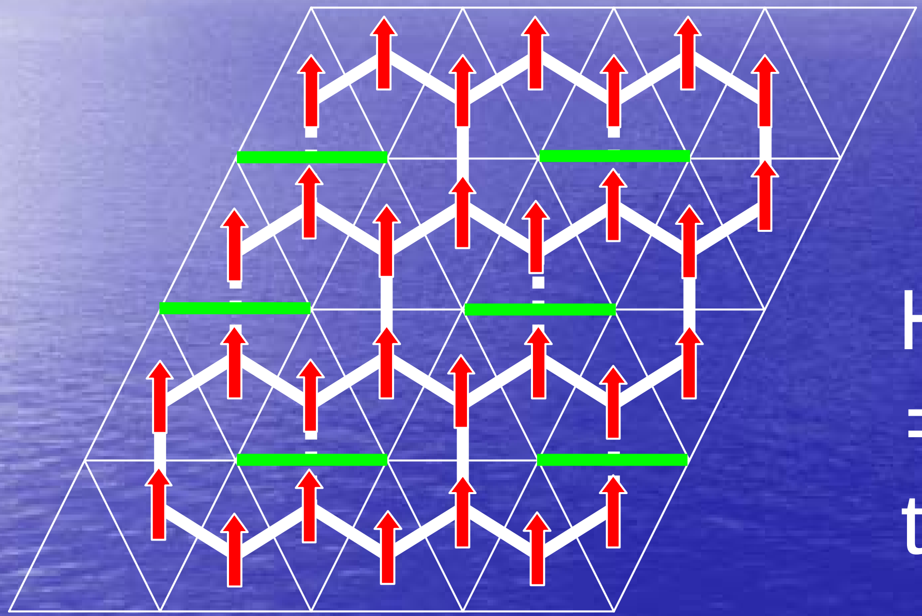
Example of a ground state



Bond unsatisfied if J>0

For that ground state, unsatisfied bonds lie on dashed lines

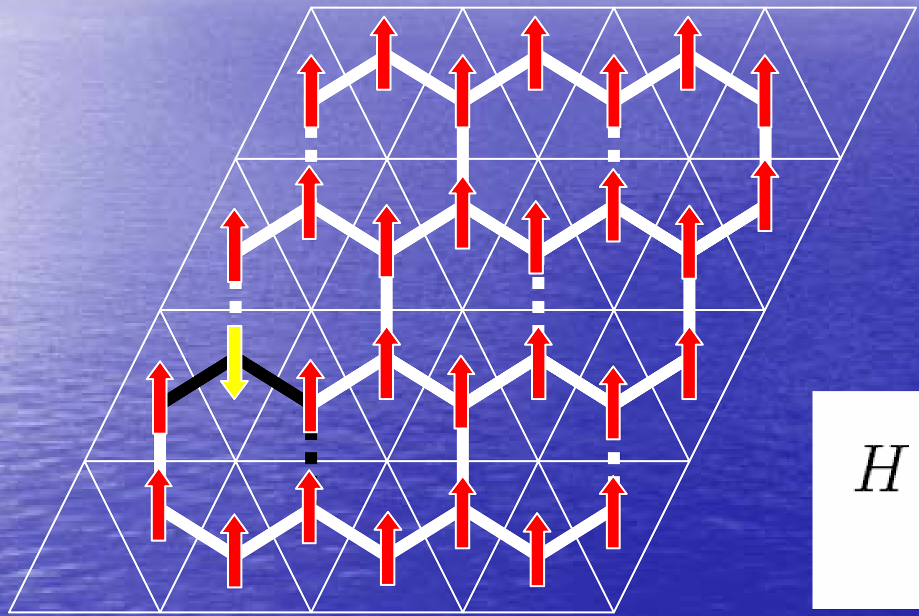
Mapping onto QDM Hilbert space



Hexagonal lattice = dual lattice of triangular lattice

Draw a bond on the triangular lattice across all unsatisfied bonds → dimer covering

