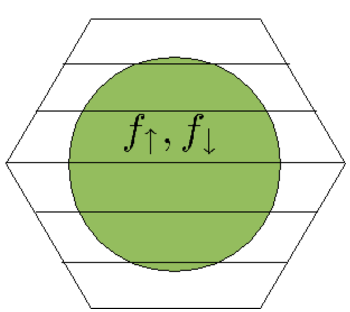
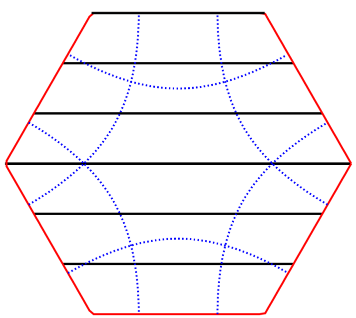
Ladder studies of a Spin Bose-Metal

Olexei Motrunich

2-leg: Donna Sheng and Matthew Fisher,
4-leg: Matt Block, Donna Sheng, and Matthew Fisher





Outline

1) What is Spin Bose-Metal? Motivation from triangular spin liquid materials

2) Spin-1/2 model with ring exchanges and ladder descendants

3) Numerical studies on the ladders
- 2-leg ladder
- 4-leg ladder
- 4-leg towards 2d, interpolating between triangular and square

4) More lessons form quasi-1d (if time permits; with Hsin-Hua Lai)
- effects of impurities
- SBM in electronic models and role of long-range repulsion
- new phases under Zeeman field

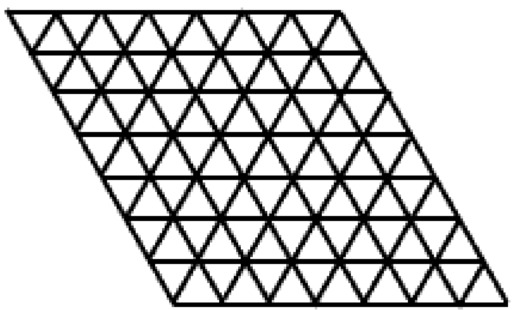
5) Outlook

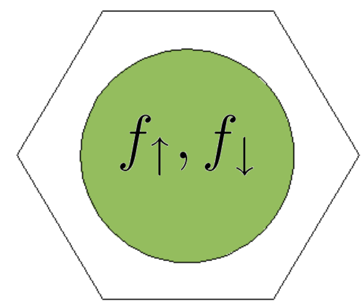
Spin Bose-Metal

(aka Spin Liquid with Spinon Fermi Sea)

"Parton" construction: $\mathbf{S}_i = f_i^\dagger \frac{\boldsymbol{\sigma}}{2} f_i;$ $\quad f_{i\uparrow}^\dagger f_{i\uparrow} + f_{i\downarrow}^\dagger f_{i\downarrow} = 1$

Mean field: hopping with no fluxes -> Fermi sea of spinons

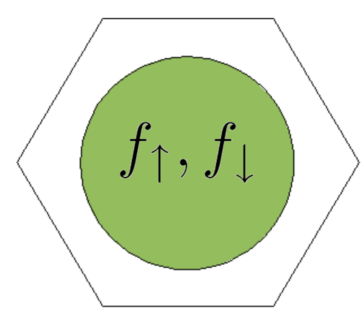




Beyond m.f.: spinon-gauge theory (aka "uniform RVB")

Beyond m.f.: Gutzwiller-project -> spin trial wavefunction

$\Psi_{spin} =$ P $_G$ (



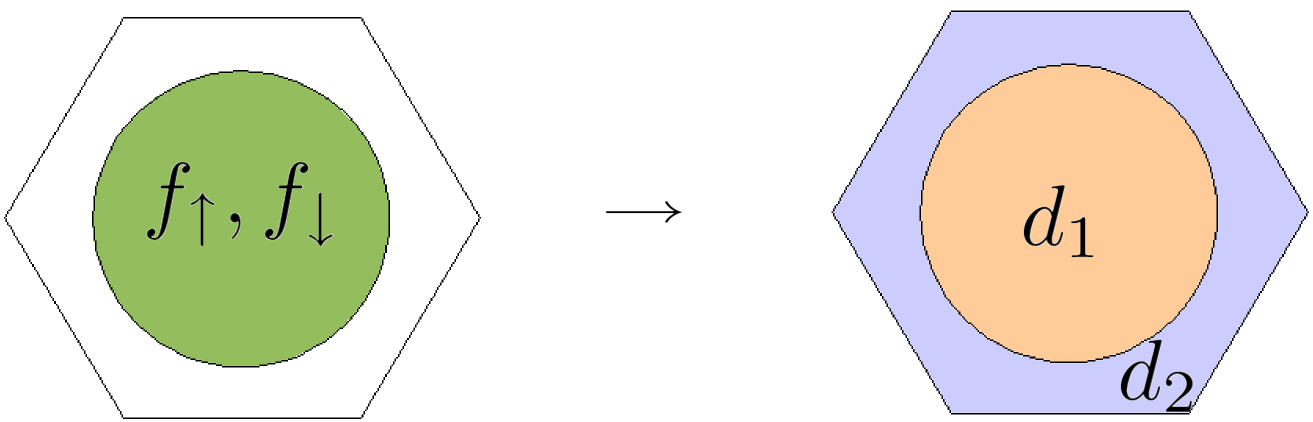
)

Determinantal structure of wavefunctions
(cf. Ryan's "Bose-Metals" talk)

Spins -> hard-core bosons and "parton" construction:

$$S^+ = f_\uparrow^\dagger f_\downarrow \quad \rightarrow \quad b^\dagger = d_1^\dagger d_2^\dagger$$

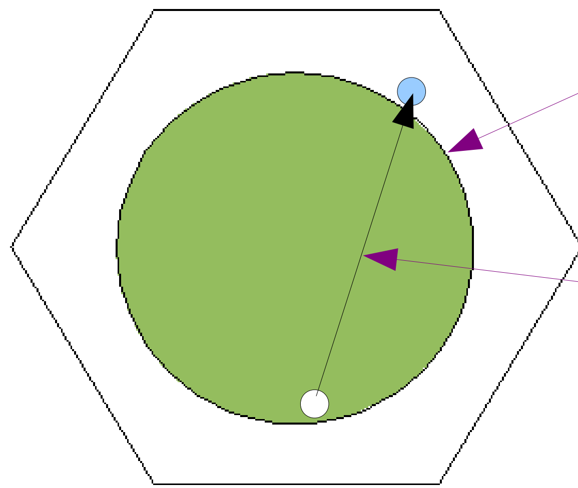
$$f_\uparrow^\dagger f_\uparrow + f_\downarrow^\dagger f_\downarrow = 1 \quad \rightarrow \quad d_1^\dagger d_1 = d_2^\dagger d_2 = b^\dagger b$$



$$\Psi_{\text{boson}}(r_1, \ldots, r_N) = det_1[r_1, \ldots, r_N] \times det_2[r_1, \ldots, r_N]$$

"Bose surface" for Spin Correlations

$$\Psi_{spin} = P_G \big($$



$$\big)$$

Absolute location of the spinon Fermi surface is gauge dependent

But relative wavevectors are gauge-independent!

Spinon particle-hole combination ~ ***boson***

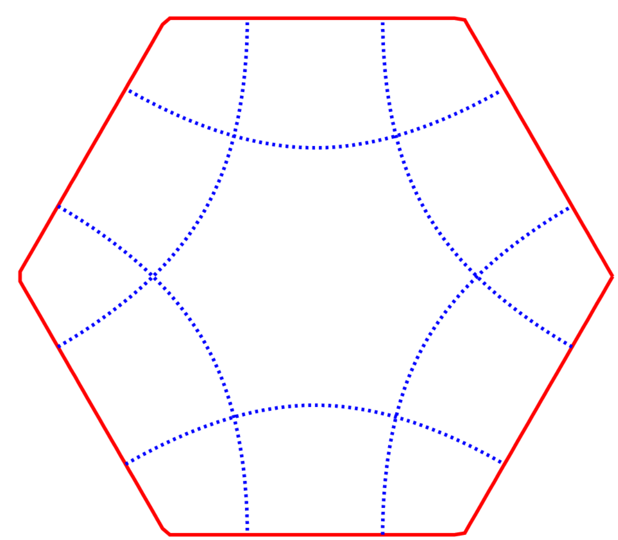
Spin correlations in r-space

$$\langle \vec{S}(r) \cdot \vec{S}(0) \rangle \sim \frac{\cos(2k_F r - \alpha)}{r^p}$$

In q-space: singular "$2k_F$"surface

$$\langle \vec{S}_q \cdot \vec{S}_{-q} \rangle \sim |q - 2k_F|^{p-3/2}$$

"$2k_F$"surface in the triangular lattice at half-filling:

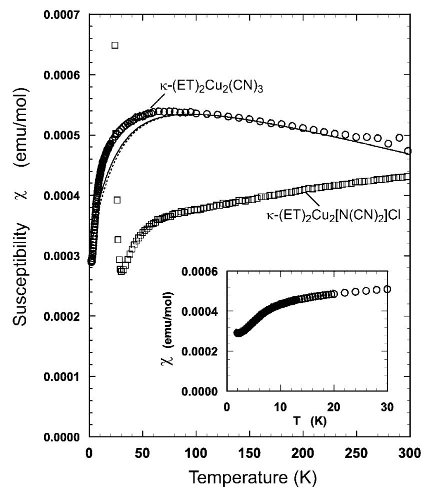


Experimental spin liquids

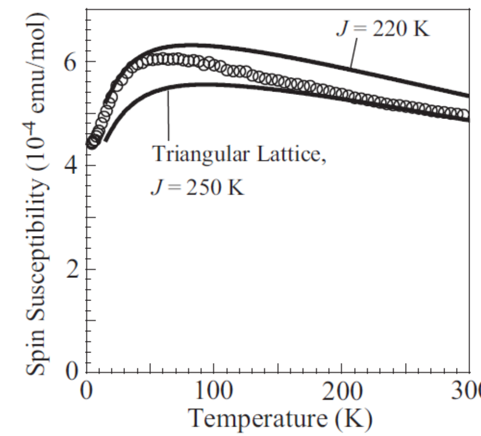
κ–$(ET)_2Cu_2(CN)_3$ and $EtMe_3Sb[Pd(dmit)_2]_2$

