Title: S=1 spin liquid with fermionic excitations

Date: Mar 28, 2013 02:30 PM

URL: http://www.pirsa.org/13030113

Abstract: In the first part of my talk I describe a search for possible quantum spin liquid ground states for spin S=1 Heisenberg models on the triangular lattice which was motivated by recent experiments on Ba3NiSb2O9. We use representation of spin-1 via three flavors of fermionic spinon operators. The ground state where one gapless flavor of spinons with a Fermi surface coexists with d+id topological pairing of the two other flavors can explain available experimental data. Despite the existence of a Fermi surface, this spin liquid state has fully gapped bulk spin excitations. This results in a linear in-temperature specific heat and constant in-plane spin susceptibility, with an unusually high Wilson ratio. Using variational Monte Carlo technique, we show that proposed spin liquid ground state is realized in an SU(3)-invariant model with sufficiently strong ring-exchange terms.

In the second part, I consider the physics of the magnetic s=1/2 impurity embedded in a S=1 spin liquid, where all three flavors of spinons have a Fermi surface. The interplay between non-Fermi-liquid behavior induced by a U(1) gauge field coupled to fermions, and a non-Fermi-liquid fixed point in the overscreened Kondo problem is studied using double expansion. The gauge field changes the physical properties of the system at the overscreened Kondo fixed point. Thus, spin-half impurity in such spin liquid can be used to probe the presence of fermionic spinons coupled to the gauge field.

References: arXiv:1108.3070, arXiv:1208.3231 and arXiv:1212.5179

S=1 spin liquid with fermionic excitations

Maksym Serbyn

Massachusetts Institute of Technology, USA

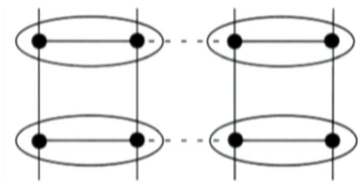
M.S., T. Senthil, P.A. Lee, PRB 84 (2011)
S. Bieri, M.S., T. Senthil, P.A. Lee, PRB 86 (2012)
M.S., T. Senthil, P.A. Lee, arXiv:1212.5179

Outline

- Introduction: possible realization of $S=1$ spin liquid
- Fermionic $S=1$ spin liquid on triangular lattice
  - ✳ Mean field approach and physical properties
  - ✳ Gutzwiller projection: variational Monte Carlo
- Kondo impurity as a probe of $S=1$ spin liquid
- Summary

Spin liquid

- No symmetry breaking; long range entanglement $\rightarrow$ fractionalized excitations, emergent gauge fields
- Realized in one dimension. RVB state in $d=2$

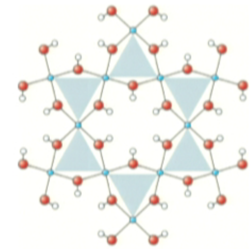


(Anderson'73)

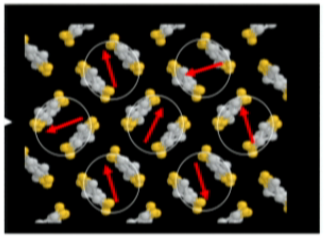
- A number of $S=1/2$ spin liquid candidates in $d=2$
  Rare when $S>1/2$ or $d>2$
- This talk: $S = 1$ spin liquid in two dimensions

Spin liquid candidates

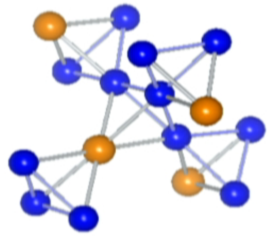
- Spin-1/2 materials:



  - ✶ herbersmithite (kagome lattice)



  - ✶ organics (triangular lattice)

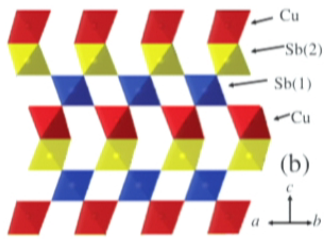


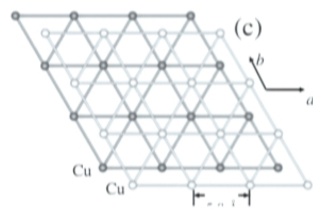
  - ✶ $Na_4Ir_3O_8$ (hyperkagome), $d=3$

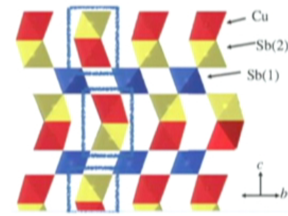
New candidate materials

- Spin-1/2 $Ba_3CuSb_2O_9$ (Zhou *et.al*. PRL'11)

  (Nakatsuji *et.al*. Science'12)



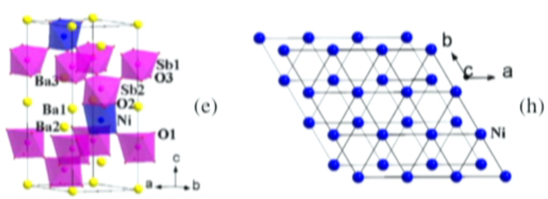


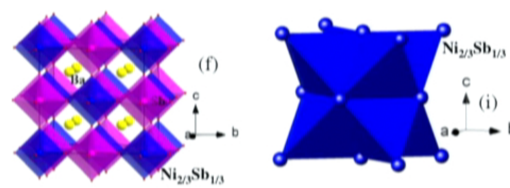


- Spin-1 $Ba_3NiSb_2O_9$ (Cheng *et.al*. PRL'11)

  6H-B phase

  6H-C phase





6H-B phase of $Ba_3NiSb_2O_9$

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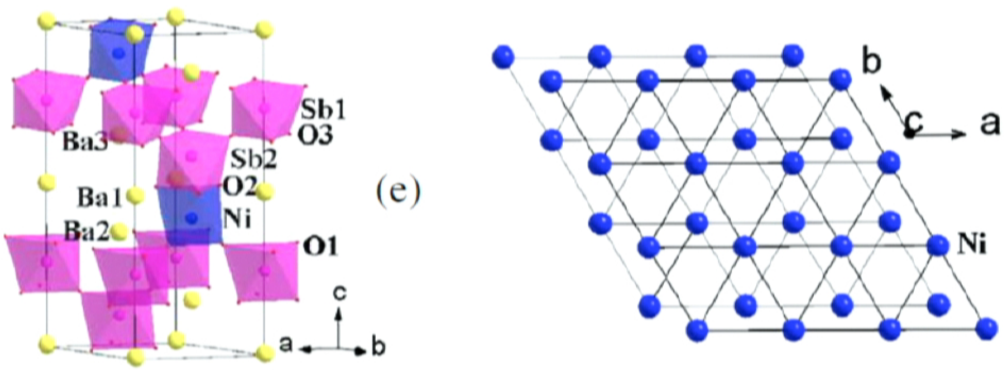
- Triangular lattice of $S = 1$ Ni^{2+} ions
- No magnetic order to T = 350 mK, but θ_{CW} = -75 K



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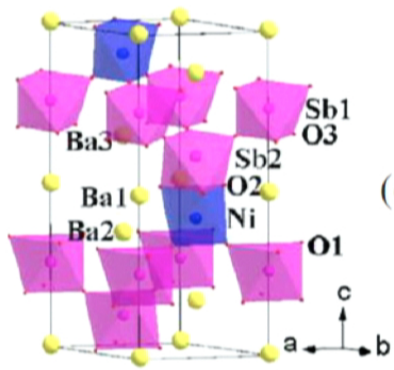

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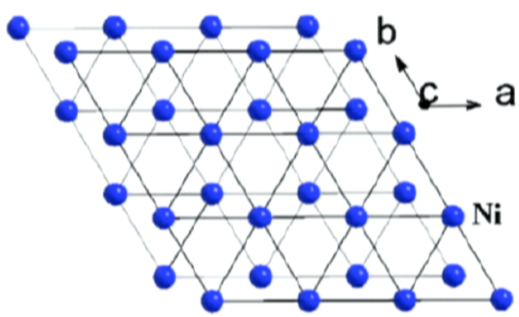