Add a transverse field



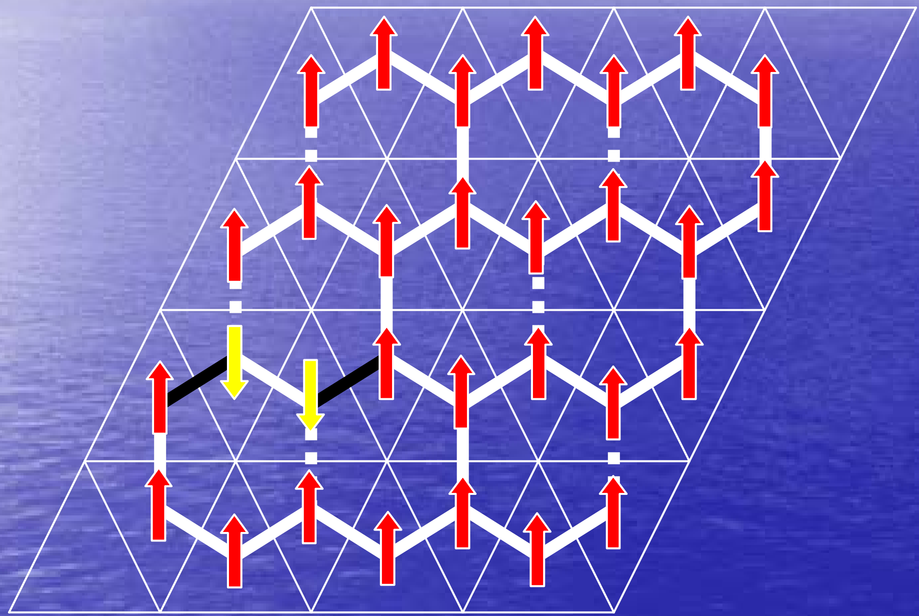
$\vec{\sigma}_i$: Pauli matrices

$$\sigma_i^x = \sigma_i^+ + \sigma_i^-$$

$$H = \sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x$$

One spin flip → outside ground state manifold

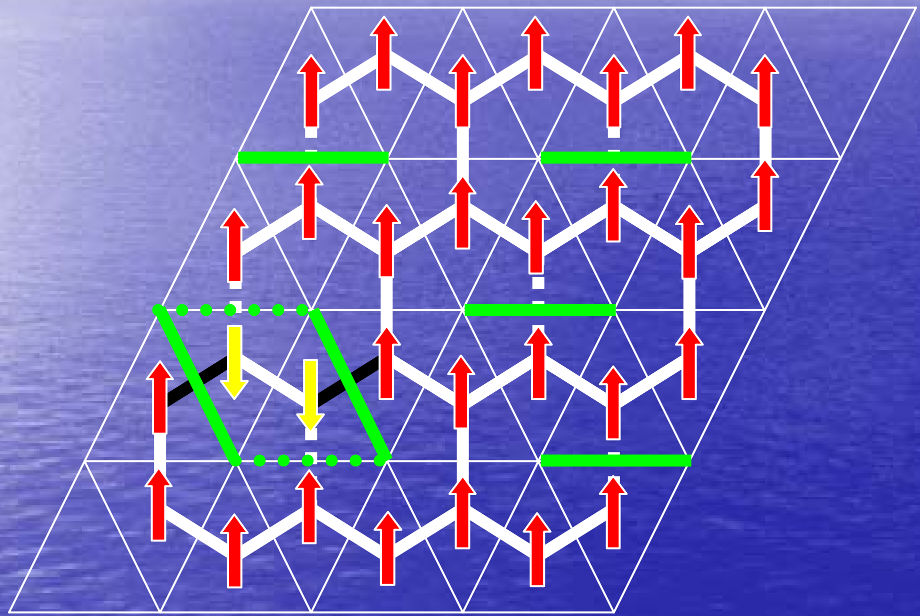
Two spin flips



Flip two spins
on neighboring
unsatisfied bonds

Stay in ground state manifold

In terms of dimers



Flip dimers around flippable plaquette

2^{nd} order perturbation theory in Γ_x

Ising model , QDM with flip term / Γ_x^2/J

Alternative I : Canonical Transformation

$$e^{iS}\hat{H}e^{-iS} \quad = \quad \hat{H} + i[S,\hat{H}] + \frac{i^2}{2!}[S,[S,\hat{H}]] + \cdots$$

Put $H = H_0 + \lambda V$. If there is an operator S such that $i[S, H_0] = -\lambda V$, then:

$$e^{iS}He^{-iS} = H_0 + \lambda^2 H^{(2)} + \lambda^3 H^{(3)} + \ldots$$

Advantages

- Possible for non degenerate GS
- Systematic expansion
- Gives access to full spectrum

Drawbacks

- Not universal: needs to find S
- Necessary condition: all linear corrections must vanish

Standard example: Hubbard → Heisenberg

Alternative II: CORE

CORE: Contractor Renormalization

1) Find numerically low-energy spectrum of largest accessible system
2) Fit it numerically with effective Hamiltonian of smaller sub-units

Advantages

- Very flexible
- Universal
- Best effective model from quantitative point of view

Drawbacks

- Not well suited for analytical treatment of effective model
- Physics of effective model not transparent

Conclusions

- Effective Hamiltonian: often a good way to understand physics at a qualitative level
- If natural small parameter, THE method to be recommended
- Several ways of deriving an effective Hamiltonian. Degenerate perturbation theory very simple and recommended if first or second order sufficient