Quantum Spin-Metals in Weak Mott Insulators

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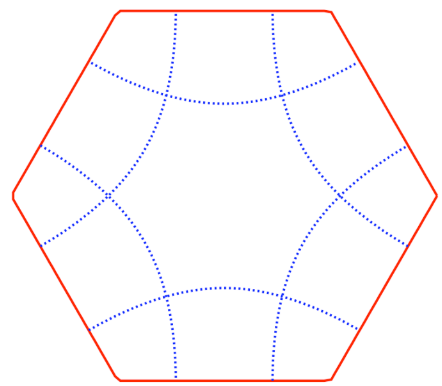
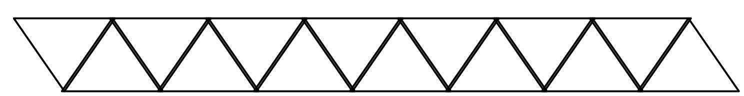
Quantum Critical Phenomena conference
Toronto 9/27/08

"Quantum Spin-metals" - spin liquids with "Bose surfaces"

singular spin correlations
on ***surfaces*** in momentum space



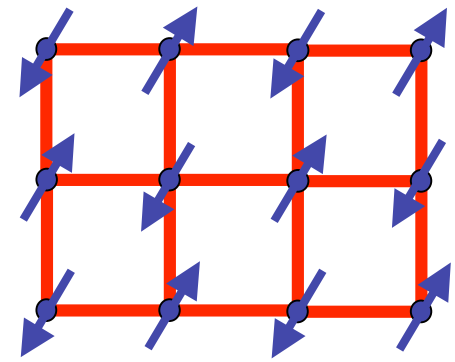
- "Spin-metals" have ***tractable quasi-1d descendents***,
- Approach/access 2d spin-metals via quasi-1d "ladders"



Spin liquids

Mott insulator - Insulating materials with an odd number of electrons/unit cell

Spin Liquids - Mott insulator with no broken symmetries



3 Classes of spin liquids

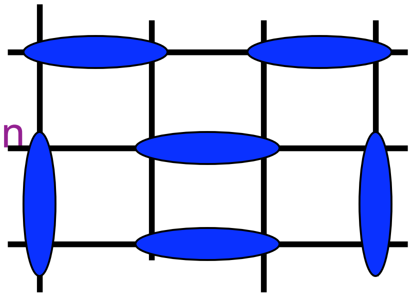
1) Topological Spin Liquids

2) Critical ("algebraic") Spin Liquids

3) "Quantum Spin Metals"

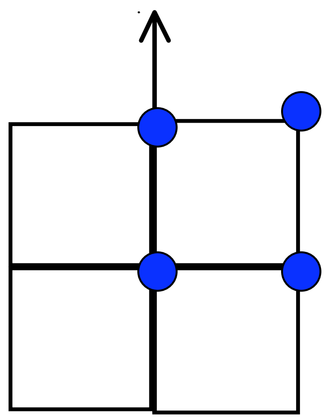
Topological Spin Liquids

- ***Spin gap***
- “Particle” excitations with fractional quantum numbers, eg spinon
- Simplest is short-ranged RVB, Z_2 Gauge structure



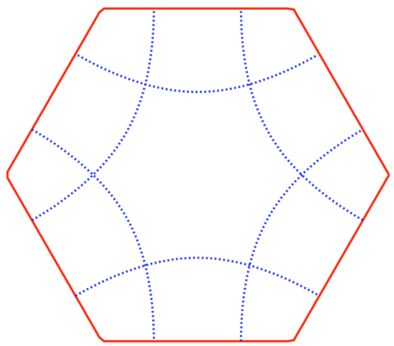
Critical Spin Liquids

- ***Stable gapless phase*** with no broken symmetries
- no free particle description
- Power-law correlations at finite set of discrete momenta



“Quantum spin metals”

Gapless spin liquids with spin correlation functions singular along surfaces in momentum space

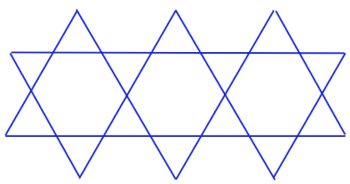


“Bose Surfaces”

2 Routes to gapless spin liquids

1.) Frustration, low spin, low coordination number

Kagome lattice AFM



- Iron Jarosite, $KFe_3\,(OH)_6\,(SO_4)_2$: Fe^{3+} s=5/2 , $f = T_{cw}/\,T_N \sim 20$
- 2d "spinels" $SrCr_8Ga_4O_{19}$ Cr^{3+} s=3/2, $f \sim 100$
- Volborthite $Cu_3V_2O_7(OH)_2\;2H_2O$ Cu^{2+} s=1/2 $f \sim 75$
- Herbertsmithite $ZnCu_3(OH)_6Cl_2$ Cu^{2+} s=1/2 , $f > 600$

(Candidate "critical" spin liquids)

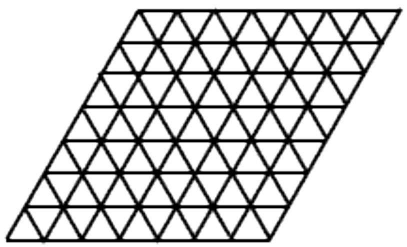
2.) Quasi-itinerancy: "weak" Mott insulator with small charge gap

Charge gap comparable to exchange J - Significant charge fluctuations

→ ***Quantum "Spin-metal" ?***

Candidate ***Triangular*** Lattice Weak Mott Insulators

- 2d Wigner crystal of electrons (eg. Si MOSFET)
- Monolayer of 3-He absorbed on a substrate
- Triangular lattice organic Mott insulators

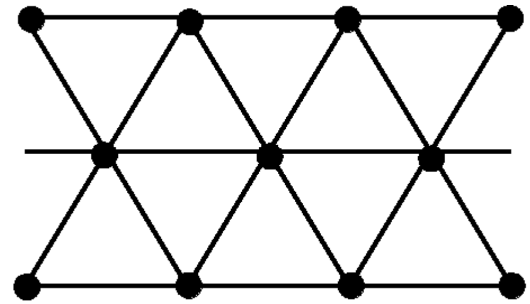


- K-$(ET)_2Cu_2(CN)_3$ Kanoda et al
- $EtMe_3Sb[Pd(dmit)_2]_2$ R. Kato et. al.