- 2d triangular lattice spin-1/2 systems; ***weak Mott insulators***
- many low-energy excitations as if Fermi sea of smth
- reviewed earlier in the program by Tarun Grover and Federico Becca

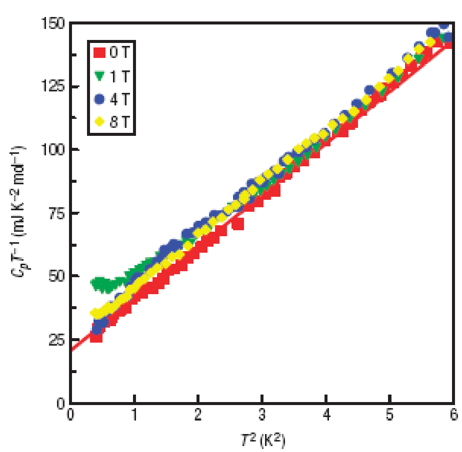
κ–(ET)
spin susceptibility
Shimizu et.al. 03



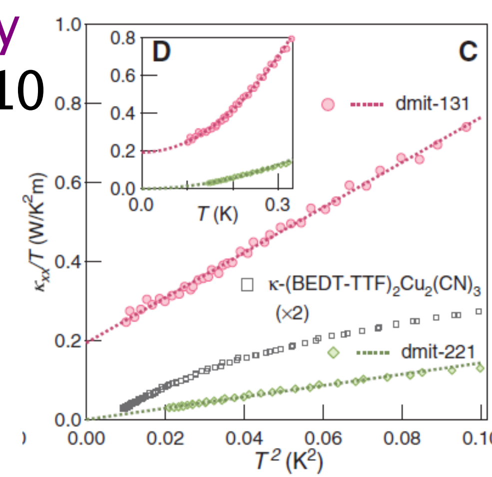
Pd-dmit
spin susceptibility
Itou et.al. 08



specific heat
S.Yamashita et.al. 08



Thermal conductivity
M.Yamashita et.al. 10



Spin model with ring exchanges

Hubbard-type model

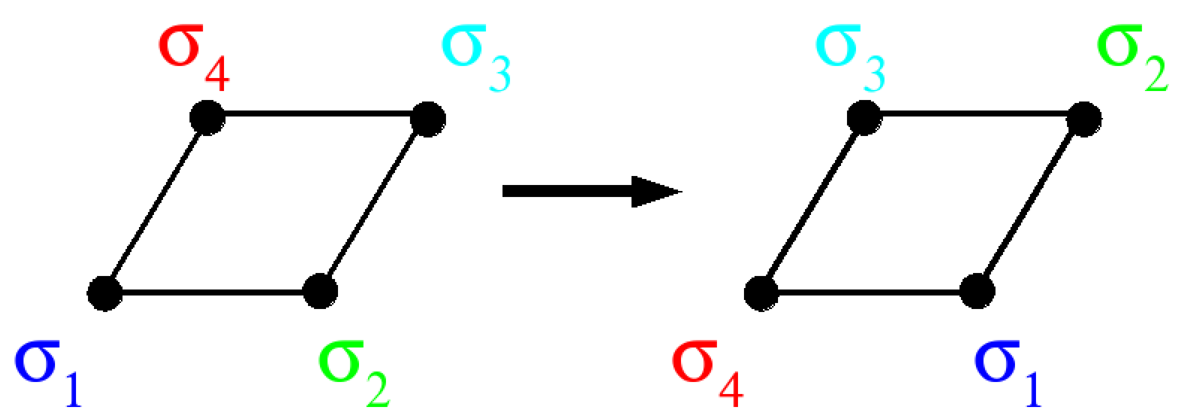
$$\hat{H}_{\text{Hubbard}} = -t \sum_{ij} c_{i\alpha}^{\dagger} c_{j\alpha} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Insulator -> effective spin model

$$\hat{H}_{\text{eff}} = \frac{2t^2}{U} \sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{20t^4}{U^3} \sum_{\text{rhombi}} (P_{ijkl} + \text{h.c.}) + \ldots$$

Ring exchange:

P_{1234} :

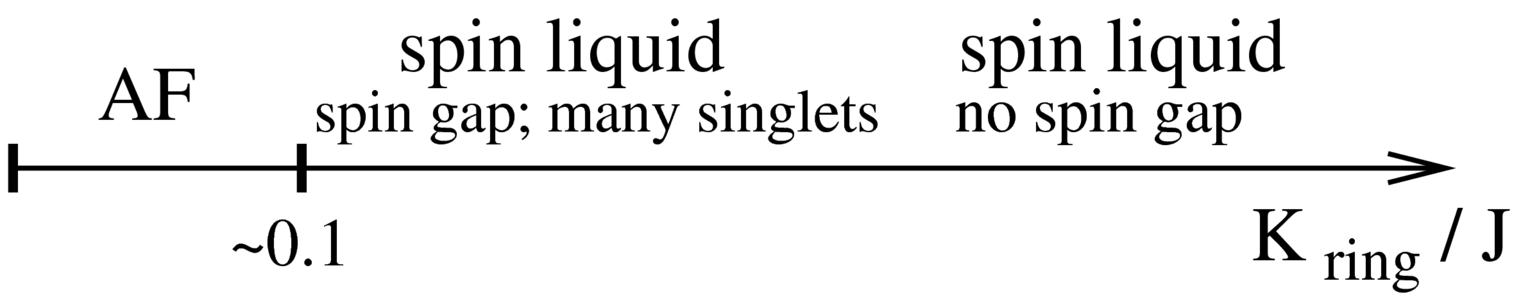


J-K_{ring} ring exchange model

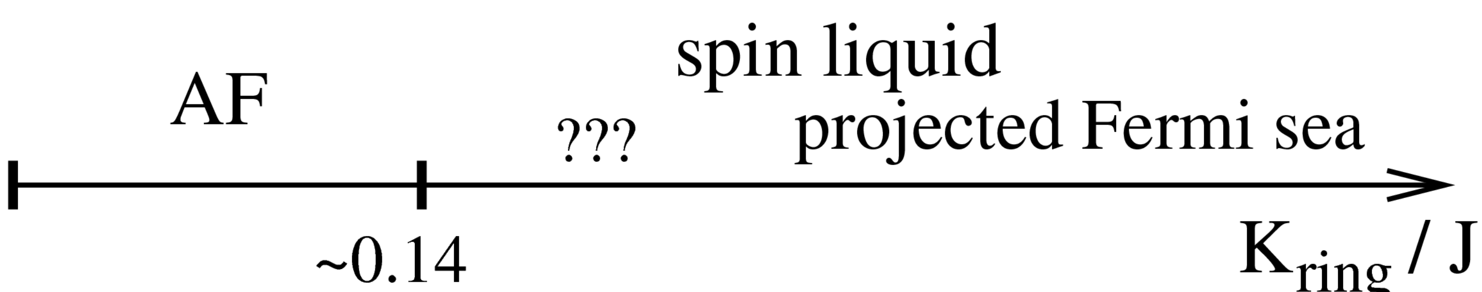
$$\hat{H}_{\text{ring}} = J \sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + K_{ring} \sum_{\text{rhombi}} (P_{ijkl} + \text{h.c.})$$

κ–$(ET)_2Cu_2(CN)_3$: $K_{ring}/J \sim 0.3$

Exact diagonalization study: (LiMing et.al. 2000, Misguich et.al. 1999)



Trial wavefunction study suggests spinon Fermi sea! (OIM 05)



Is Spin Bose-Metal actually the ground state of the triangular ring model?

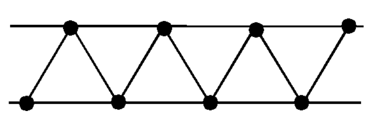
Unbiased numerical studies –difficult in 2d (perhaps some techniques developed in this program, like branching MERA?)