Spin liquid behavior in 6H-B phase

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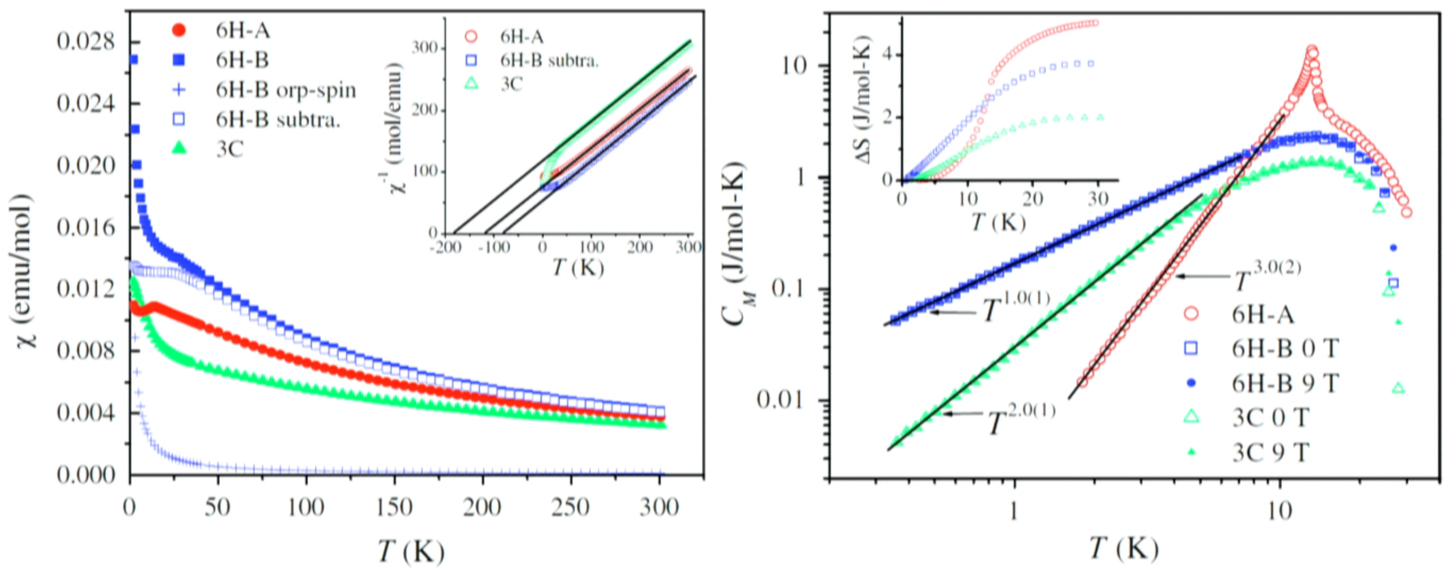
- Constant spin susceptibility as $T \to 0$
- Linear in T specific heat, Wilson's ratio $R_W = 5.6$



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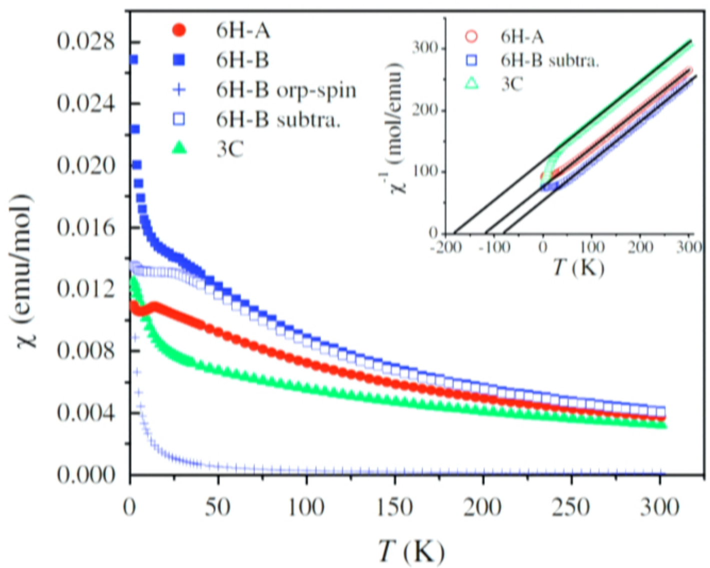

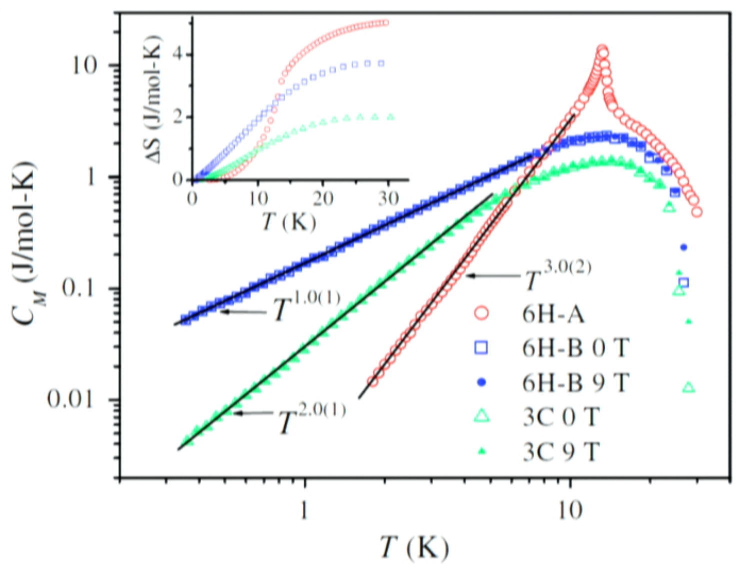

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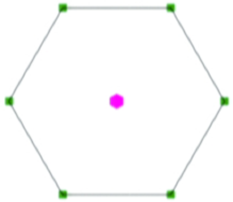

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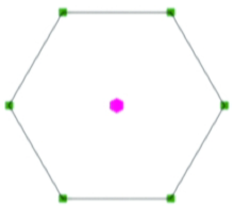

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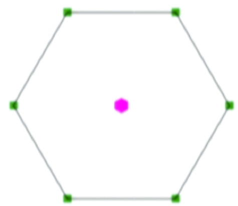

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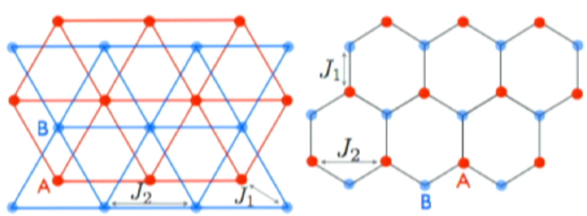
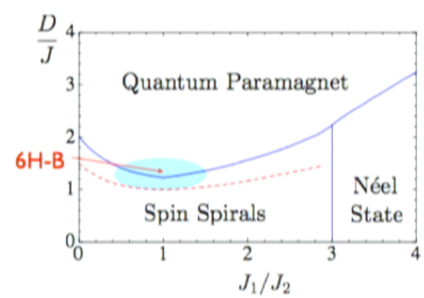
  - ✶ Proximity to quantum critical (Chen *et.al*.,PRL'12)





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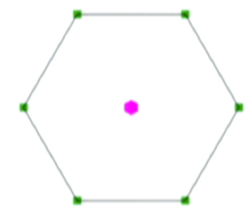

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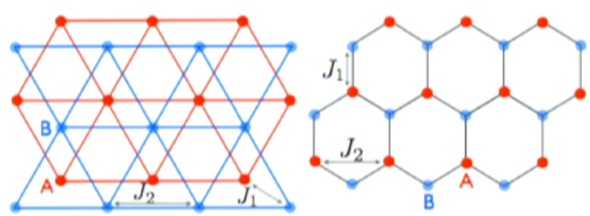

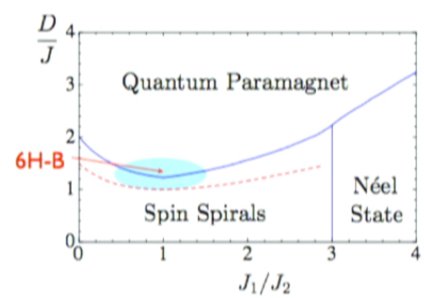

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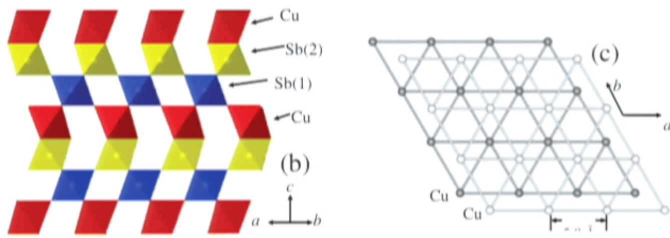

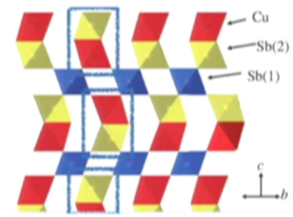

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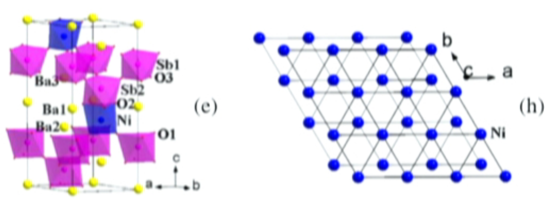
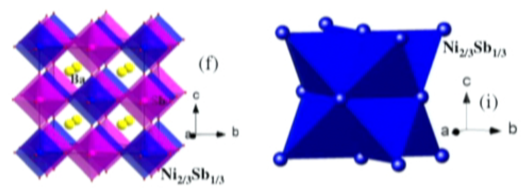