Also, possibly 3d hyper-kagome compound, $Na_4Ir_3O_8$

“Best” Candidate spin-metal: $\kappa-(ET)_2Cu_2(CN)_3$

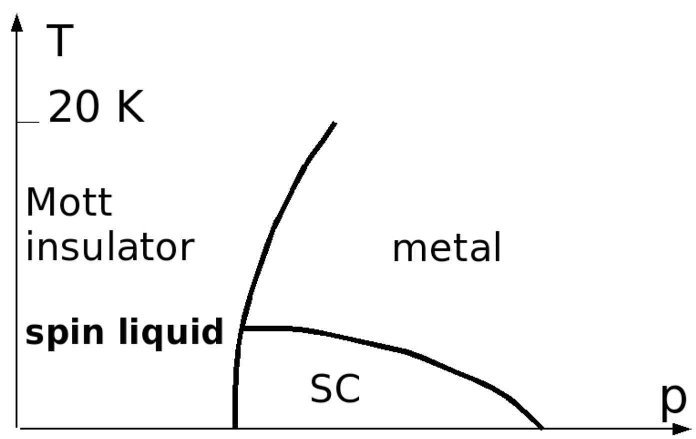
Motrunich (2005) , S. Lee and P.A. Lee (2005)
suggested spin liquid with spinon Fermi surface



- Modelled as triangular Hubbard at half-filling
- Just on the Insulator side
- No magnetic order down to 20mK ~ 10^{-4} J
- Many gapless spin excitations – as many as in a metal with Fermi surface
- Large spin entropy – more than in a metal!

NMR, μSR, χ

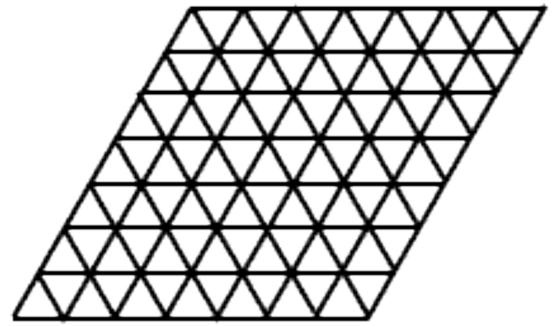
t = 55meV; U/t = 8
-> J ~ 250K



Kurosaki et.al. 05; Shimizu et.al. 03

Hubbard model on triangular lattice

$$\mathcal{H} = -t \sum_{\langle ij \rangle} [c^\dagger_{i\alpha} c_{j\alpha} + h.c.] + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

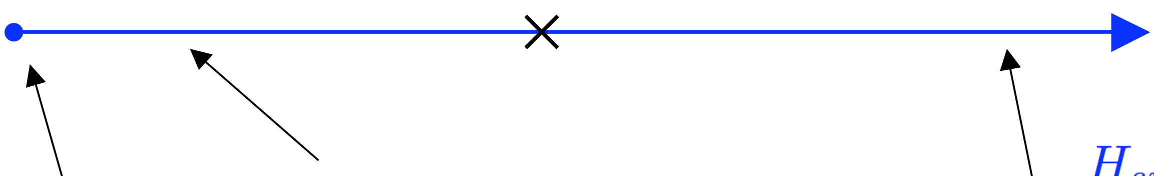


Phase diagram at Half filling?

Weak coupling

Strong coupling

metal ????? insulator



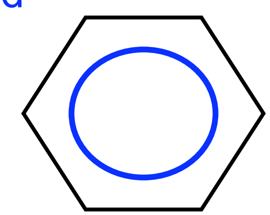
U/t

0

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

Free Fermi gas,
un-nested

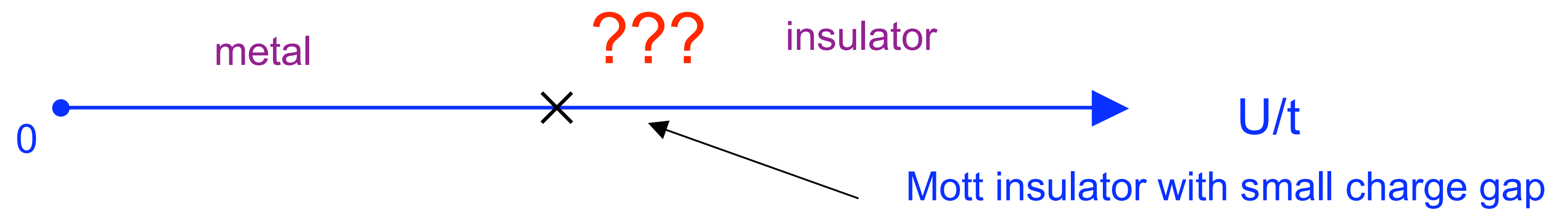
Fermi liquid



Heisenberg n.n. AFM
3-sublattice Neel state

$J = t^2/U$

"Weak" Mott insulator - Ring exchange



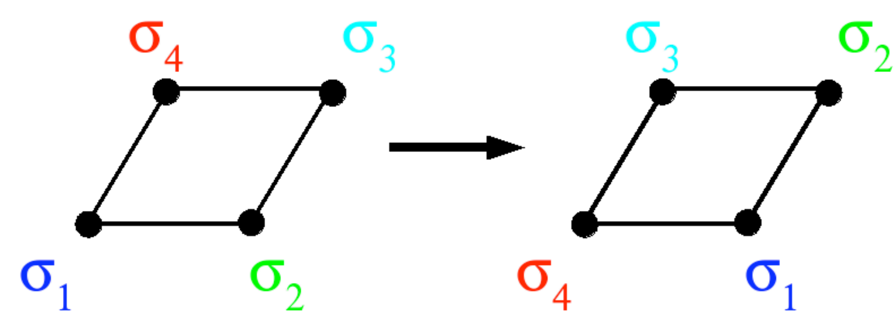
$$\hat{H}_{\mathrm{Hubbard}} = -t \sum_{ij} c^{\dagger}_{i\alpha} c_{j\alpha} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Insulator --> effective spin model

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

Ring exchange:
(mimics charge
fluctuations)

P_{1234} :



Slave-fermion approach: Only game in town

Fermionic representation of spin-1/2

$$\mathbf{S}_i = f_i^\dagger \frac{\boldsymbol{\sigma}}{2} f_i; \qquad f_{i\alpha}^\dagger f_{i\alpha} = 1;$$

General “Hartree-Fock” in the singlet channel

$$\mathcal{H}_{\rm trial} = -\sum_{ij} t_{ij} f_{i\alpha}^\dagger f_{j\alpha}$$

$$\longrightarrow \quad |\Psi_0\rangle \quad \longrightarrow \quad |\Psi_{\rm spin}\rangle = P_G(|\Psi_0\rangle)$$

free fermions — spins — Gutzwiller projection

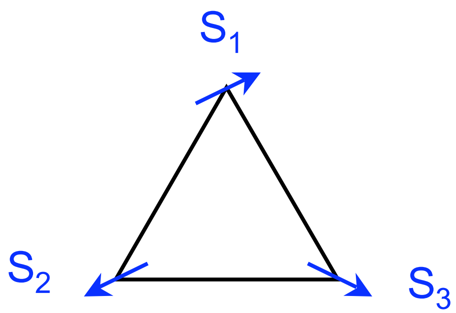
- easy to work with numerically – VMC (Ceperley 77, Gros 89)