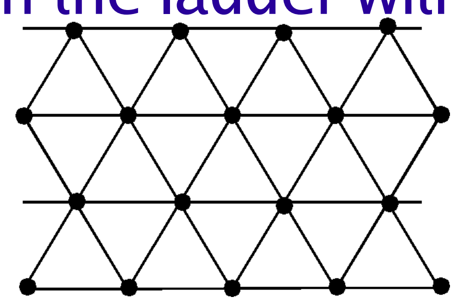
Our approach: fully controlled numerical DMRG studies on ladders (Ryan's talk, Steve White's discussion)

- compare with variational ladder descendant states
- treat spinon-gauge theory with controlled bosonization techniques

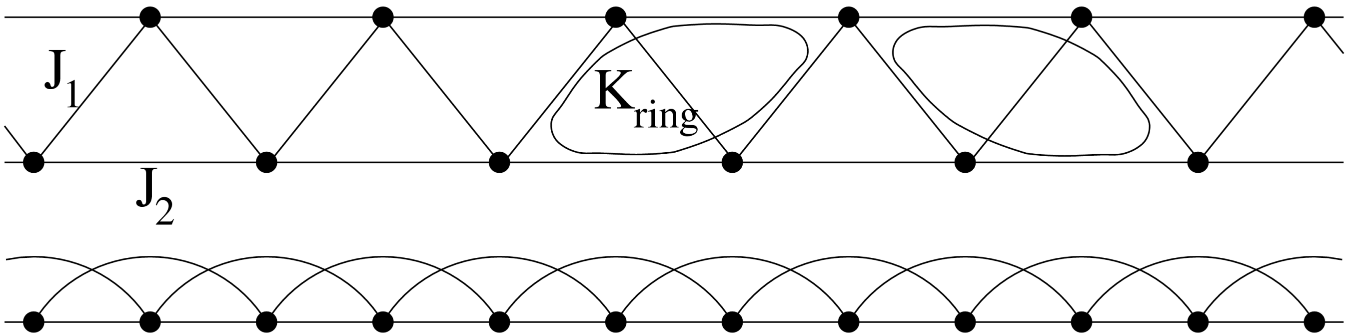
In the limit of long ladders, "SBM descendants" are multi-mode Luttinger liquids that inherit some properties from the 2d state such as singular wavevectors in correlations

Trial wavefunction: spinon hopping on the ladder with no fluxes





Ring exchange model on the 2-leg strip



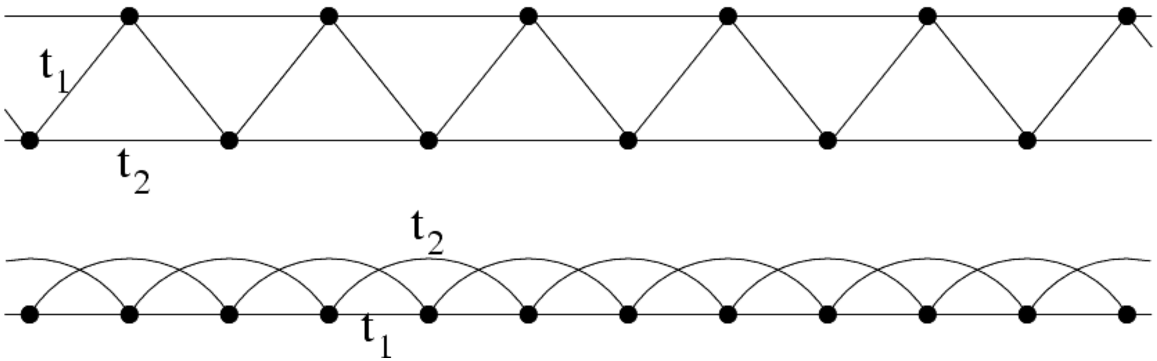
$$\hat{H} = \sum_i 2J_1 \vec{S}_i \cdot \vec{S}_{i+1} + 2J_2 \vec{S}_i \cdot \vec{S}_{i+2} + K_{\rm ring} \left(P_{i,i+2,i+3,i+1} + {\rm h.c.} \right)$$

Analysis of the J_1- J_2- K_{ring} model

D.N.Sheng, OIM, and M.P.A.Fisher, Phys. Rev. B 79, 205112 (2009)

- exact diagonalization (prior ED work L=24 Klironomos et al 07)
- **DMRG!**
- Variational Monte Carlo with Gutzwiller wavefunctions
- **Bosonization solution of gauge theory!**

Gutzwiller wavefunction on the 2-leg strip

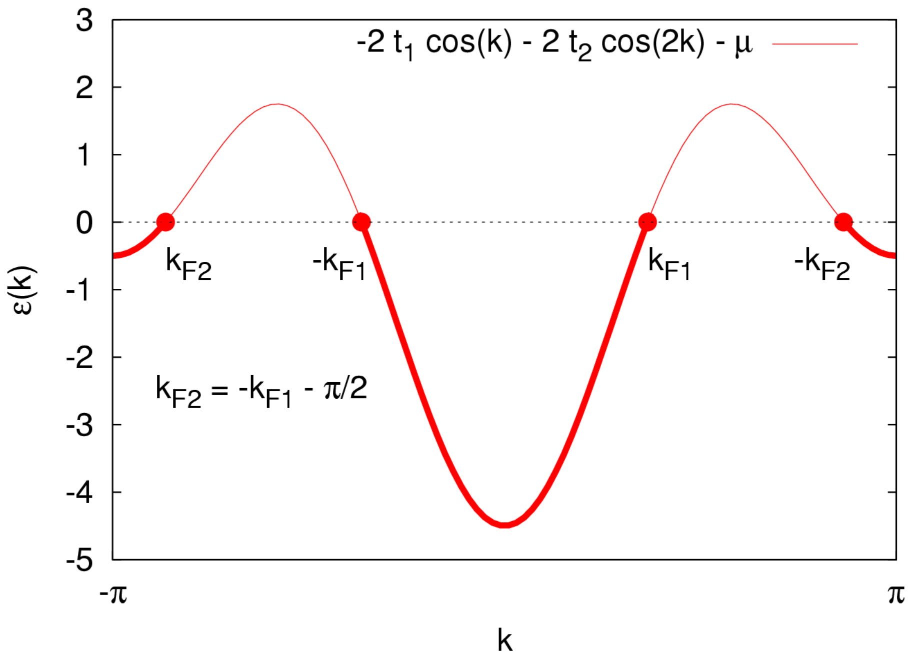


t_1- t_2 chain hopping

$t_2 < 0.5\ t_1$ –one Fermi segment → Bethe phase

$t_2 > 0.5\ t_1$ –two Fermi segments → SBM descendant!