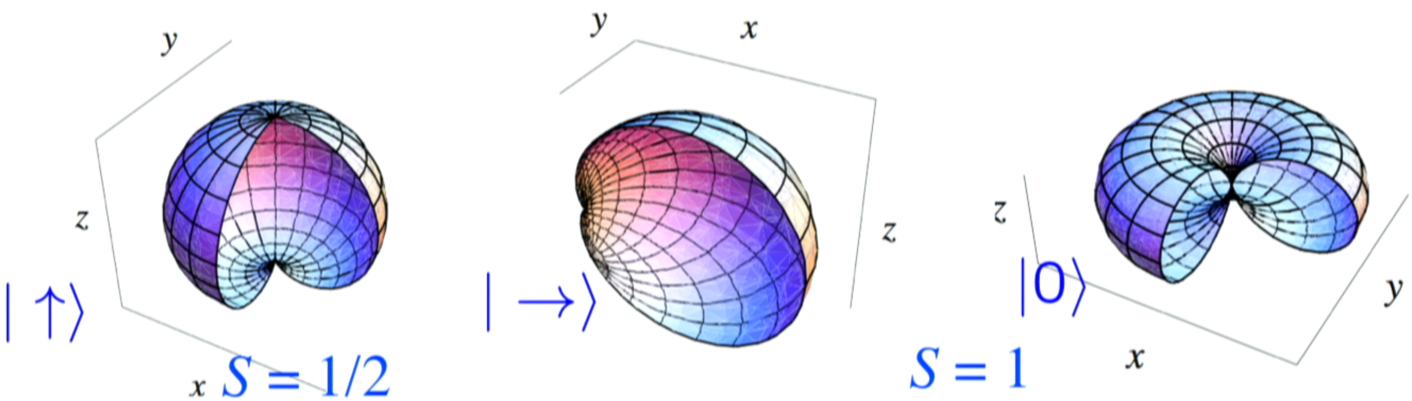


Spin-1 vs Spin-1/2

- $S = 1/2$: any state is a spin-coherent state $|\mathbf{n}\rangle$

$$(\mathbf{n}\cdot\mathbf{S})|\mathbf{n}\rangle = S|\mathbf{n}\rangle, \quad |\mathbf{n}\rangle = \cos\frac{\theta}{2}e^{-i\phi/2}|\uparrow\rangle + \sin\frac{\theta}{2}e^{i\phi/2}|\downarrow\rangle$$

- $S = 1$: 4 parameters, *superposition* of coherent states
  $\rightarrow$ coexisting *spin* and *quadrupolar* order

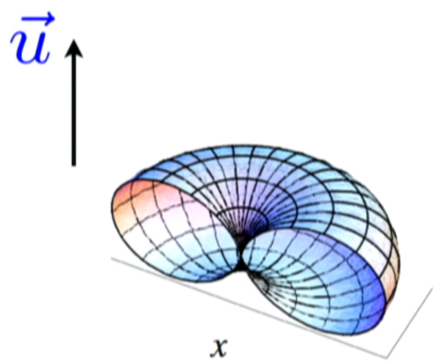


Basis for spin-1

- Change basis from conventional to:

$$|x\rangle = \frac{i(|1\rangle - |-1\rangle)}{\sqrt{2}}, \quad |y\rangle = \frac{|1\rangle + |-1\rangle}{\sqrt{2}}, \quad |z\rangle = -i|0\rangle$$

$$|\vec{d}\rangle = \sum_{\alpha=x,y,z} d_\alpha \, |\alpha\rangle, \quad \vec{d} = \vec{u} + i\vec{v}, \quad \begin{array}{c} \vec{u} \perp \vec{v} = 0 \\ \vec{u}^2 + \vec{v}^2 = 1 \end{array}$$



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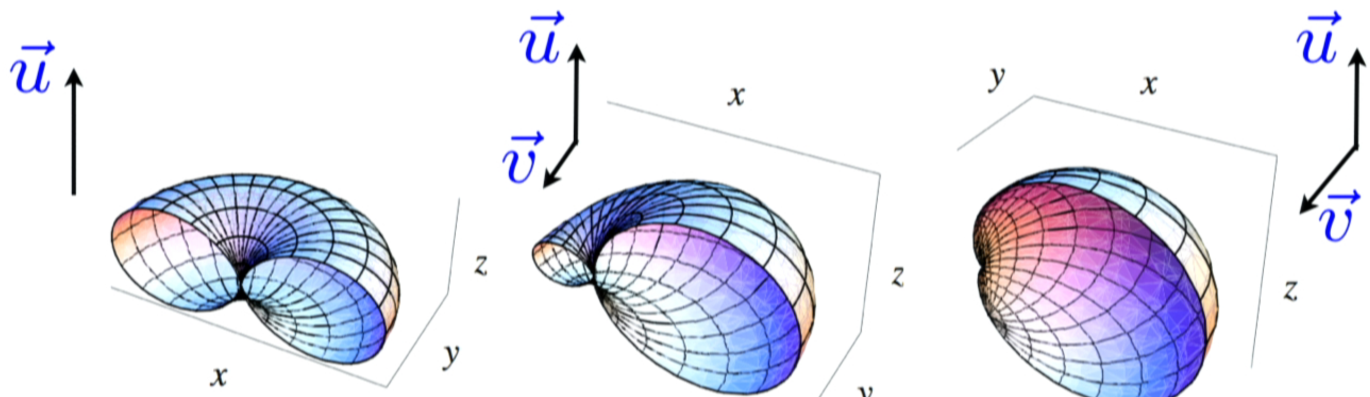

$S_z = 0$ $\quad \langle S_x \rangle = 1/2$ $\quad S_x = 1$

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Fermionic spinons

- Three spinons $\vec{f}=(f_x, f_y, f_z)$ to represent spin

$$\vec{S}_i = -i\vec{f}_i^\dagger \times \vec{f}_i, \qquad \vec{f}_i^\dagger \cdot \vec{f}_i = 1.$$

- Local $U(1)\times Z_2$ symmetry in spin representation

$$f_i \to e^{i\phi} f_i, \qquad f_i \to f_i^\dagger$$

- Mean field decoupling $\rightarrow$ quadratic Hamiltonian with $U(1)\times Z_2$ gauge field

$$H = \sum_{\langle ij\rangle}[J\vec{S}_i \cdot \vec{S}_j + K(\vec{S}_i \cdot \vec{S}_j)^2] + D\sum_i (S_i^z)^2$$

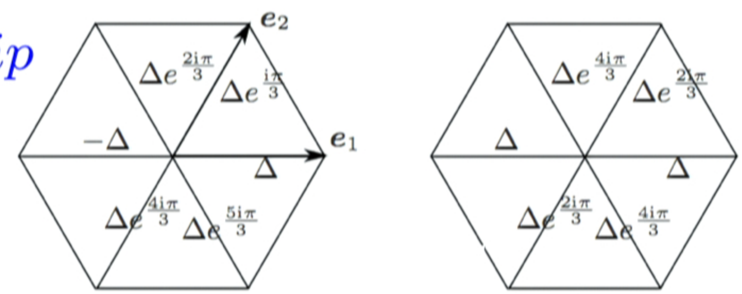
Mean field approach

- Hopping and pairing of fermions:

$$H = \sum_{i,j} [\chi_{ij} f^\dagger_{i\alpha} f_{j\alpha} + \Delta^{\alpha\beta}_{ij} f^\dagger_{i\alpha} f^\dagger_{j\beta} + \text{h.c.} + \ldots]$$

$\chi^\alpha = \langle f^\dagger_{i\alpha} f_{j\alpha} \rangle$ and $\begin{bmatrix} \Delta^{xy} = \langle f_{ix} f_{jy} \rangle & s, d\text{–wave} \\ \Delta^{\alpha} = \langle f_{i\alpha} f_{j\alpha} \rangle & p, f\text{–wave} \end{bmatrix}$

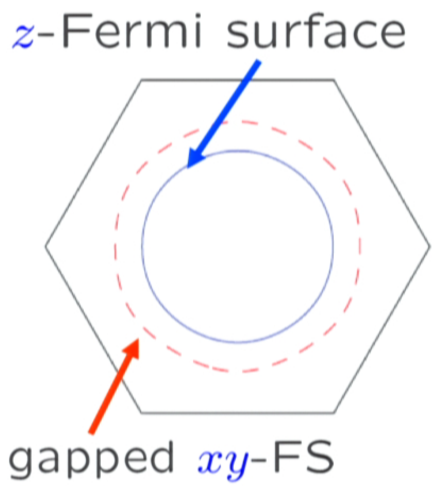
$p + ip$



$d + id$

Pairing and Fermi surface together

- State with pairing $\Delta^{xy} = \langle f_x f_y \rangle$
- f_x and f_y are gapped $\rightarrow$ gauge field is massive
  f_z particles have Fermi surface
- Realized at the mean field level with $d+id$ pairing



Physical properties

- Gapless f_z particles with Fermi surface result in
  - ✶ linear in T specific heat
  - ✶ anisotropic spin susceptibility $\chi_{zz} = 0$, $\chi_{xx} = \chi_{yy} = const$
  - ✶ Wilson ratio $R_W \simeq 2.6 \div 5.3$ for $D \gtrsim \Delta$
  - ✶ exponentially small NMR relaxation rate $1/T_1 T$
- $d+id$ pairing: $\mathcal{T}$-reversal symmetry breaking, chiral order parameter, pair of edge modes

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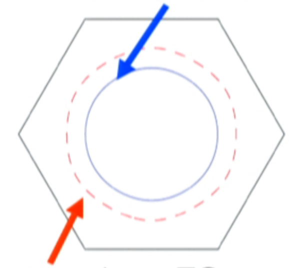
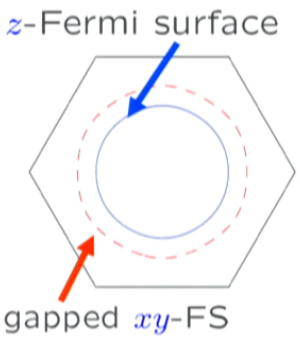
Variational Monte Carlo

- Mean field: spin liquid state for $S=1$



Variational Monte Carlo

- Mean field: spin liquid state for $S=1$
- Q: Spin model, realizing this state?