Gauge structure

$$\mathcal{H}_{\text{trial}} = -\sum_{ij} t_{ij} f^\dagger_{i\alpha} f_{j\alpha} = -\sum_{ij} |t_{ij}| e^{i a_{ij}} f^\dagger_{i\alpha} f_{j\alpha}$$

variational parameter

Slow spatial variation of the phases a_{ij} produces only small trial energy change ~ (curl a)^2

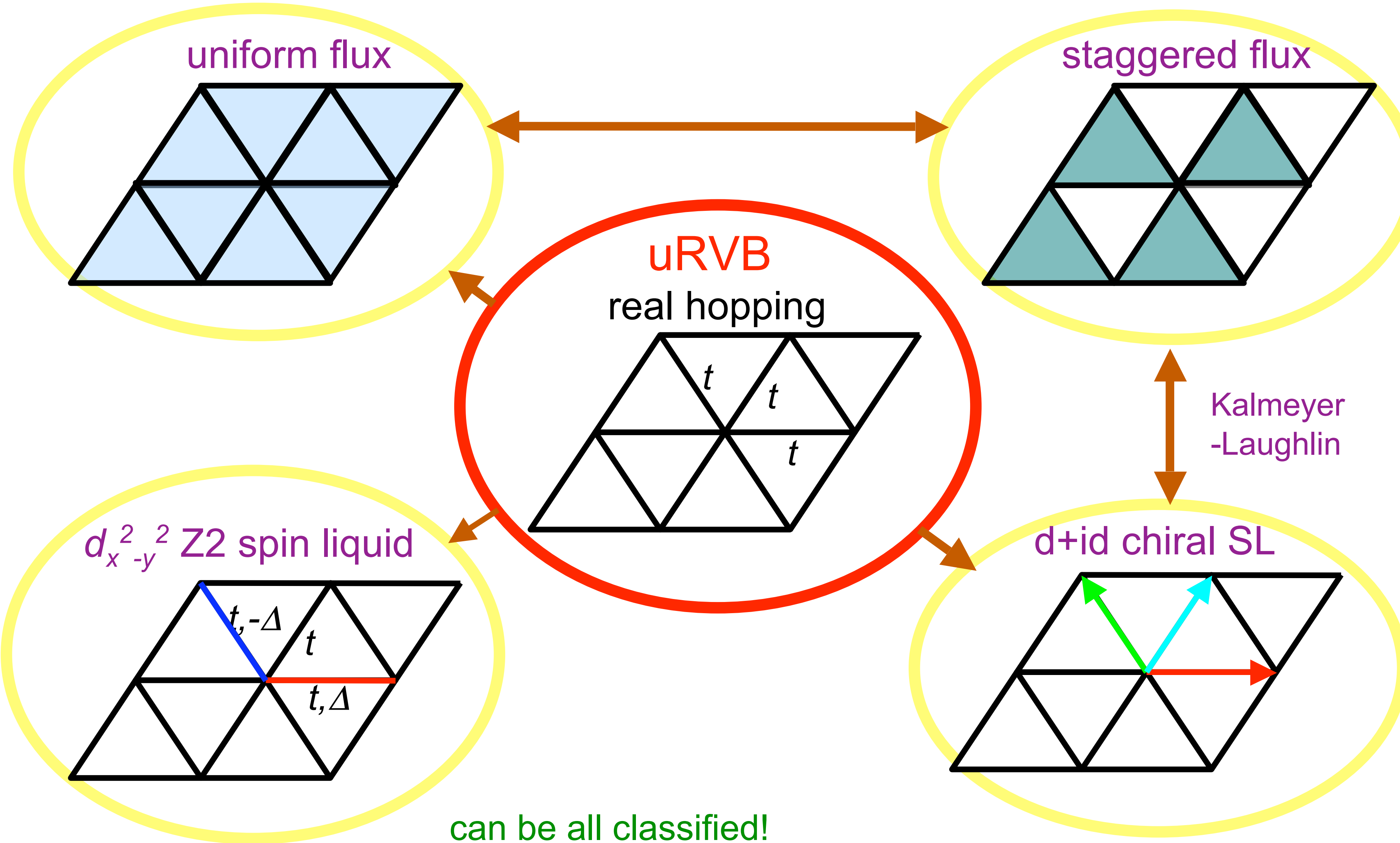


Physics of gauge flux: Spin chirality

$$\nabla \times a \sim \vec{S}_1 \cdot (\vec{S}_2 \times \vec{S}_3)$$

→ need to include a_{ij} as dynamical variables

Examples of “fermionic” spin liquids



can be all classified!

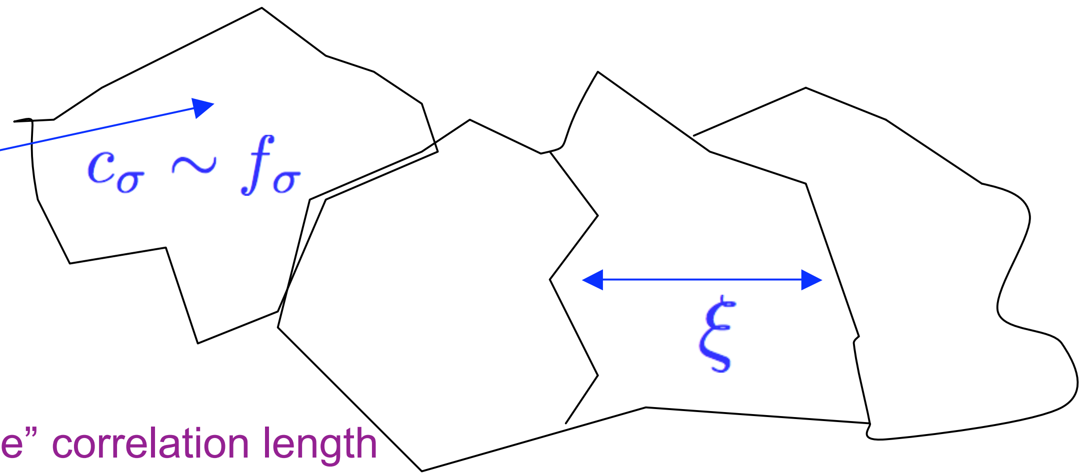
Wen 2001; Zhou and Wen 2002

Weak Mott insulator: Which spin liquid?