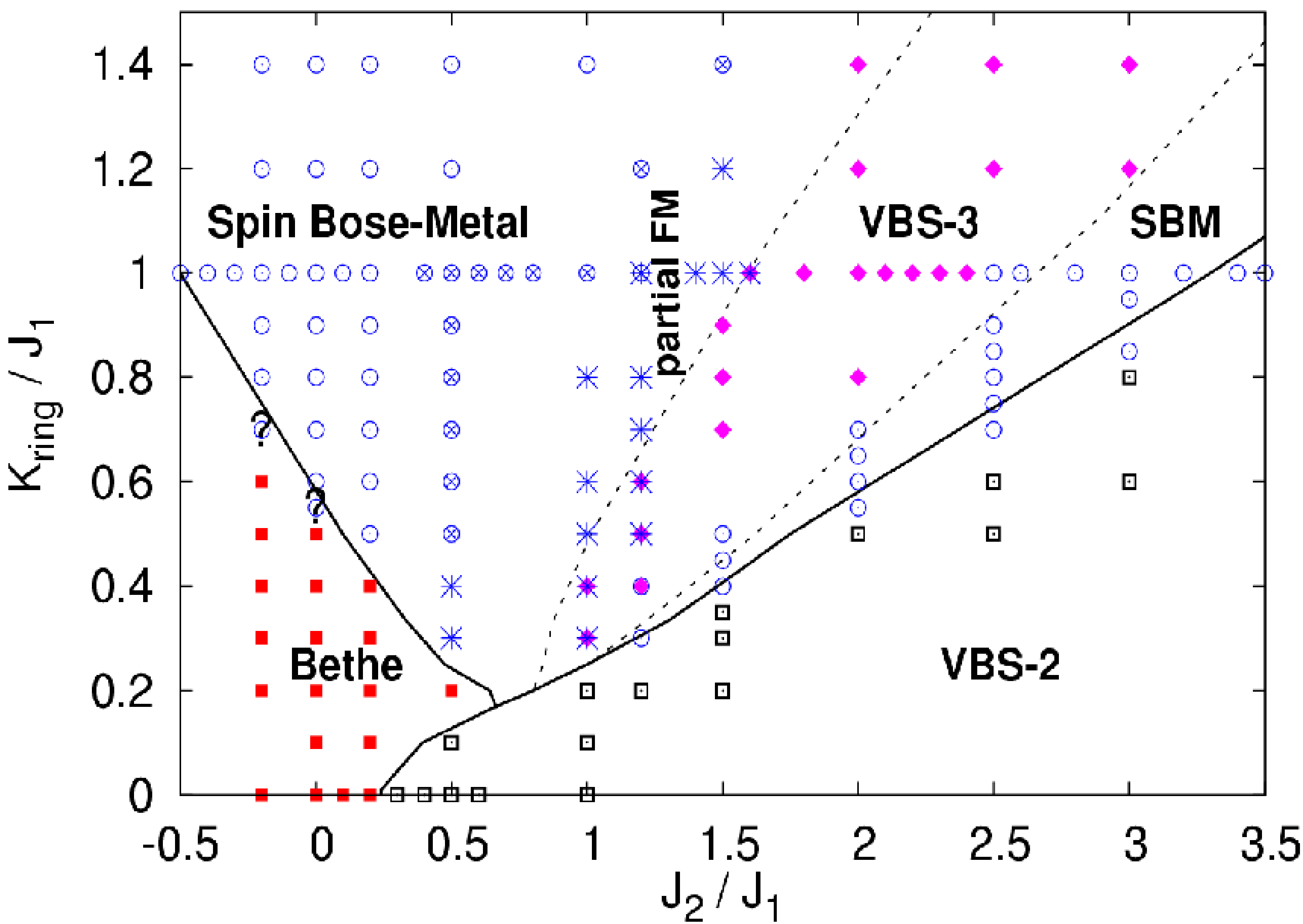
$$\Psi_{spin} = P_G (\quad)$$



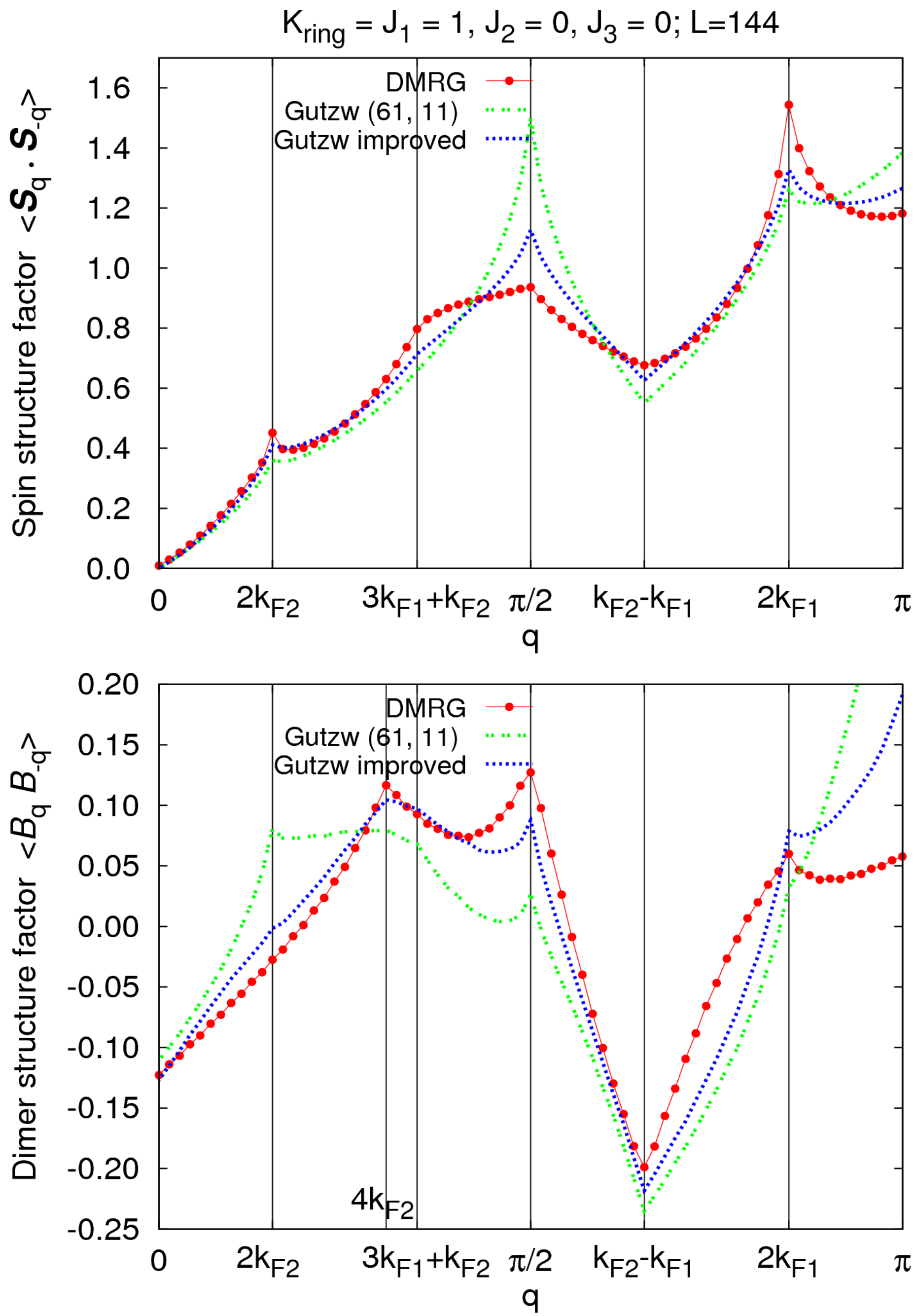
single variational parameter t_2/ t_1 or k_{F2}

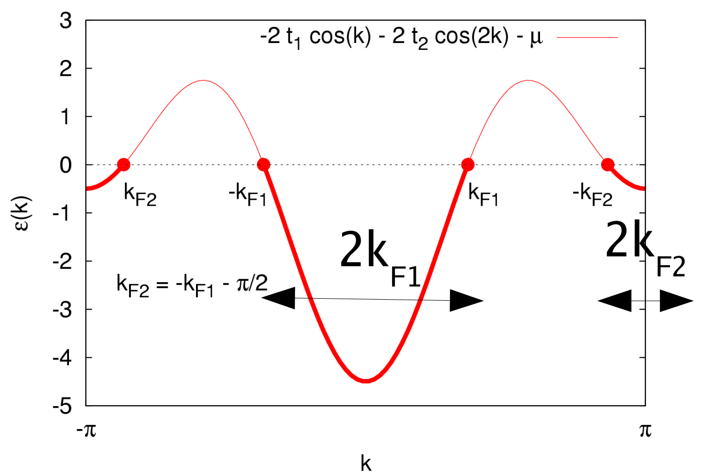
Does this phase happen in the ring model? - YES!