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Spin liquid variational states

- Ground state of quadratic trial Hamiltonian

$$H = \sum_{i,j} [f^\dagger_{i\alpha} f_{j\alpha} + \Delta^{\alpha\beta}_{ij} f_{i\alpha} f_{j\beta} + \text{h.c.}] - \mu_\alpha n_\alpha$$

- Gutzwiller projection → spin wave function

$$|\psi\rangle = \mathcal{P}(n_j = 1)|\psi_0\rangle$$

- RVB states not breaking any lattice symmetries
  - ✶ U(1) state: $\Delta^{\alpha\beta} = 0$
  - ✶ odd pairing: $\Delta^{xx} = \Delta^{yy}, \Delta^{zz}$ (f-wave, $p+ip$-wave)
  - ✶ even pairing: Δ^{xy} (s-wave, $d+id$-wave)

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Bilinear-biquadratic model

- Energies at D = -0.4: ordered state wins

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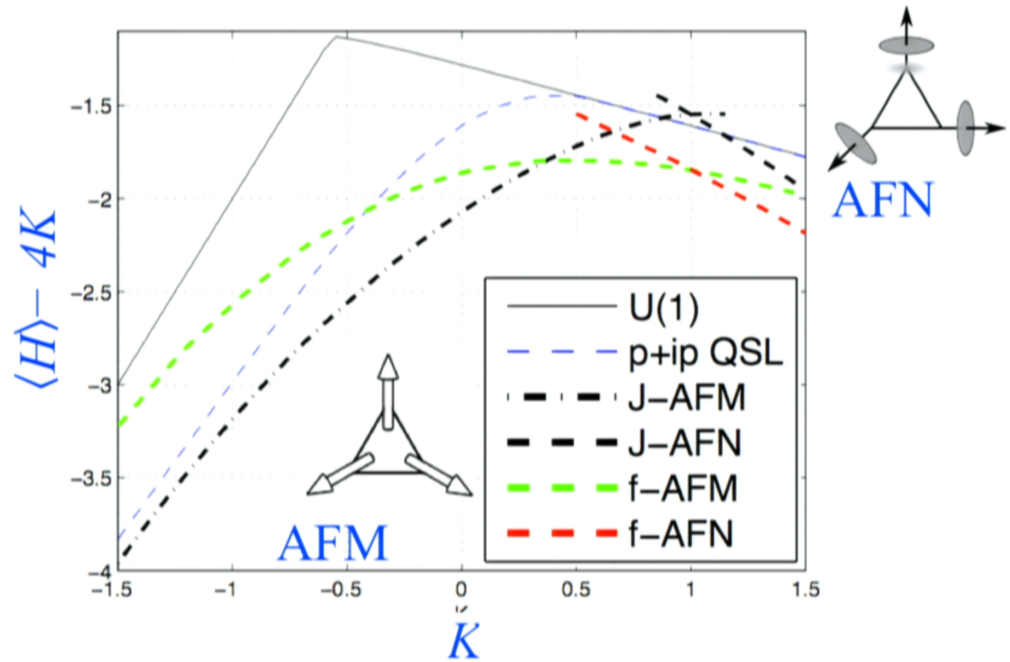

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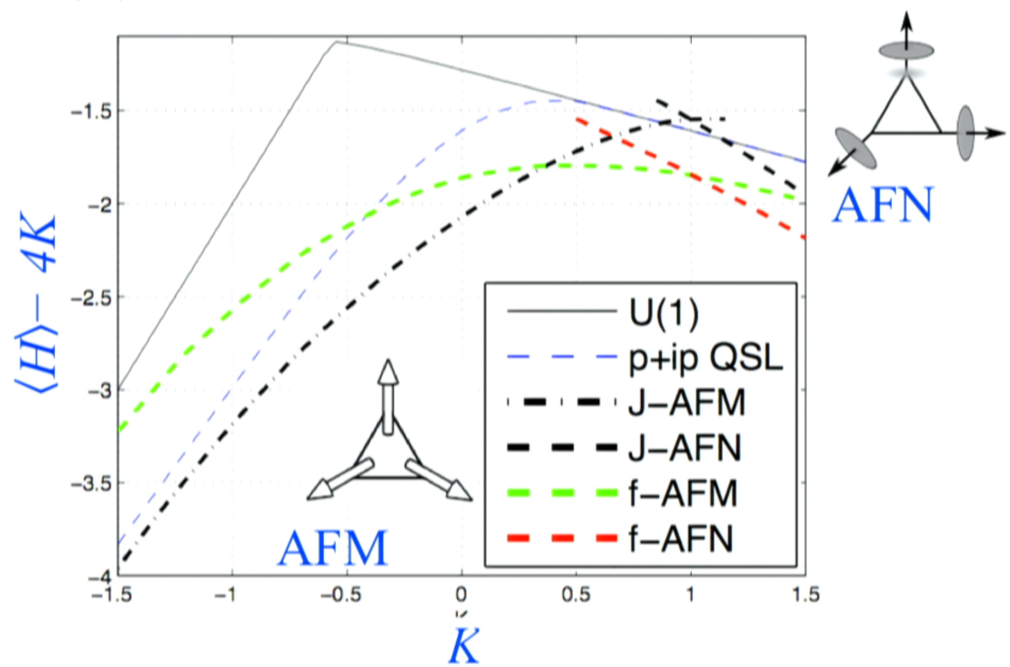
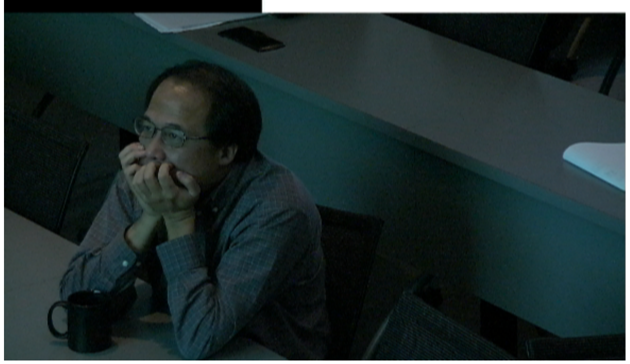


SU(3) symmetric Hamiltonian

- Energies at J = K compared to DMRG

State	$SU(3)$ energy
Fermionic f-AFM	-0.57(8)
Huse-Elser $\mathcal{J}$-AFM	-0.27(7)
$U(1)$ spin liquid	-0.34(3)
DMRG [29] ($N = 8 \times 10$)	-0.678

(Bauer *et. al.*, 2011)



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- SU(3) symmetric Hamiltonian with ring exchange

$$H_\triangle = \cos\alpha \sum_{\langle ij \rangle} P_{ij} + \sin\alpha \sum_{\langle ijk \rangle} P_{ij} P_{jk} + \text{h.c.}$$

$$P_{ij} = \vec{S}_i \cdot \vec{S}_j + (\vec{S}_i \cdot \vec{S}_j)^2 - 1$$

SU(3) symmetric Hamiltonian

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State	$SU(3)$ energy
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Huse-Elser $\mathcal{J}$-AFM	-0.27(7)
$U(1)$ spin liquid	-0.34(3)
DMRG [29] ($N = 8 \times 10$)	-0.678

(Bauer *et. al.*, 2011)

- SU(3) symmetric Hamiltonian with ring exchange

$$H_\triangle = \cos\alpha \sum_{\langle ij \rangle} P_{ij} + \sin\alpha \sum_{\langle ijk \rangle} P_{ij} P_{jk} + \text{h.c.}$$

$$P_{ij} = \vec{S}_i \cdot \vec{S}_j + (\vec{S}_i \cdot \vec{S}_j)^2 - 1$$

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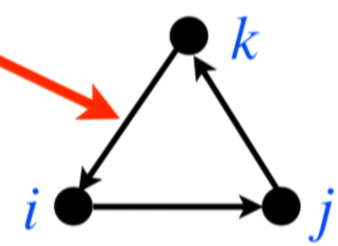