Motrunich (2005)

Long charge correlation length, $\langle c_\sigma(x) c_\sigma^\dagger(0) \rangle \sim e^{-x/\xi}$ $\xi >> a$

Inside correlation region electrons do not "know" they are insulating, they are "essentially" spinons

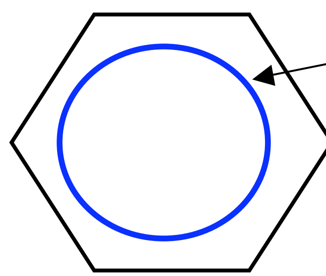


Guess: ***Spin*** correlations "inside" correlation length "resemble" spin correlations of free fermion metal. oscillating at $2k_F$

$$\langle \vec{S}(x) \cdot \vec{S}(0) \rangle \sim \cos(2k_F x)/x^{3/2}$$

Appropriate spin liquid:

Gutzwiller projected Filled Fermi sea ("spin-metal")



Spinon fermi surface

Gutzwiller-projected Fermi Sea

$$P_G \left(|\text{Fermi Sea}\rangle = \prod_{k<k_F} c^{\dagger}_{k\uparrow} c^{\dagger}_{k\downarrow} |vac\rangle \right)$$

$$= a|(\uparrow)\ (\uparrow)\ (\downarrow)\ (\uparrow)\ (\downarrow)\ (\uparrow)\rangle + b|(\uparrow\downarrow)\ (0)\ (\downarrow)\ (\uparrow)\ (\uparrow)\ (\downarrow)\rangle$$

$$+c|(\uparrow)\ (\downarrow)\ (\downarrow)\ (\uparrow\downarrow)\ (\uparrow)\ (0)\rangle + d|(\downarrow)\ (\uparrow)\ (\uparrow)\ (\downarrow)\ (\uparrow)\ (\downarrow)\rangle + \ldots$$

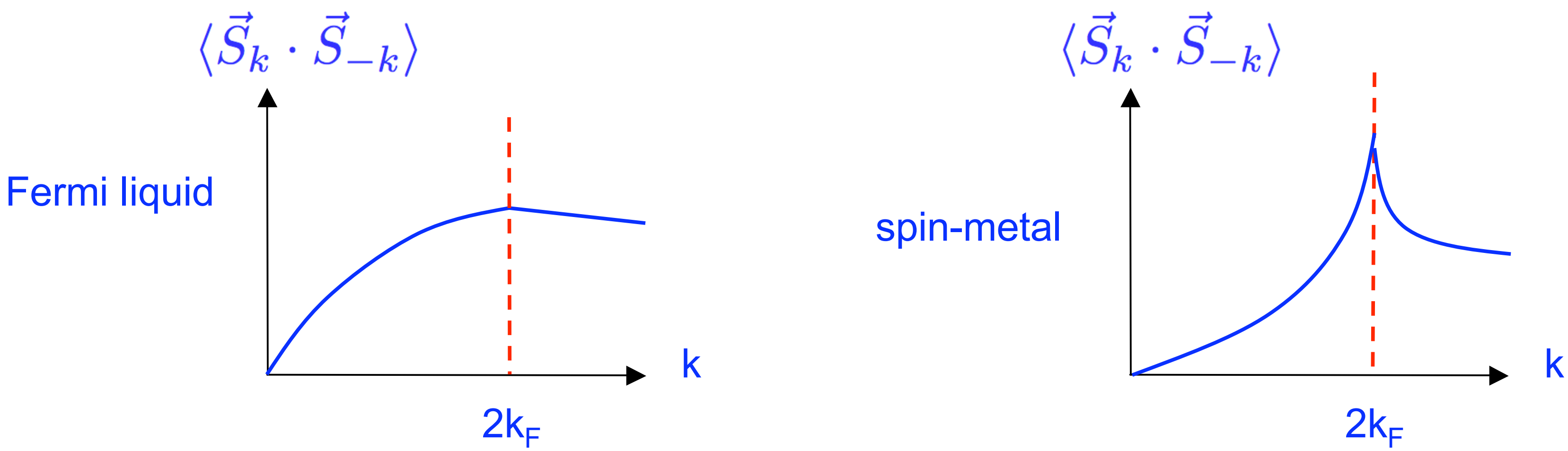
real-space configurations

-- insulator wave function (Brinkman-Rice picture of Mott transition)

$$\Psi_{\text{spin}}(\{R\uparrow\},\{R'\downarrow\}) = \det[R\uparrow]\det[R'\downarrow](-1)^{p(\{R\uparrow\},\{R'\downarrow\})}$$

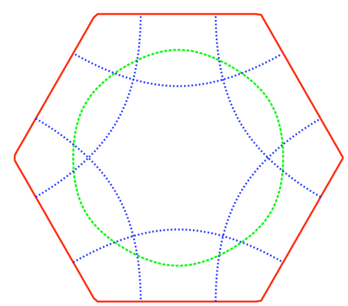
Phenomenology of Spinon Fermi sea state; Gauge theory

Singular spin structure factor at $2k_F$ in “spin-metal”
(more singular than in Fermi liquid metal)



Spin-metal: more low energy excitations than a real metal, “soft” spin-chirality fluctuations

$$C_{\mathrm{uRVB}} \sim k_B t_{\mathrm{spinon}}^{1/3} (k_B T)^{2/3} > C_{\mathrm{metal}} \sim k_B (k_B T)$$

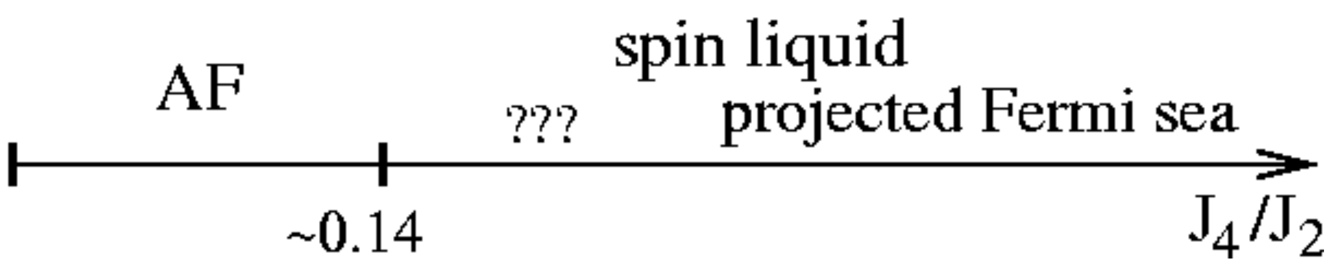


$2k_F$ “Bose surface” in triangular lattice spin-metal

But is Spinon Fermi sea actually the ground state of Triangular ring model (or Hubbard model)?

$$\hat{H}_{\rm ring} = J_2 \sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + J_4 \sum_{\rm rhombi} (P_{ijkl} + {\rm h.c.})$$

Variational Monte Carlo analysis suggests it might be for $J_4/J_2 > 0.3$ (O. Motrunich - 2005)