Phase diagram of the 2-leg ring model



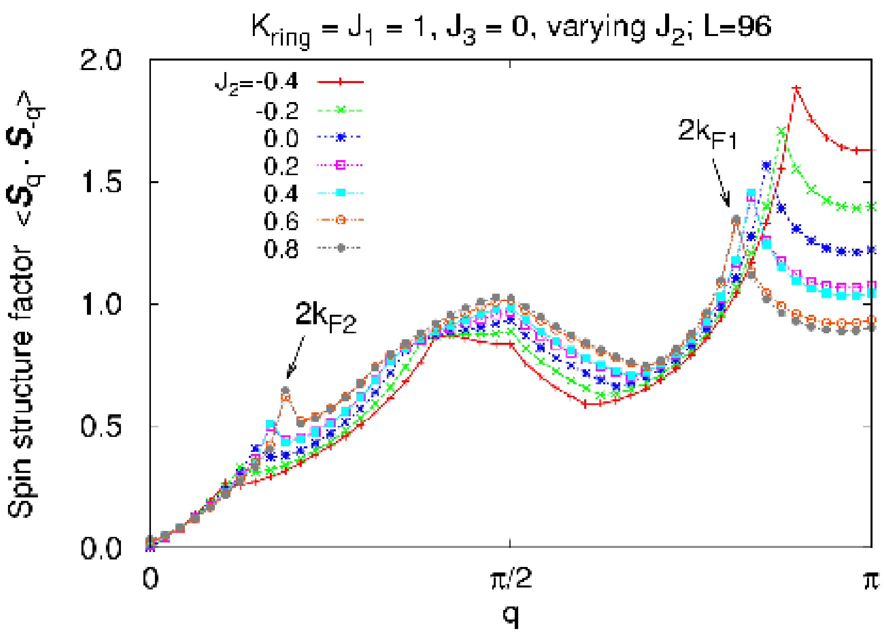
Comparison of DMRG and Gutzwiller

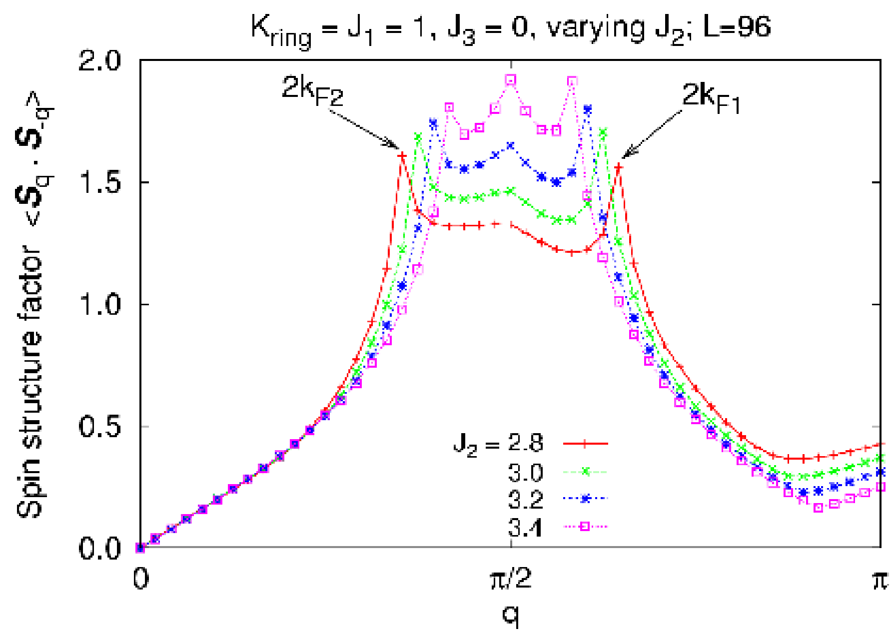


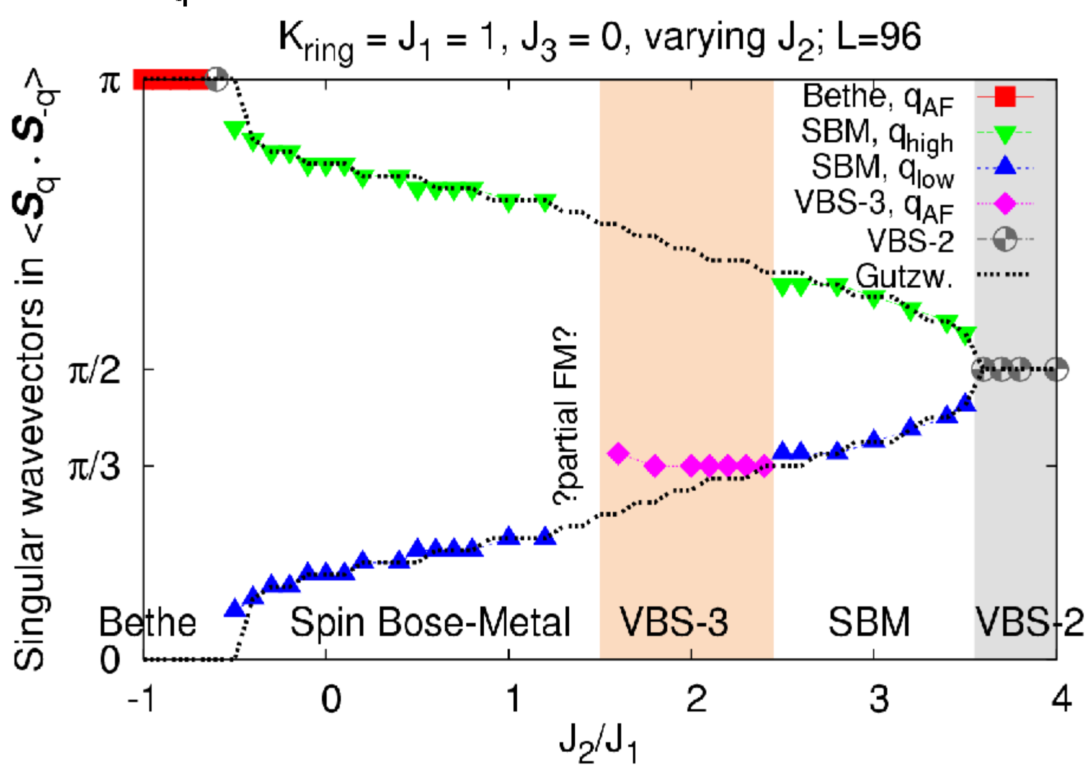


singular wavectors -- ladder remnants of the 2d critical surfaces

Evolution of the singular wavevectors



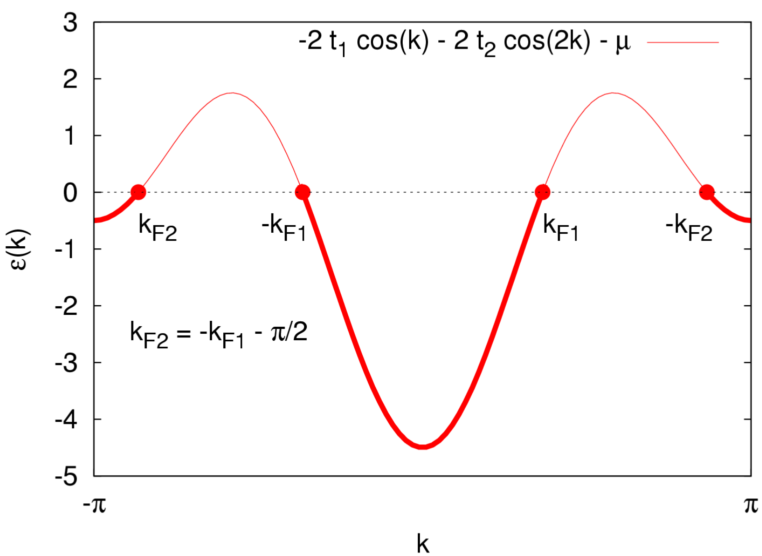




Bosonization description of the 2-leg SBM

Can solve parton-gauge treatment of the spin model by bosonization

Equivalent long wavelength description starting from physical electrons



"C2S2"metal:

$$\{\phi_{1\uparrow}, \theta_{1\uparrow}\}, \{\phi_{1\downarrow}, \theta_{1\downarrow}\}, \{\phi_{2\uparrow}, \theta_{2\uparrow}\}, \{\phi_{2\downarrow}, \theta_{2\downarrow}\}$$

$$\theta_{a\rho} = \frac{\theta_{a\uparrow} + \theta_{a\downarrow}}{\sqrt{2}}, \quad \theta_{a\sigma} = \frac{\theta_{a\uparrow} - \theta_{a\downarrow}}{\sqrt{2}}$$

$$\theta_{\rho+} = \frac{\theta_{1\rho} + \theta_{2\rho}}{\sqrt{2}}$$ - overall charge mode

$$\theta_{\rho-} = \frac{\theta_{1\rho} - \theta_{2\rho}}{\sqrt{2}}$$ - "transverse charge"mode (non-transporting!)

$\theta_{1\sigma}, \theta_{2\sigma}$ - two spin modes

Bosonization description of the 2-leg SBM

* Gap out the overall charge mode $\theta_{\rho+}$ [possible at intermediate coupling if an eight-fermion Umklapp ~$\cos(4\theta_{\rho+})$ becomes relevant] while keeping $\theta_{\rho-}$, $\theta_{1\sigma}$, $\theta_{2\sigma}$ gapless -> "C1[ρ-]S2" Mott insulator

* 3 gapless modes: 2 in the spin sector (Luttinger parameters $g_{1\sigma} = g_{2\sigma} = 1$ by SU(2) spin invariance); 1 in the charge sector (Luttinger parameter $g_{\rho-}$)

* In the spin model, the "ρ–" mode represents local spin chirality fluctuations: $\chi_{Q=0} \sim \partial_x \phi_{\rho-}$

$$\chi(x) \equiv \vec{S}(x-1) \cdot [\vec{S}(x) \times \vec{S}(x+1)]$$

Bosonization description of the 2-leg SBM

* Can analyze all residual interactions and affirm that this can be a stable phase (requires $g_{\rho-} < 1$)

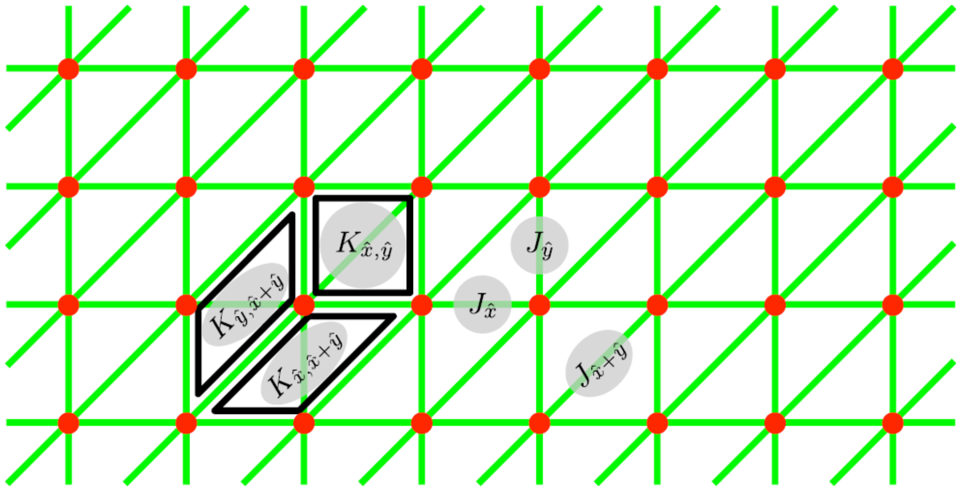
* Can understand all observables (e.g., dominant correlations are spin and bond at wavevectors $2k_{Fa}$ with scaling dimension $\Delta = ½ + g_{\rho-}/4$)

* Gutzwiller wavefunctions appear to be fine-tuned states corresponding to $g_{\rho-}=1$

* Can understand nearby phases found in the DMRG (VBS-2, Chirality-4, Dimer-3)