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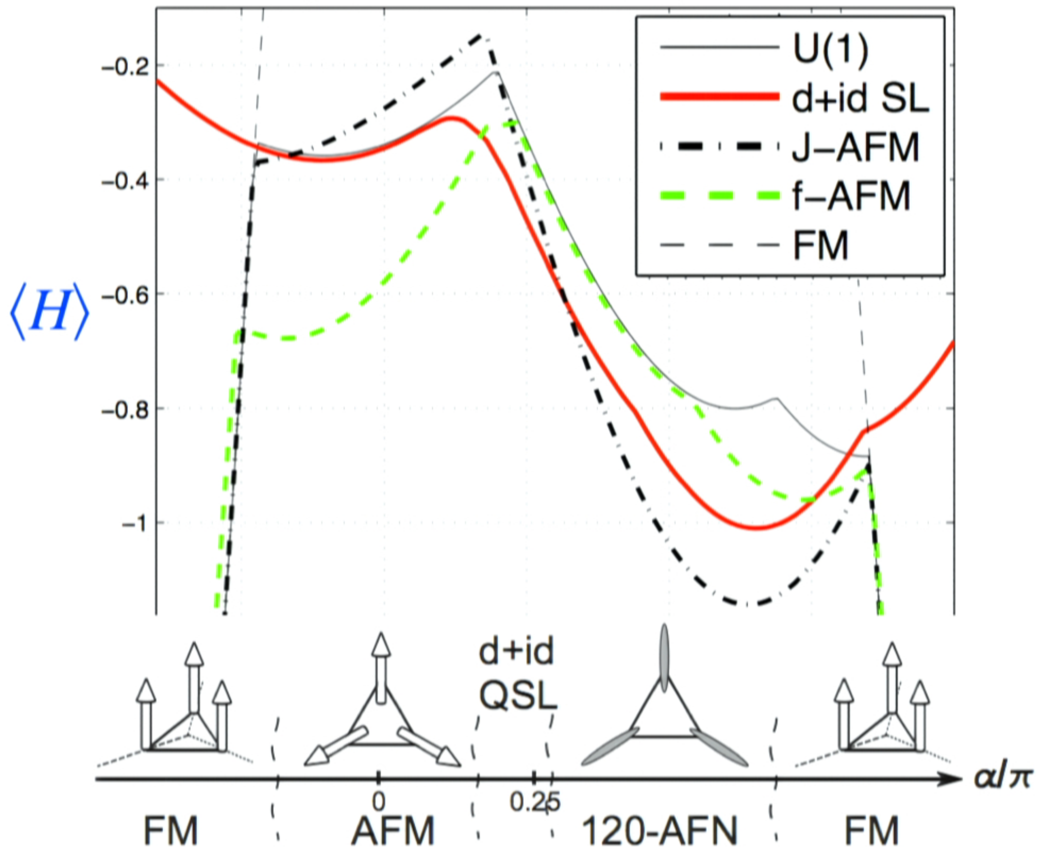
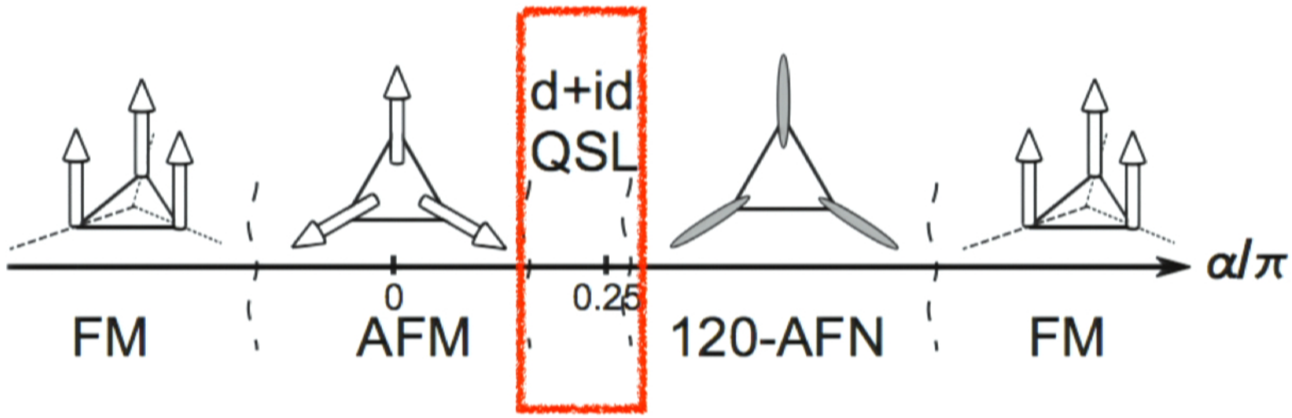


Phase diagram



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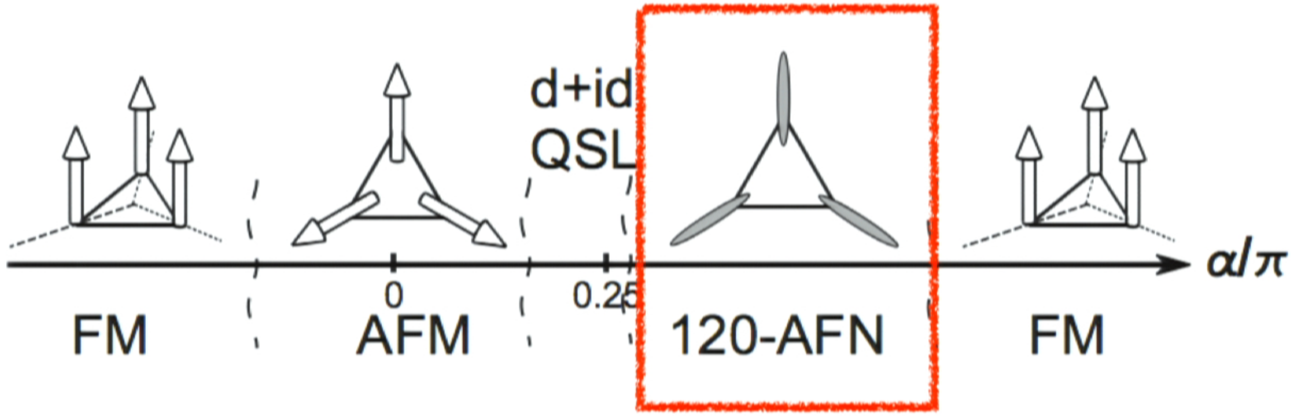
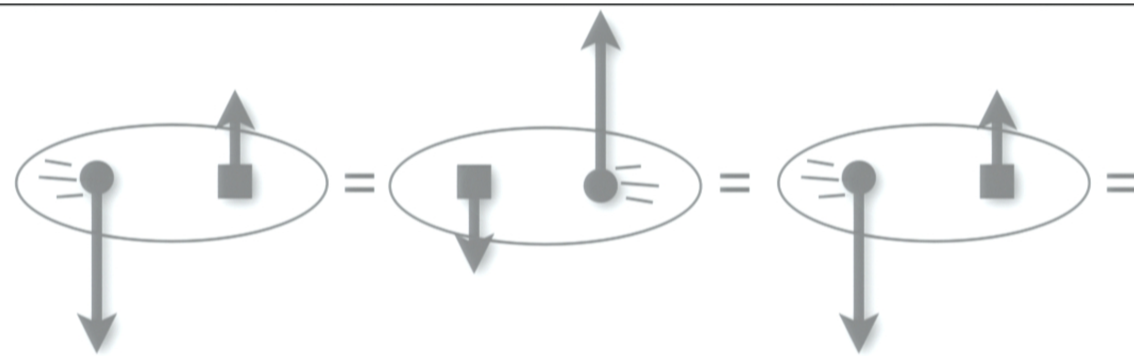


- QSL with *d+id* pairing wins for $\alpha = 0.17\pi \div 0.33\pi$
- For $\alpha > 0.33\pi$ 120°AFN: spontaneous polarization develops, no f_z spinons → $S=1$ reduces to $S=1/2$

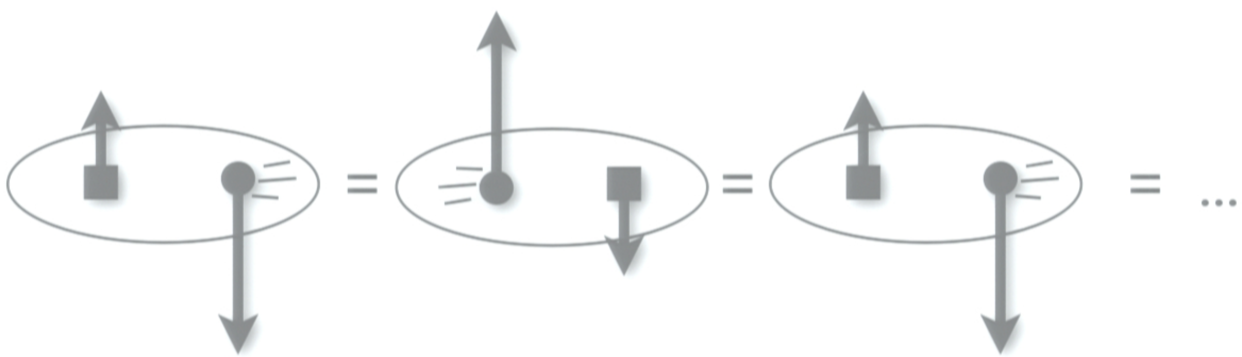
Summary of part I

- Spin liquid ground state for $S = 1$ on triangular lattice with fermionic excitations
- Exotic physical properties: gapless nematic excitations in the bulk, topological edge modes
- Realized in the ring exchange model within VMC

Open questions: 6H-B phase microscopic Hamiltonian, further experiments; ground state of ring exchange model?