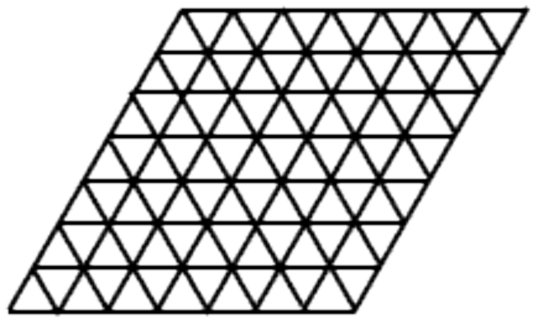
A theoretical quandary: Triangular ring model is intractable

- Exact diagonalization: so small,
- QMC - sign problem
- Variational Monte Carlo - biased
- DMRG - problematic in 2d

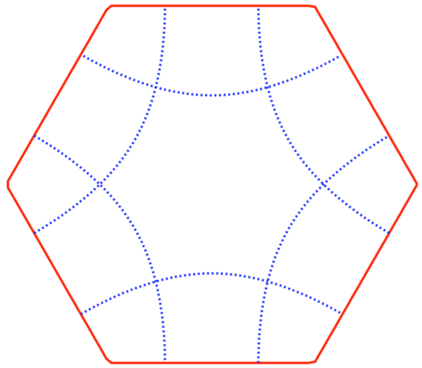
?????

Ladders to the rescue:

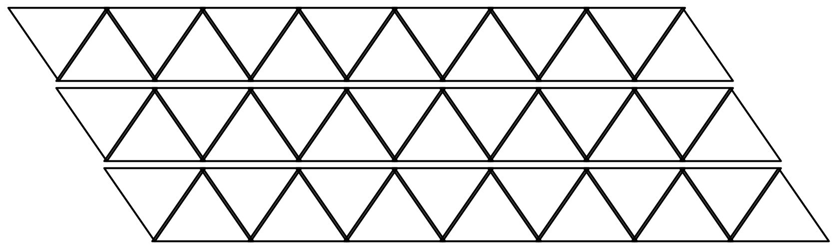
2d Triangular lattice



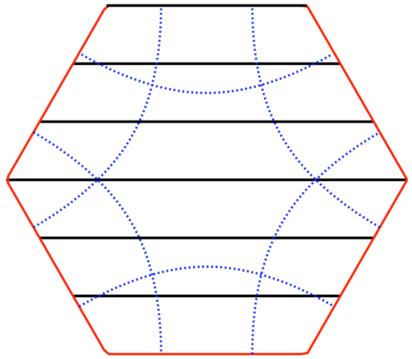
2d Bose surfaces



Quasi-1d Zigzag “strips”:

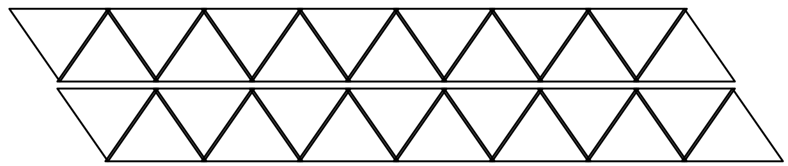


Fingerprint of 2d Bose surface
many gapless 1d modes, of order N

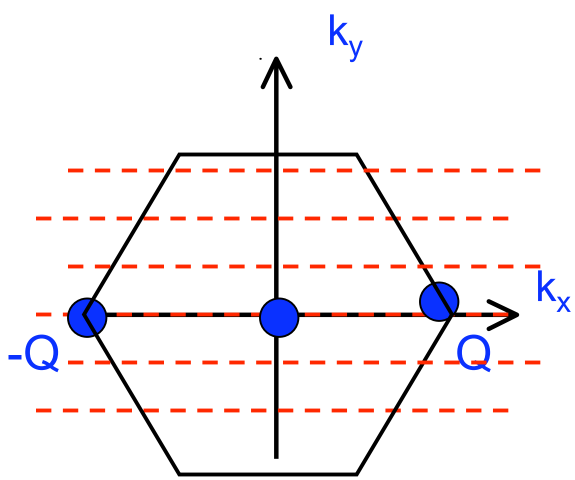


Quasi-1d route to "Spin-Metals"

Triangular strips:

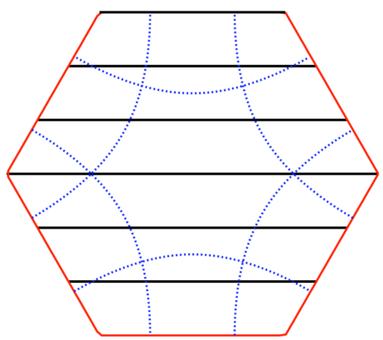


Neel or Critical Spin liquid



Few gapless 1d modes

Spin-Metal

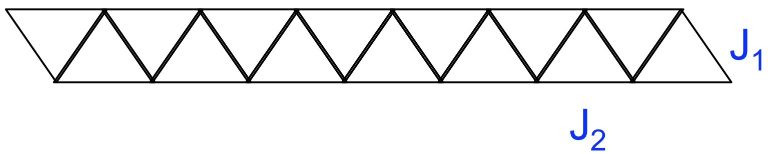


Fingerprint of 2d singular surface - many gapless 1d modes, of order N

New spin liquid phases on quasi-1d strips, each a descendent of a 2d spin-metal

2-leg zigzag strip

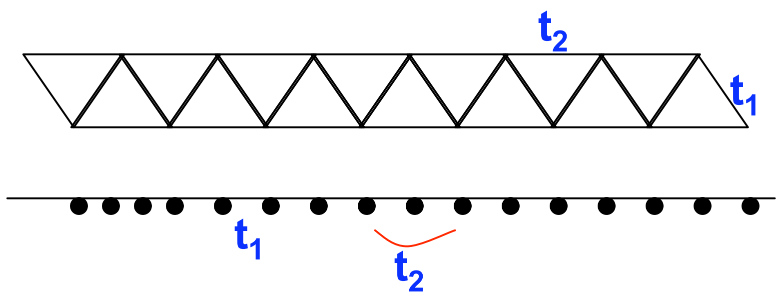
$$\mathcal{H}_\Delta = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + K \sum_{\langle 1234 \rangle} [\mathcal{P}_{1234} + \mathcal{P}^{-1}_{1234}]$$