Ring exchange model on the 4-leg ladder

Matt Block, Donna Sheng, OIM, and Matthew Fisher, arXiv 1009.1179

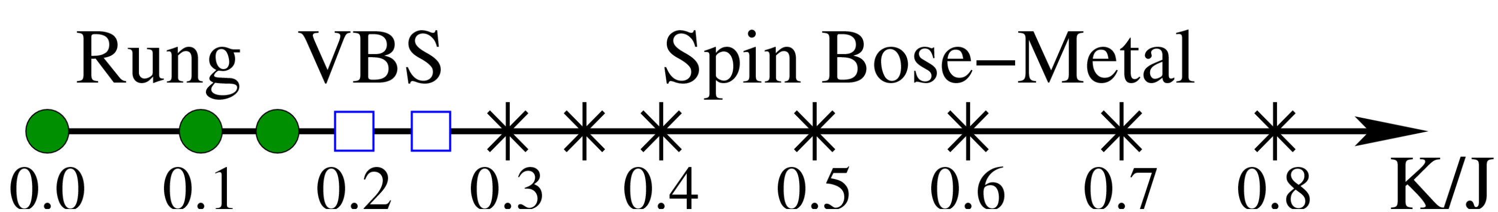


"Isotropic" (or "triangular") model

$$J_{\hat{x}} = J_{\hat{y}} = J_{\hat{x}+\hat{y}} = J$$

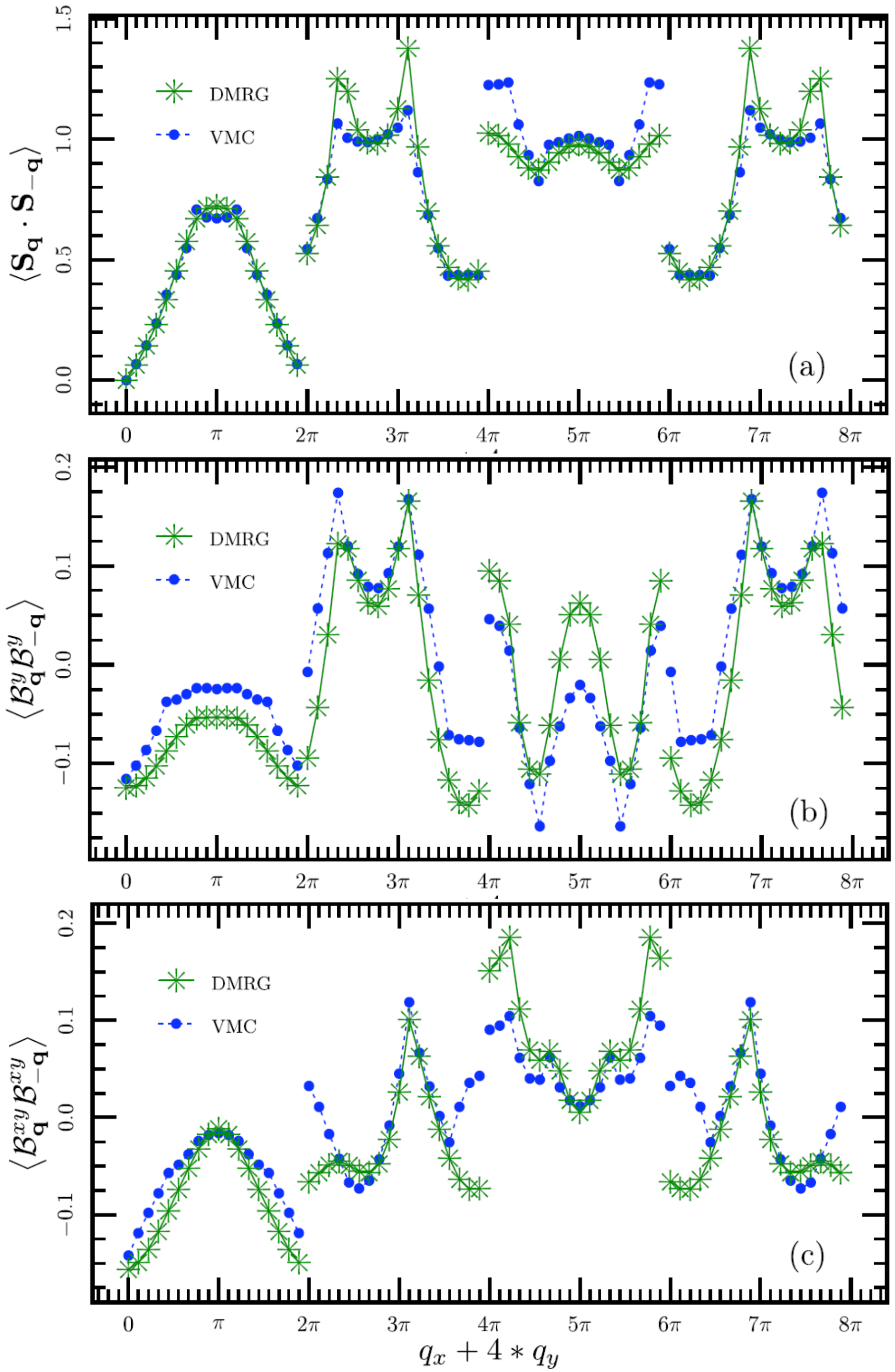
$$K_{\hat{x},\hat{y}} = K_{\hat{x},\hat{x}+\hat{y}} = K_{\hat{y},\hat{x}+\hat{y}} = K$$

Numerical phase diagram from ladders up to 18x4:



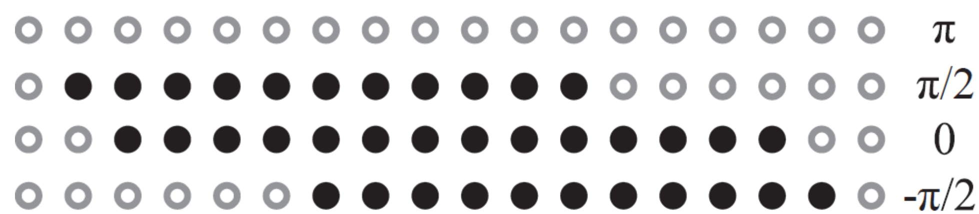
VMC/DMRG comparison

K/J=0.6 on 18x4



DMRG/VMC structure factors essentially do not change for K/J > 0.3

Optimal VMC state:



Low-energy theory:
c=6-1=5 gapless modes,
3 in the spin sector and
2 in the "transverse charge"
(need 2 Luttinger parameters)

Critical evaluation of the 4-leg SBM

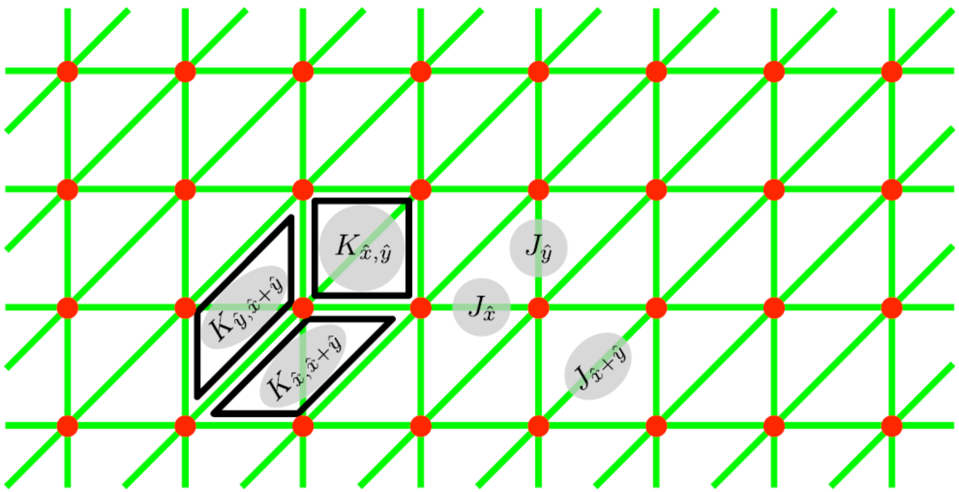
* VMC/DMRG comparisons are not stellar, but reasonable, and we do not know any other states to rationalize the complicated structure factors; note that the apparent features in the spin and dimer correlators occur at the same wavevectors and are of comparable strength –these are properties of the SBM!

* The SBM can in principle be stable, but there many possible instability channels

* The DMRG data so far is suggestive of the SBM phase, but cannot rule out eventual instability and small gaps

* Would like to study larger sizes. Challenge: the state is very entangled and already for 12x4 ladder our maximal DMRG block size barely captures the entanglement entropy

4-leg study interpolating between triangular and square regimes



$$J_{\hat{x}+\hat{y}} < J_{\hat{x}} = J_{\hat{y}}$$

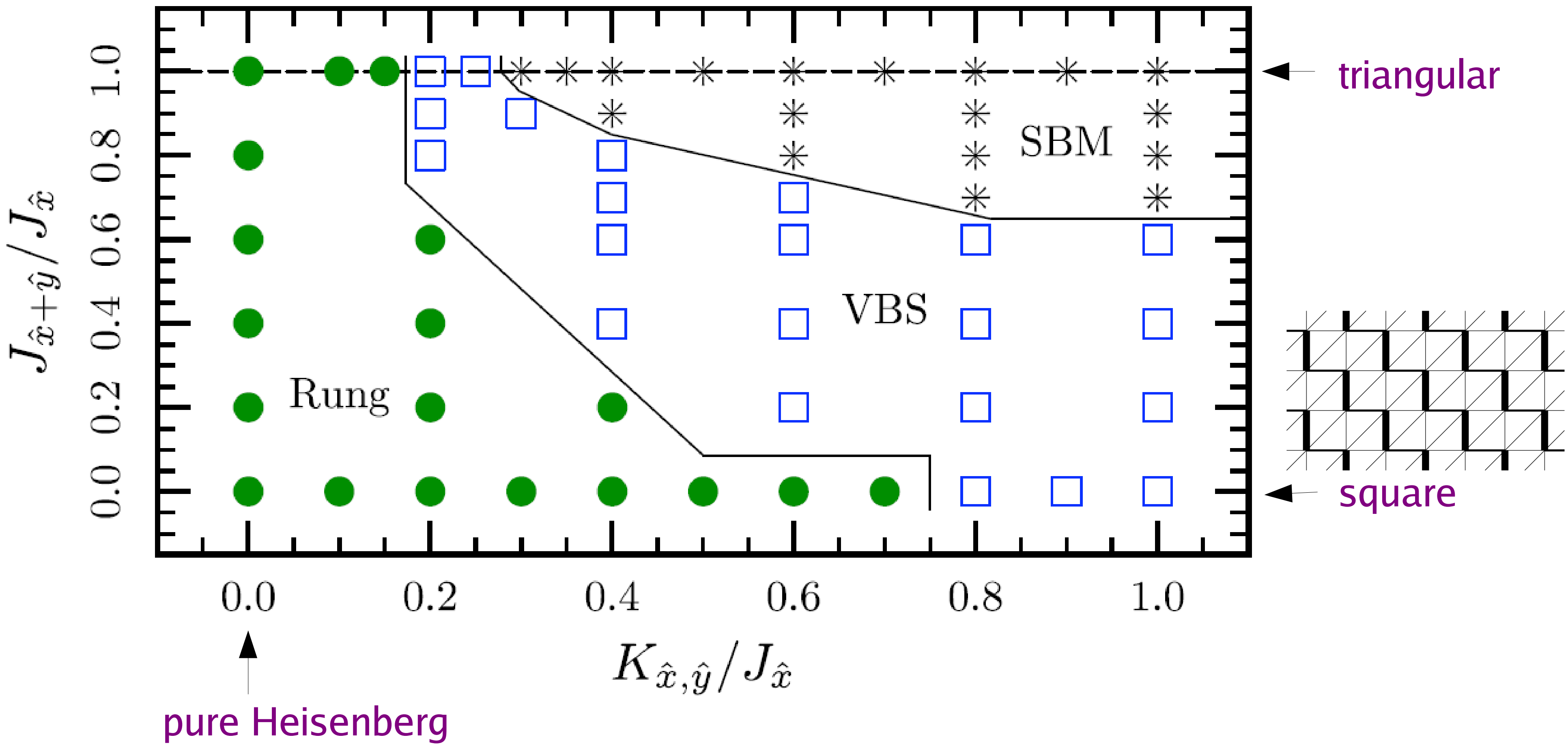
square + weaker frustrating diagonal, appropriate for broader κ–$(ET)_2X$ and $X[Pd(dmit)_2]_2$ families of materials

$$K_{\hat{x},\hat{x}+\hat{y}} = K_{\hat{y},\hat{x}+\hat{y}} = \frac{J_{\hat{x}+\hat{y}}}{J_{\hat{x}}} K_{\hat{x},\hat{y}}$$