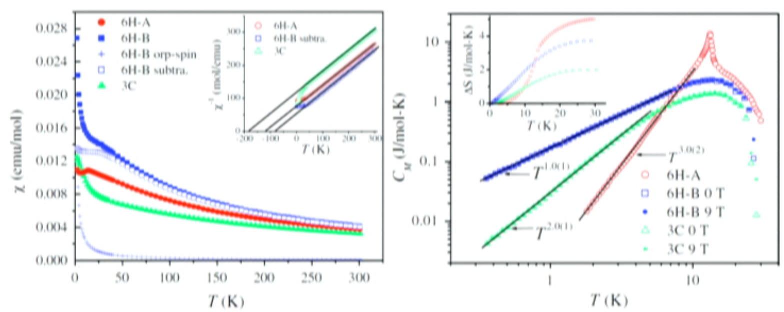


Kondo impurity in S=1 spin liquid



Hunting for spin liquids

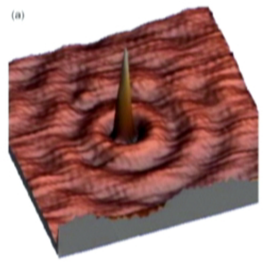
- Spin liquid: elusive phase, difficult to detect
- Signatures: absence of order, χ, C

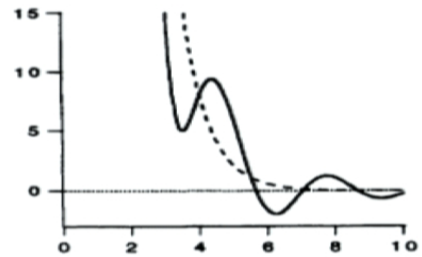


- Other probes? Transport, neutron scattering, phonons, impurity

Impurity in a Fermi liquid

- Charged impurity: Friedel oscillations

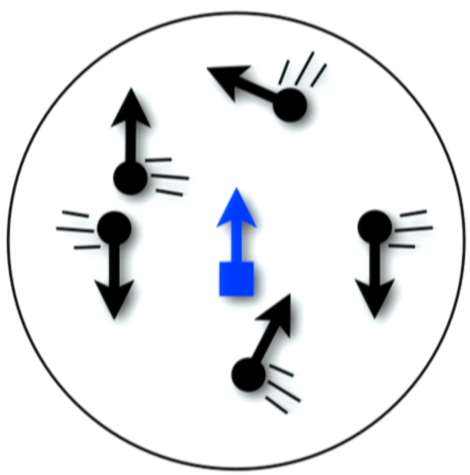


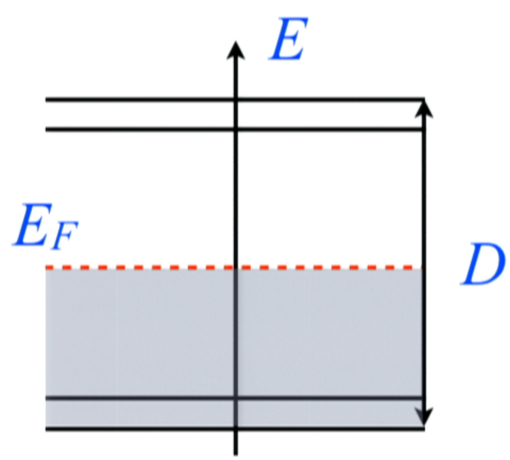


- Impurity with spin (→ coupling to spinons)
  - ✶ RKKY interaction between impurity spins
  - ✶ Kondo effect: screening of local moment

Kondo effect in a Fermi liquid

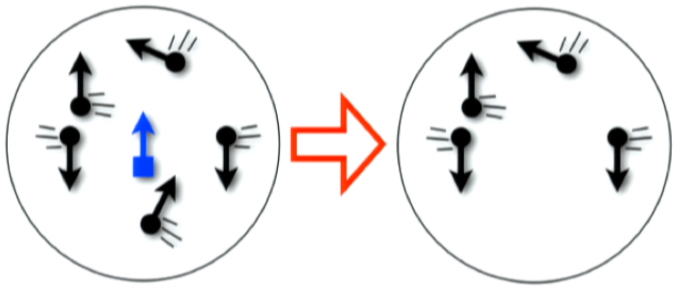
- A simplest strongly correlated system
- Renormalization Group in bandwidth D
- Different regimes: impurity spin $\gtrless$ fermionic spin





Overscreened Kondo

- $s_{\text{imp}} \geqq S$: perfect (under) screening: strong coupling



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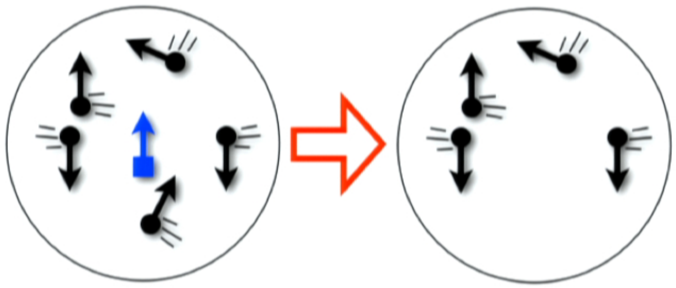

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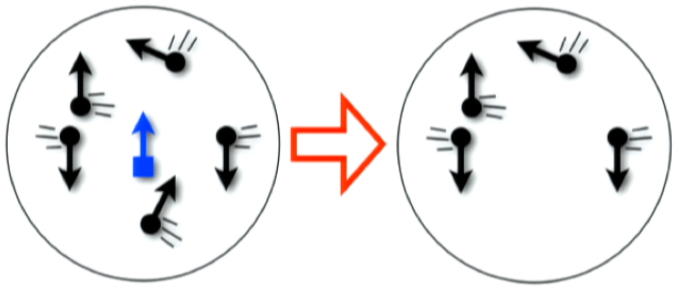

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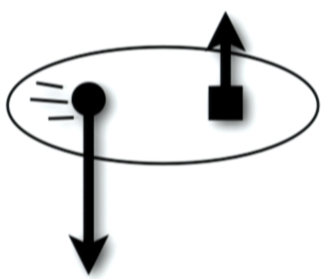

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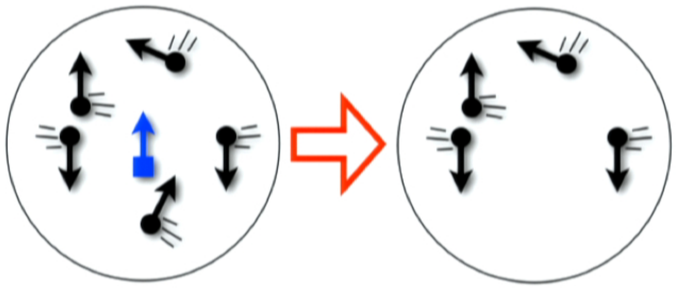

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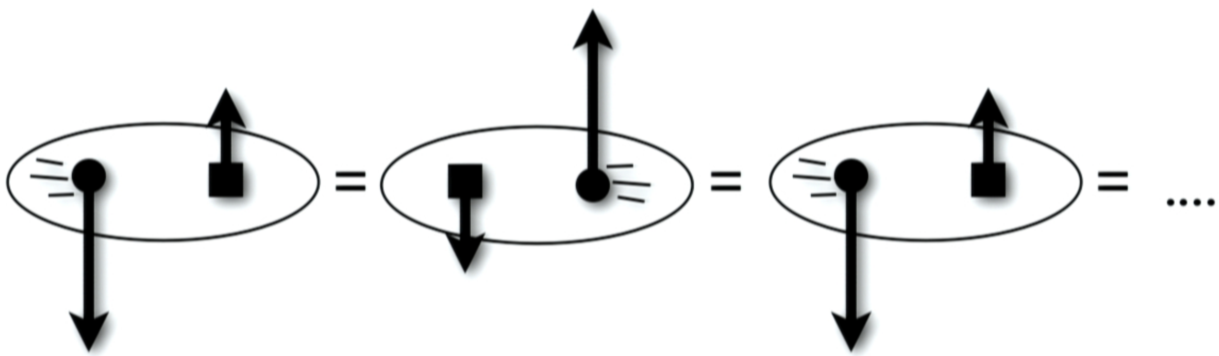

Impurity in S=1 fermionic spin liquid

- $s=1/2$ impurity in $S=1$ spin liquid with three spinons
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  - ✳ gauge field strongly coupled to spinons

  ?