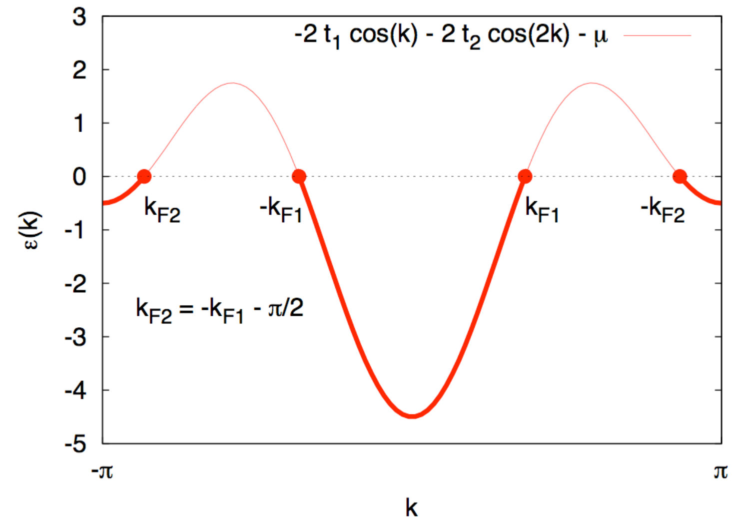
Analysis of J_1-J_2-K model on zigzag strip

Exact diagonalization
Variational Monte Carlo of Gutzwiller wavefunctions
Bosonization of gauge theory
DMRG

Gutzwiller Wavefunction on zigzag



$$\mathcal{H}_{\text{trial}} = -\sum_{ij} t_{ij} f^\dagger_{i\alpha} f_{j\alpha}$$



Spinon band structure

$\rightarrow |\Psi_0\rangle \rightarrow |\Psi_{\text{spin}}\rangle = P_G(|\Psi_0\rangle)$

free fermions — spins — Gutzwiller projection

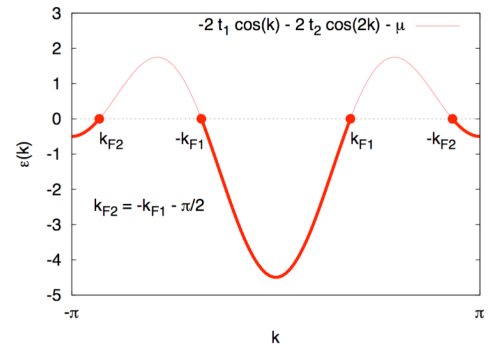
Single Variational parameter: t_2/t_1 or k_{F2}

$(k_{F1}+k_{F2} = \text{pi}/2)$

Bosonize Quasi-1d Gauge Theory

Linearize around the
two sets of Fermi points

$$f_\alpha(x) = \sum_{a,P} e^{iPk_{Fa}x} f_{Pa\alpha}$$



Bosonize

$$f_{Pa\alpha} \sim e^{i(\varphi_{a\alpha} + P\theta_{a\alpha})}$$

Integrate out the gauge field

"Fixed-point" theory of zigzag spin-metal, $\mathcal{L}_{s\ell} = \mathcal{L}_\sigma + \mathcal{L}_\chi$

Two gapless spin modes

$$\mathcal{L}_\sigma = \frac{1}{2\pi} \sum_{a=1,2} \left[\frac{1}{v_a} (\partial_\tau \theta_{a\sigma})^2 + v_a (\partial_x \theta_{a\sigma})^2 \right]$$

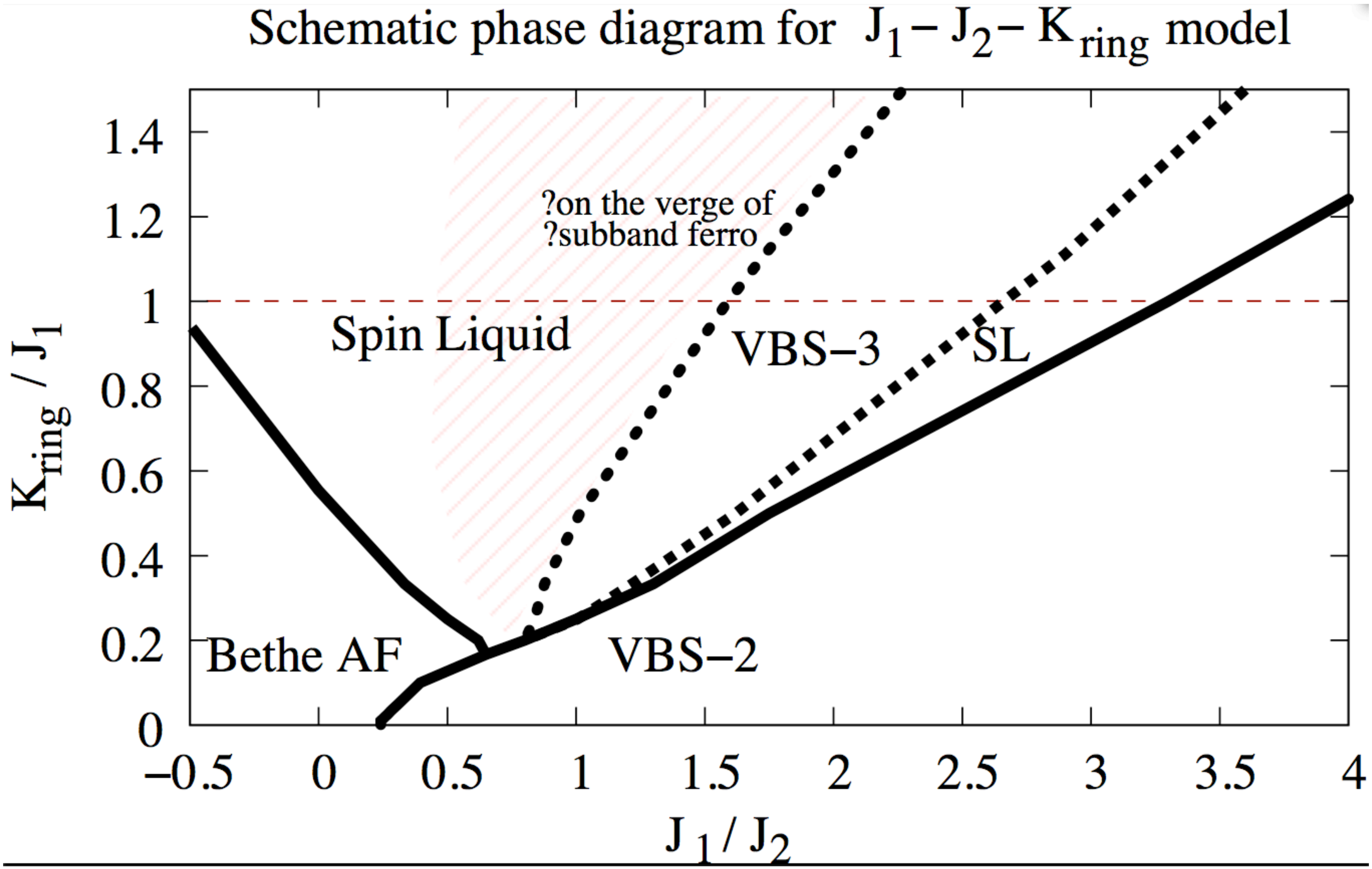
Gapless spin-chirality mode

$$\mathcal{L}_\chi = \frac{1}{2\pi g} \left[\frac{1}{v} (\partial_\tau \theta_\chi)^2 + v (\partial_x \theta_\chi)^2 \right]$$

$$\chi = \vec{S}_{x-1} \cdot [\vec{S}_x \times \vec{S}_{x+1}] \qquad \chi \sim \partial_x \varphi_\chi$$