-- model anisotropy in the ring exchange couplings, motivated by Hubbard to spin model thinking

$$J_{\hat{a}} \sim t_{\hat{a}}^2/U, \quad K_{\hat{a},\hat{b}} \sim t_{\hat{a}}^2 t_{\hat{b}}^2/U^3 \implies K_{\hat{a},\hat{b}} \sim J_{\hat{a}} J_{\hat{b}}/U$$

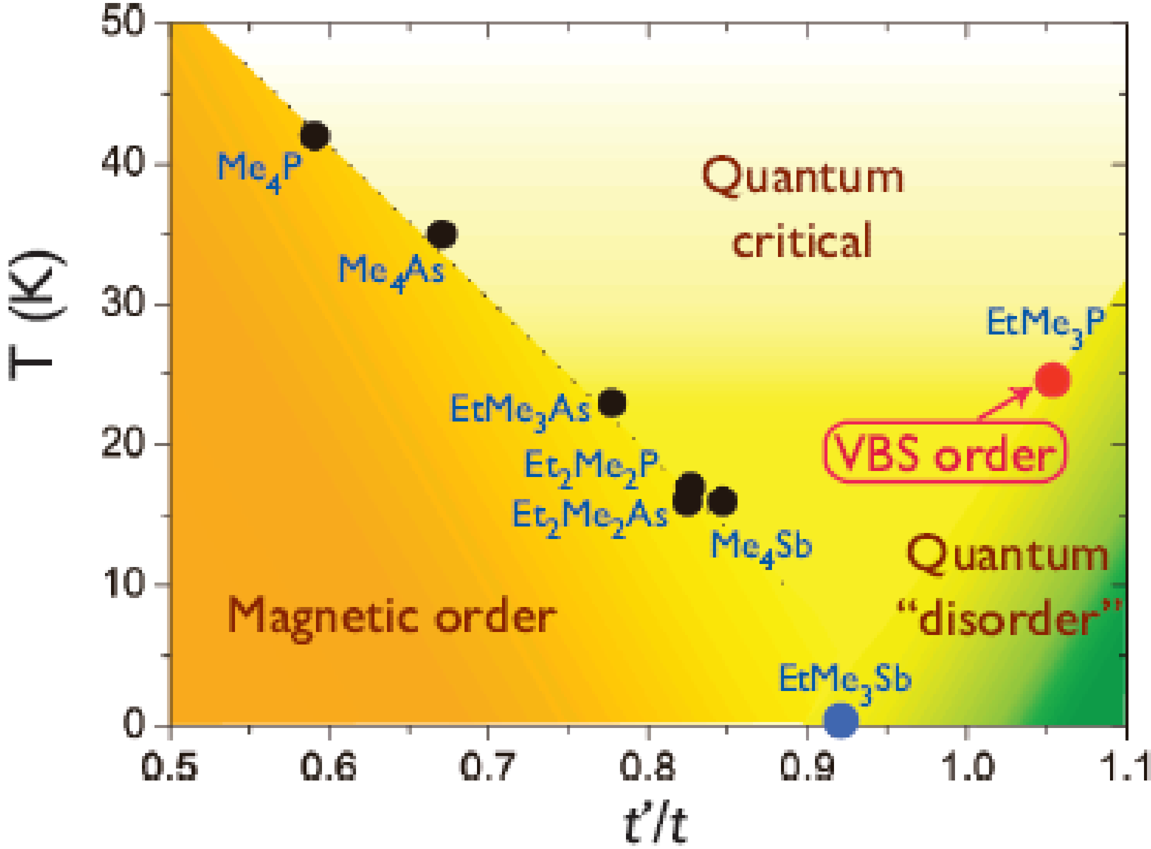
Interpolating between triangular and square



* VBS in the square limit –staggered dimer state (Lauechli et al 05); on the ladder, orients in the transverse direction

* Square rung phase –morally Neel phase restricted to even number of legs

Phases of the $X[Pd(dmit)_2]_2$ family



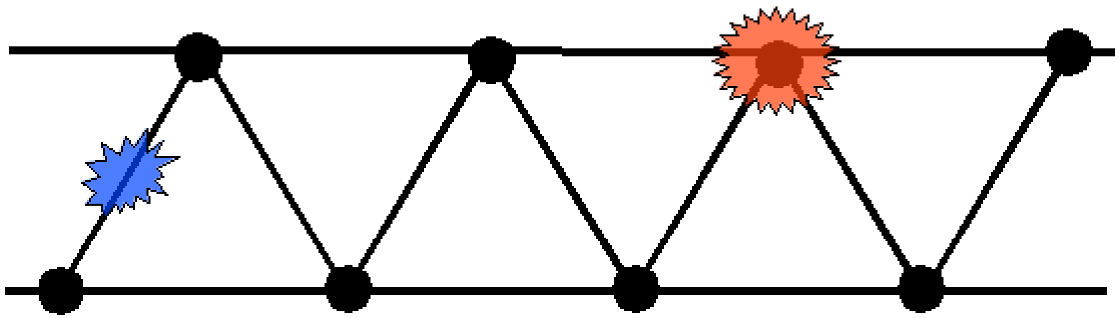
Shimizu et.al. 07
Sachdev 09

- Neel order near the square limit and over large anisotropy range
- spin liquid close to the isotropic regime
- interestingly, realizes VBS order close to the isotropic regime

(caution: material physics may be more complex and/or the simple ring model may be not appropriate)

More lessons from ladders: Textures around non-magnetic impurities

Hsin-Hua Lai and OIM, Phys. Rev. B 79, 235120 (2009)



Static texture in the local energy: $\langle B_{2k_{Fa}}(x) \rangle \sim \dfrac{\cos(2k_{Fa}x + \delta_{2k_{Fa}})}{x^{\frac{1}{2}+\frac{g}{4}}}$

-- slow power law decay (half of the bulk exponent)

Local spin susceptibility: $\chi^{osc}_{2k_{Fa}}(x) \sim x^{\frac{1}{2}-\frac{g}{4}} \cos\left(2k_{Fa}x + \delta'_{2k_{Fa}}\right)$

-- grows away from impurity! (Eggert and Affleck 95)

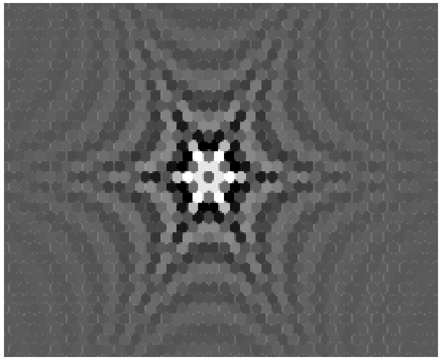
Textures in the 2d spin liquid

Karol Gregor and OIM, Phys. Rev. B 79, 024421 (2009)

Static texture in the local energy density (mean field calculation):

$$\epsilon_{\rm loc}(r) - \bar{\epsilon} \sim \frac{\cos(2k_F r + \phi')}{r^2}$$

Local susceptibility has stronger texture (mf calculation):



$$\chi_{\rm loc}(r) - \bar{\chi} \sim \frac{\cos(2k_F r + \phi)}{r}$$

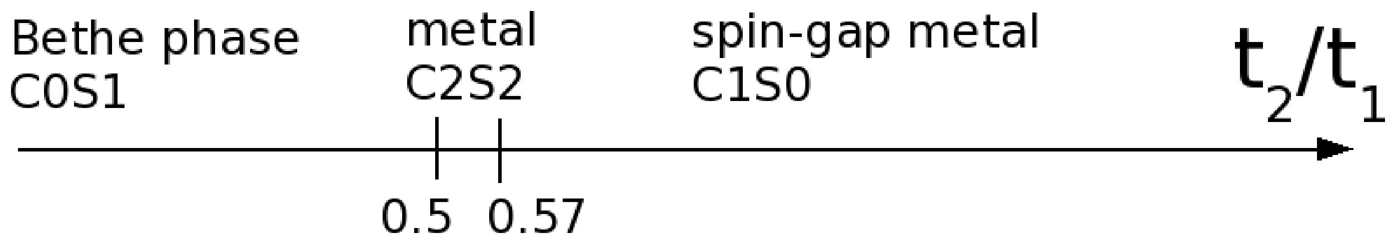
- can lead to strong broadening of NMR lines
- power laws are expected to be modified beyond mean field

(Altshuler et.al. 94, Mross and Senthil 10)

SBM in electronic models (e.g. Hubbard)?