(M.S., T. Senthil, P.A. Lee, arXiv:1212.5179)

- Impurity in Dirac spin liquid (Kim&Kim'06)
  also in $S=1/2$ spin liquid with Fermi surface (Ribeiro&Lee PRB'11)

Hamiltonian

- Spin Hamiltonian → low energy theory

$$H_{\mathsf{f}} = \sum_{\mathbf{k},\alpha} \frac{1}{2m} f^{\dagger}_{\vec{k}\alpha} (\vec{k} - \vec{a})^2 f_{\vec{k}\alpha} + \frac{J}{N} \vec{S}(0) \cdot \vec{s}$$

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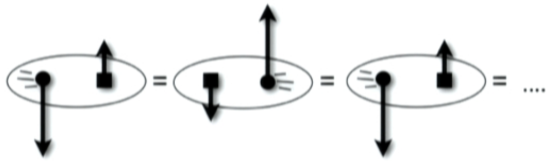

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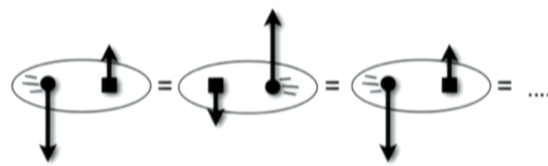

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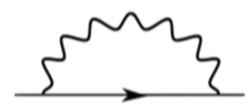

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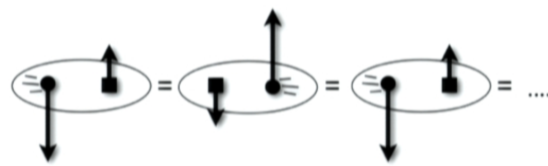

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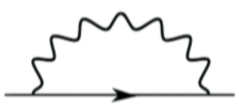

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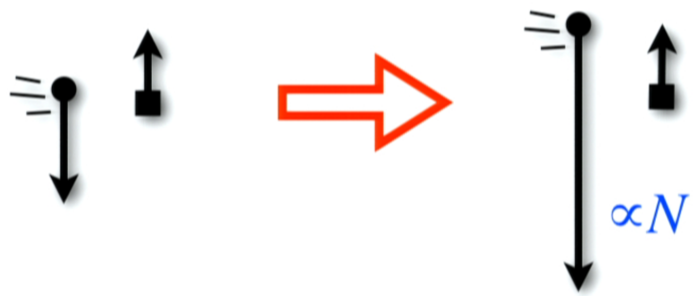
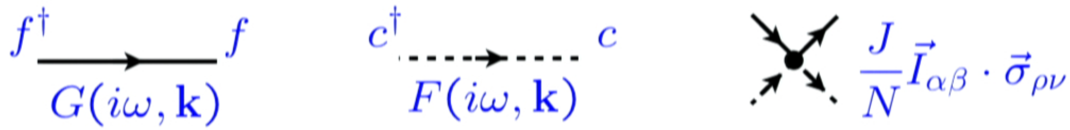


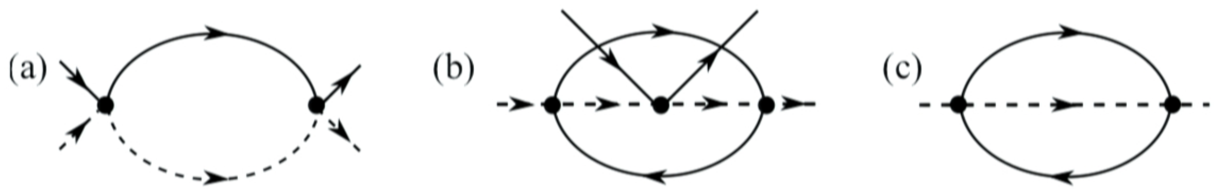
- RG flow of dimensionless coupling g with bandwidth (Abrikosov;Nozieres&Blandin)

$$g = \nu J, \qquad \beta(g) = -\frac{d \log g}{d \log D}$$

Perturbative β-function

- β-function is calculated perturbatively in g:





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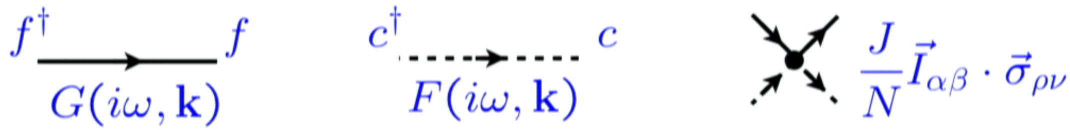

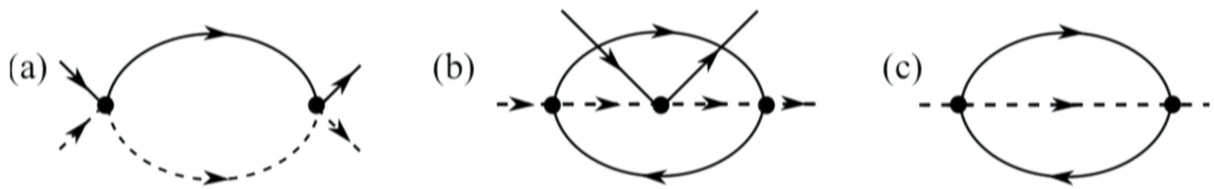

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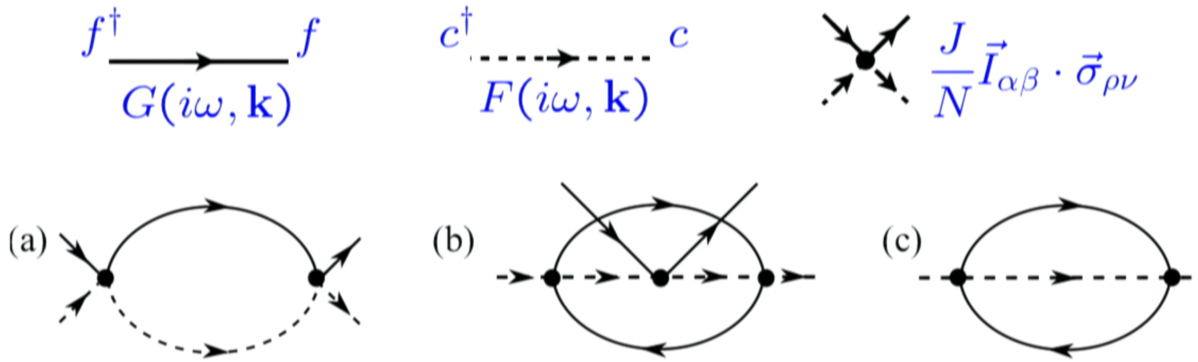

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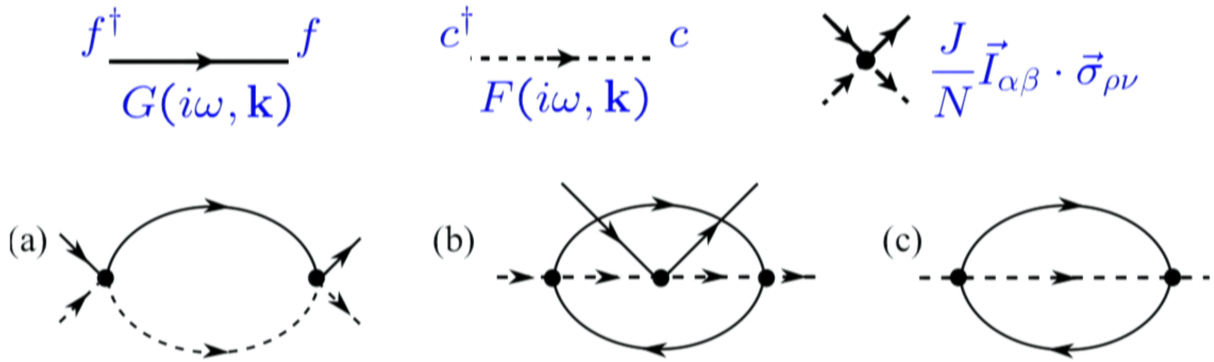

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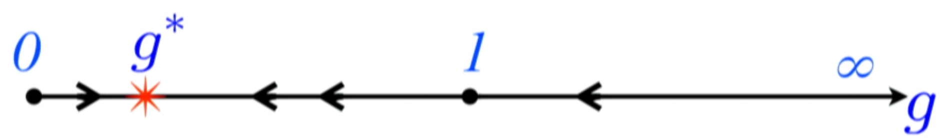

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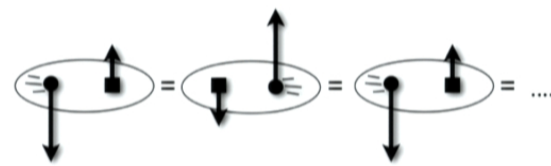

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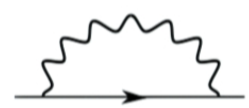

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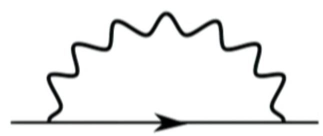
Spinons coupled to U(1) gauge field