3 harmonic modes, 3 velocities + one Luttinger
parameter g<1

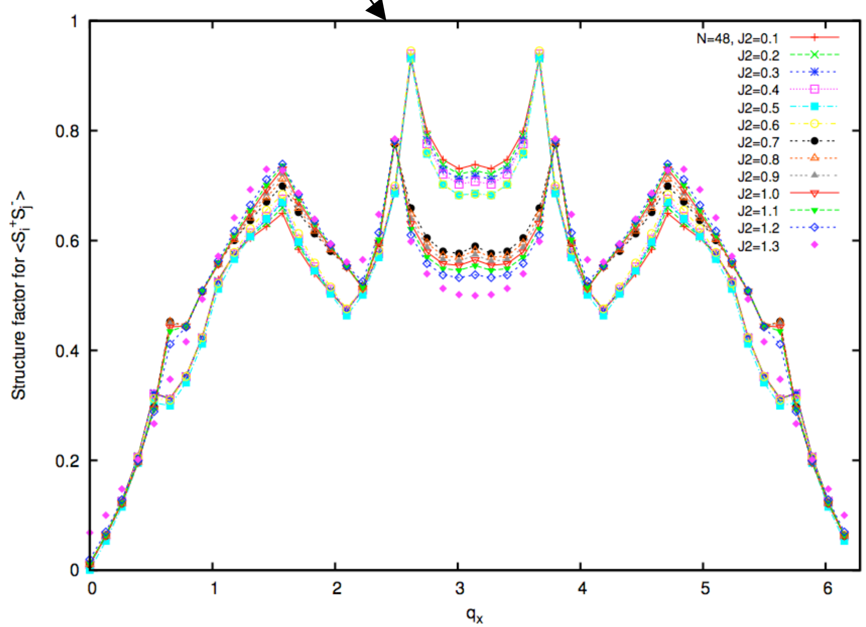
Phase diagram of zigzag ring model



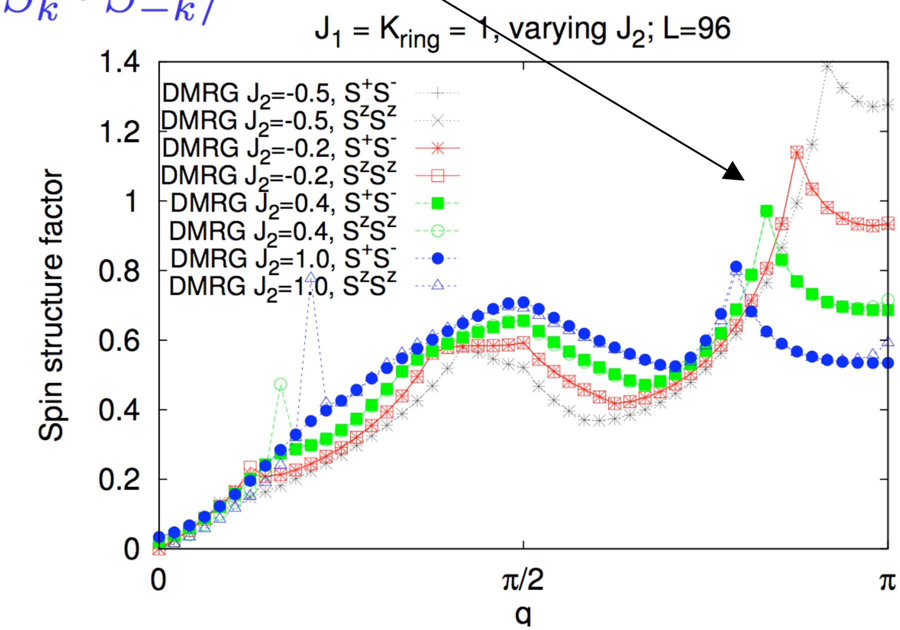
Spin Structure Factor in Spin-liquid; DMRG

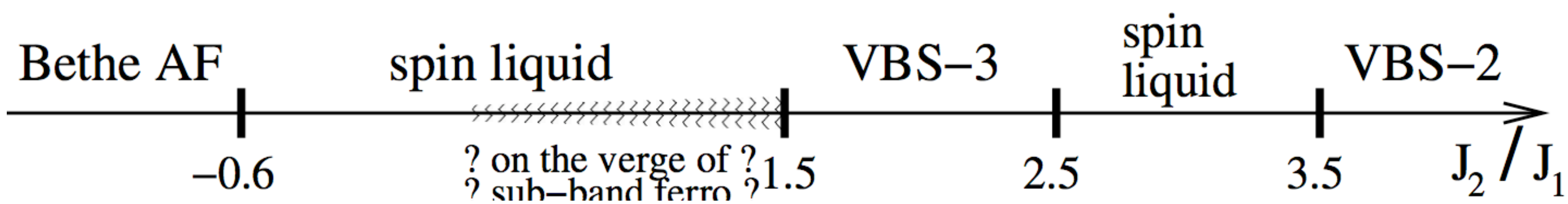
Singularities in momentum space locate the "Bose" surface (points in 1d)