* 2d: need K/J ~ 0.3 to get into the SBM
  Naive estimates from the 2d Hubbard model:
  max(K/J) ~ 0.2-0.3 while remaining in the Mott insulator
– perhaps the SBM can indeed happen, as suggested by a recent study of high-order effective spin model (Yang, Laeuchli, Mila, Schmidt arxiv:1006.5649)

* 2-leg Hubbard model likely does not have the SBM:
  The SBM is C1[ρ-]S2 Mott insulator and is expected to be proximate to the C2S2 metal. However, on-site Hubbard-U gives same weight at all wavevectors and easily causes instabilities in the spin sector. Already in the weak coupling phase diagram (Gros et al), there is only a small sliver of the C2S2 metallic phase:

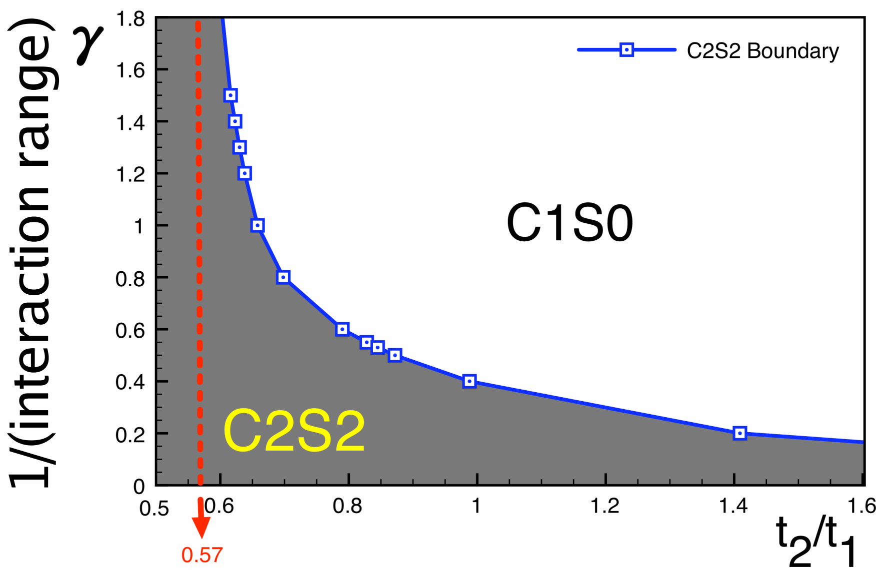


Electronic models with extended repulsion

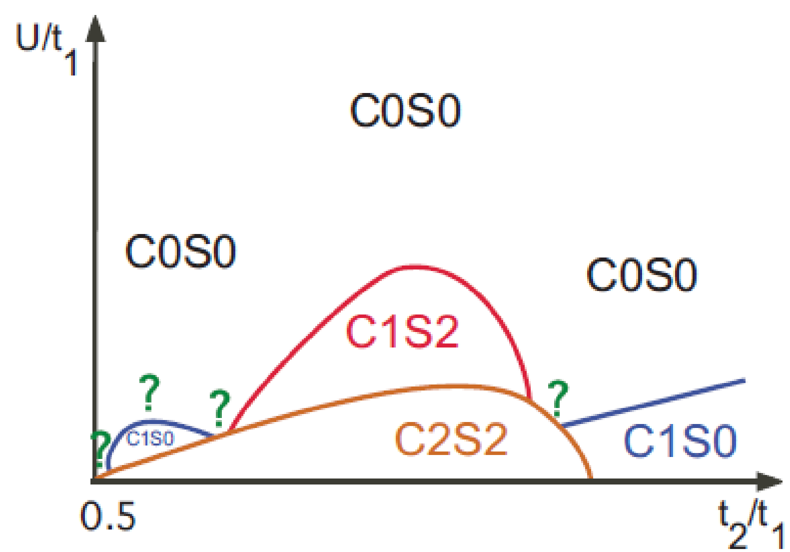
Hsin-Hua Lai and OIM, Phys. Rev. B 81, 045105 (2010)

Idea (Kane, Balents, and Fisher 97): Longer-ranged interactions feed mostly into $V_{q=0}(\partial\theta_{\rho+})^2$, and this overall repulsion suppresses instabilities of the "Fermi surface". Furthermore, increasing this interaction is precisely what we need to make the Umklapp $v_8 \cos(4\theta_{\rho+})$ relevant and induce the C1[ρ-]S2 Mott insulator (SBM) phase

Weak coupling phase diagram with extended interactions:



Schematic intermediate coupling phase diagram proximate to extended C2S2 metal:



Stabilizing role of extended interactions? Strong-coupling thinking

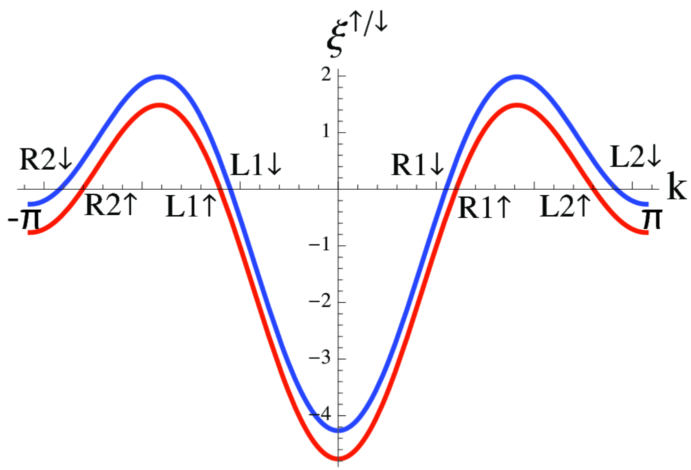
* If the Mott insulating state is driven by longer-ranged repulsion, the role of ring exchanges (also more extended) is likely increased, since local charge motion is less costly compared to the Hubbard-only case. This probably favors the SBM phase.

* In real materials the Coulomb interaction is long-ranged and interactions beyond Hubbard can be important (Nakamura et al 09). Furthermore, the Coulomb is poorly screened near the Mott transition. Perhaps this is helping to stabilize the spin liquids in the 2d triangular materials κ–$(ET)_2Cu_2(CN)_3$ and $EtMe_3Sb[Pd(dmit)_2]_2$?

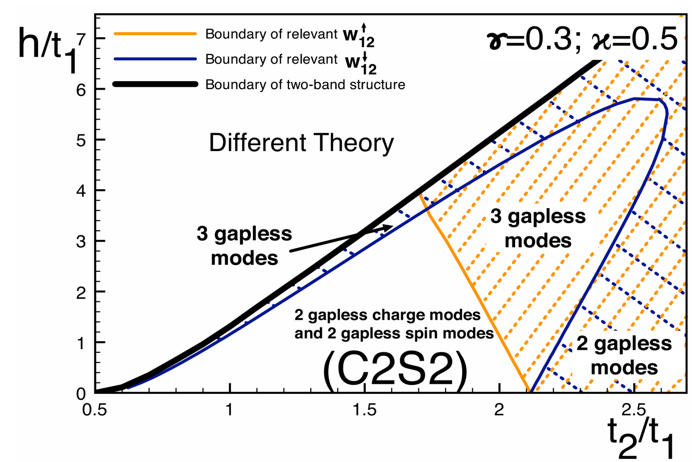
Instabilities of the SBM in Zeeman field?

Hsin-Hua Lai and OIM, Phys. Rev. B 82, 125116 (2010)

2-leg ladder study; dispersion with Zeeman-split Fermi seas



Weak coupling phase diagram, starting from the C2S2 metal stabilized by extended interactions



Instabilities of the C2S2 metal driven by terms like

$$w^{\uparrow}_{12}(c^{\dagger}_{R1\uparrow}c^{\dagger}_{L1\uparrow}c_{L2\uparrow}c_{R2\uparrow} + H.c.)$$

-- smth like "Cooper pairing" in the up-spin system

Mott insulating states are obtained by further gapping out the overall charge mode ("Gutzwiller projection")

Possible generalizations to 2d

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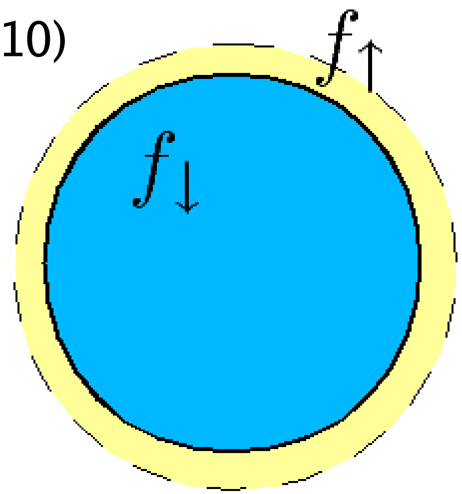

1) Pair the $f_\uparrow$ spinons, while leaving the $f_\downarrow$ Fermi sea intact

Interesting properties:

* gapless Fermi sea of spin-down spinons, hence metal-like specific heat, Pauli spin susceptibility, thermal conductivity (note that the gauge field is Higgsed out)

* spin-1 excitations are gapped (S^+ correlations decay exponentially) –can look like a gapped system in NMR with spin-1/2 nuclei

* spin-2 excitations are gapless (spin-nematic $N(r)=S^+(r)S^+(r+a)$ has $1/r^3$ power law correlations)

* S^z correlations are power law oscillating at $2k_F$ of the down-FS

2) Pairing within each spinon species --> spin-nematic order

Summary, open questions, outlook

1) Does the spinon Fermi sea state persist in the ring model to 2d?

- 2-leg, 4-leg suggest "maybe", but with the DMRG we hit entanglement wall with periodic bc already on the 4-leg
- use open-bc? try more 2d-like samples? use SU(2) invariance? target momentum eigenstates?
- new algorithms? (branching MERA?)

2) Is the resulting 2d phase described by 2d spinon-gauge theory?

- our quasi-1d treatment "2N -> 2N-1 gapless modes"(eliminating the overall charge mode) are fun on 2-leg, 4-leg, but likely fails to connect to the 2d spinon-gauge theory
- how to improve the Gutzwiller wavefunctions (which likely become less accurate and fail qualitatively to capture spatial gauge fluctuations)? How do gauge fluctuations affect the degree of entanglement?
- maybe there is some Spin Bose-Metal phase but the spinon-gauge is not a good description; non-(parton-gauge) descriptions?