- Large-N expansion: three $\to N$ flavors of spinons
- Non-Fermi-liquid: singular self-energy due to gauge field dominates at small ω

$$\Sigma(i\omega) =$$



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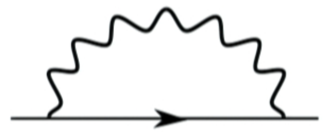

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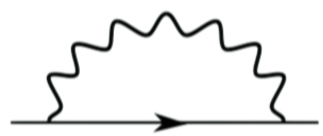

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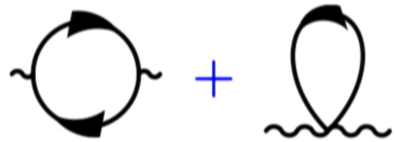
- Greens function has $1/N$ in denominator; power counting is destroyed (S.-S. Lee; Metlitski&Sachdev)

Double expansion

- Double expansion: dynamical exponent of gauge field as a control parameter (Mross *et.al*. PRB'10)

$D(i\omega, \mathbf{q}) =$  $= \gamma \frac{|\omega|}{q} + \chi_0 q^{1+\varepsilon}$

- Instead of $\varepsilon = 1$ as in physical case, we consider limit

$$N \to \infty, \quad \varepsilon \to 0, \quad N\varepsilon = \text{const}$$

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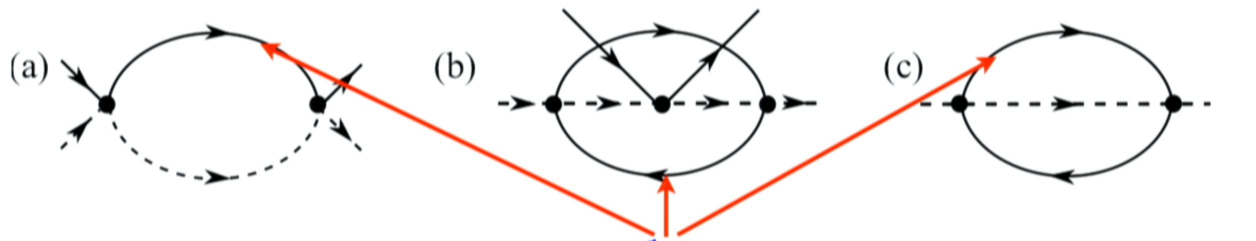
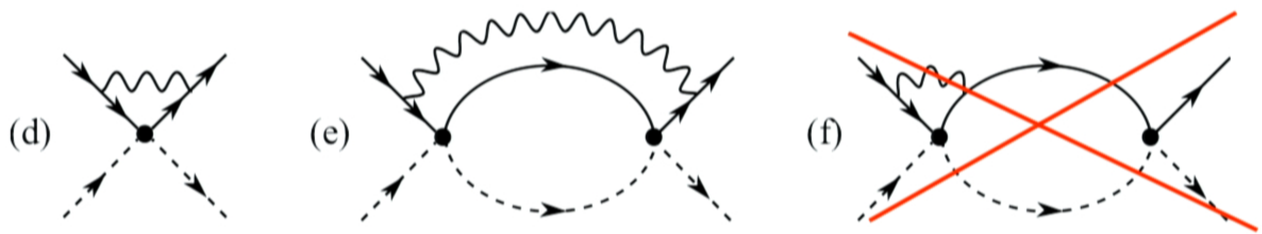
Kondo with gauge field

- Flow of Kondo coupling g assuming that e is fixed:



$$G^{-1}(\mathbf{k}, i\omega) = i\omega - \xi_{\mathbf{k}} - \Sigma(i\omega)$$

- Vertex corrections do not contribute



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- Position of fixed point is intact up to $O(1/N^3)$, *but* the scaling exponent *is* modified:

$$\Delta = -\beta'(g^*) = \frac{2}{N} \qquad + \ldots$$

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- Δ becomes smaller → softening of singularities from the decoherence of quasiparticle excitations

Behavior of physical quantities

- Power-law behavior of running coupling constant:

$$g_R(\omega) = g^* - \zeta\,(\omega/T_K)^{\triangle} \qquad \triangle = \frac{2}{N}(1-\kappa) + \ldots$$

- Scattering rate due to impurity, thermal conductivity

$$\nu\tau^{-1}(\omega) \propto 1 - N\zeta(\omega/T_K)^{\triangle}$$

$$\delta\kappa_{\mathrm{th}}/\kappa^0_{\mathrm{th}} \propto n_{\mathrm{imp}}(1 - N\zeta\,(\omega/T_K)^{\triangle})$$

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- Power-law behavior of running coupling constant:

$$g_R(\omega) = g^* - \zeta\,(\omega/T_K)^{\Delta} \qquad \Delta = \frac{2}{N}(1-\kappa) + \ldots$$

- Scattering rate due to impurity, thermal conductivity

$$\nu\tau^{-1}(\omega) \propto 1 - N\zeta(\omega/T_K)^{\Delta}$$

$$\delta\kappa_{\text{th}}/\kappa^0_{\text{th}} \propto n_{\text{imp}}(1 - N\zeta\,(\omega/T_K)^{\Delta})$$

- Thermodynamic properties

$$C_{\text{imp}} \sim \left(\frac{T}{T_K}\right)^{2\Delta} \quad \chi_{\text{imp}} \sim \frac{1}{T}\left(\frac{T}{T_K}\right)^{2\Delta} \quad M \sim \left(\frac{h}{T_K}\right)^{\Delta}$$

Summary of part II

- $N \to \infty$, $\varepsilon \to 0$ limit: Kondo fixed point survives but it is modified by the gauge field

- Critical behavior → fermionic excitations
  Softening compared to Fermi liquid → gauge field

- Specific heat, spin susceptibility and NRM relaxation rate as probes (M.S., T. Senthil, P.A. Lee, arXiv:1212.5179)

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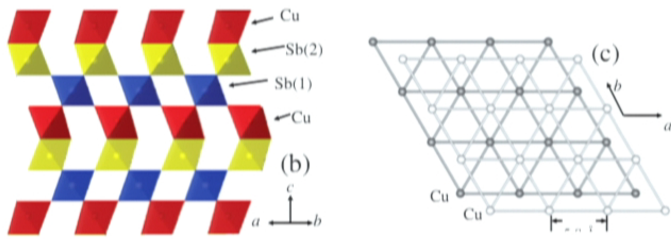
Outlook

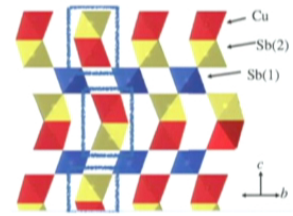
- S=1 spin liquid with emergent fermionic excitations
  - ✶ $d+id$ pairing of spinons
  - ✶ all spinons have Fermi surface: overscreened Kondo to probe spinons and gauge field
- Possible further directions
  - ✶ material-oriented questions
  - ✶ ED, DMRG,...: search for spin models

New candidate materials

- Spin-1/2 $Ba_3CuSb_2O_9$ (Zhou *et.al*. PRL'11)

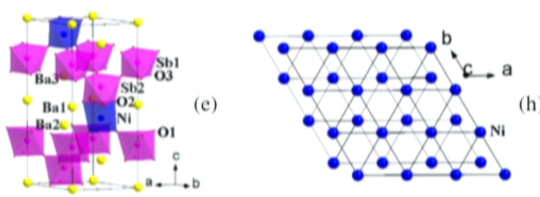
  (Nakatsuji *et.al*. Science'12)

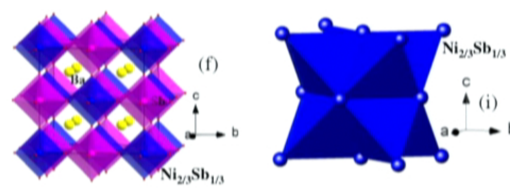




- Spin-1 $Ba_3NiSb_2O_9$ (Cheng *et.al*. PRL'11)

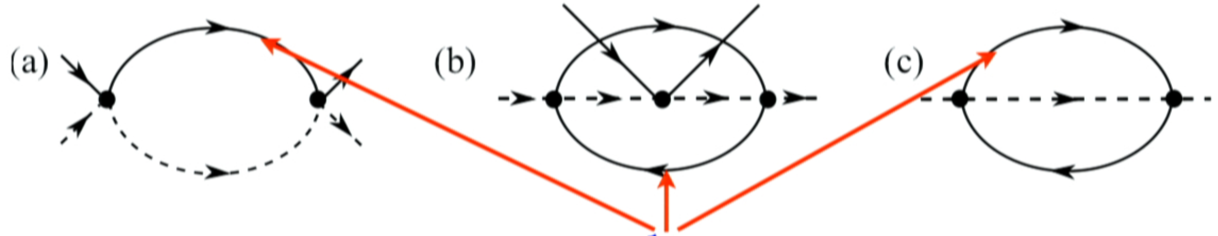
  6H-B phase 6H-C phase





Kondo with gauge field

- Flow of Kondo coupling g assuming that e is fixed:



$$G^{-1}(\mathbf{k}, i\omega) = i\omega - \xi_{\mathbf{k}} - \Sigma(i\omega)$$

- Vertex corrections do not contribute