$\langle \vec{S}_k \cdot \vec{S}_{-k} \rangle$



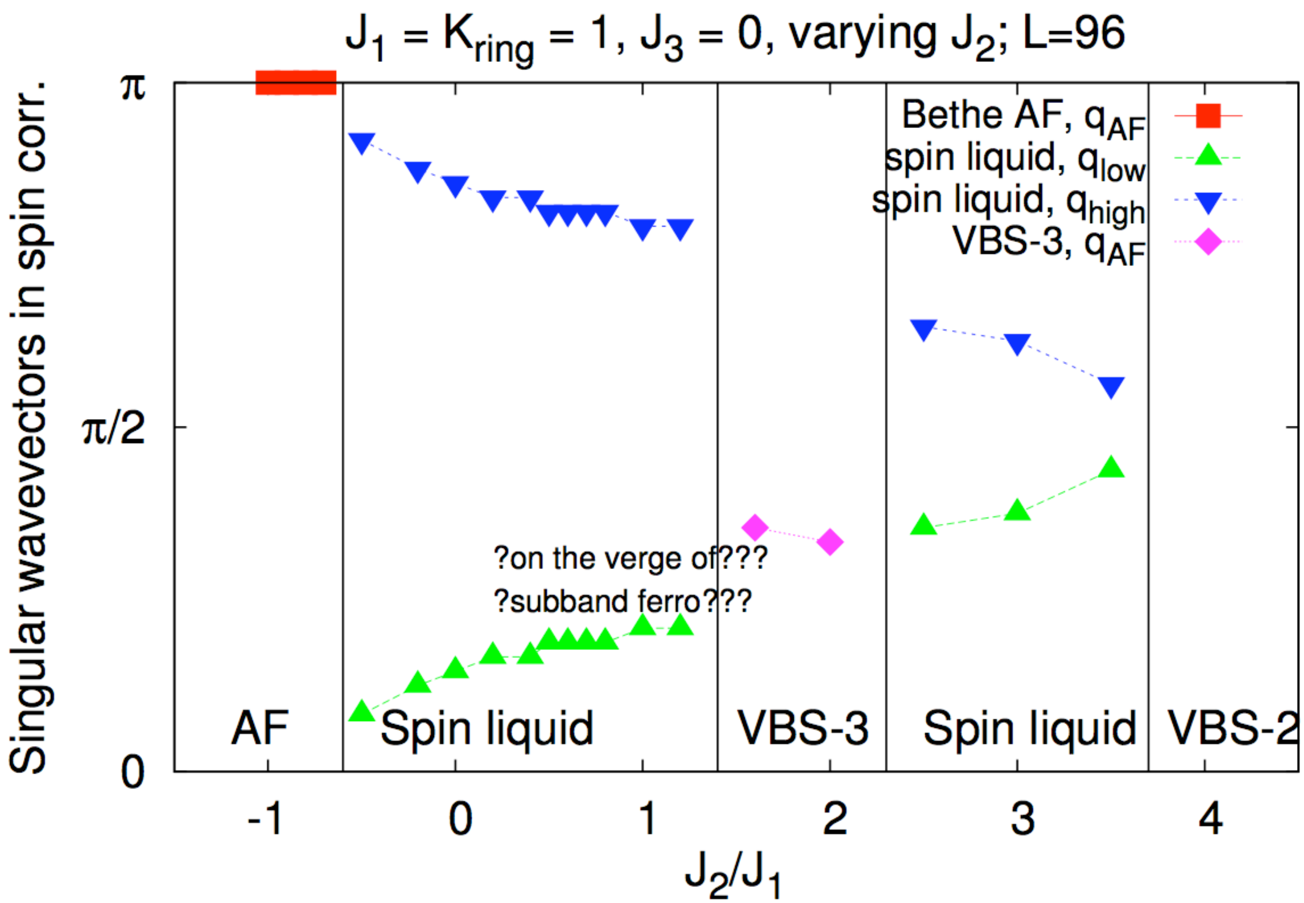
$\langle \vec{S}_k \cdot \vec{S}_{-k} \rangle$





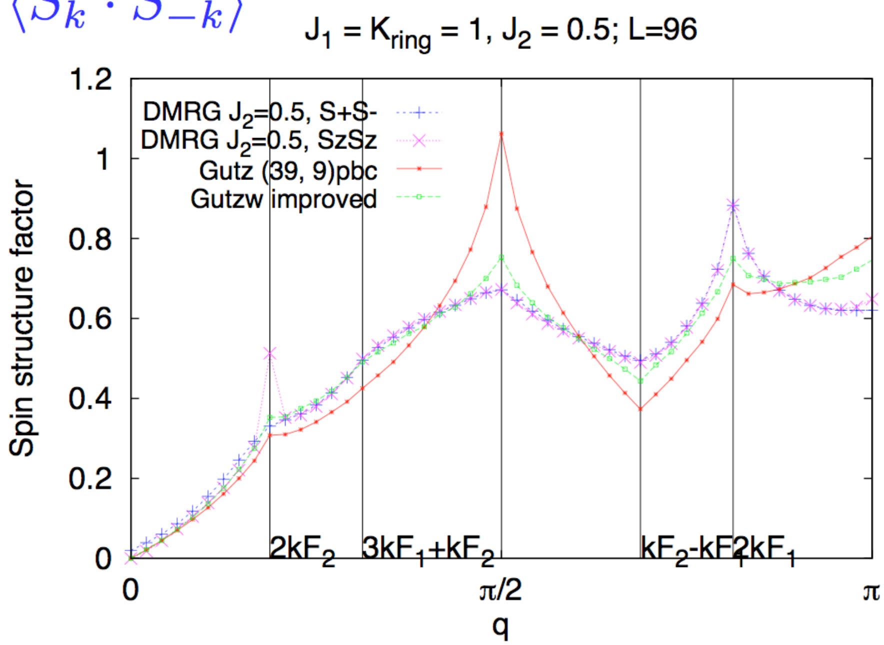
Evolution of singular momentum ("Bose" surface)

DMRG

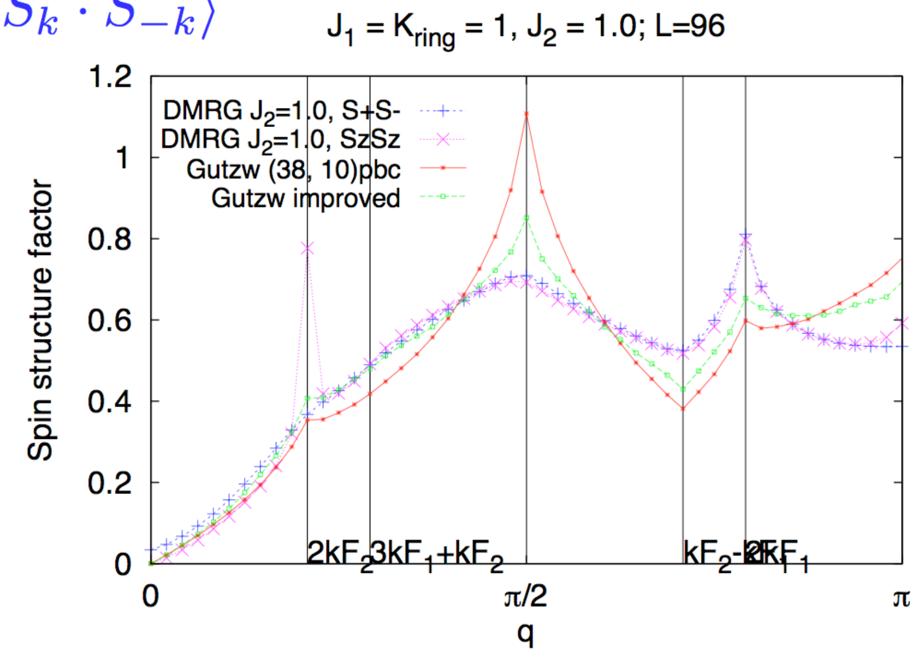


DMRG ***and*** VMC spin structure factor

$\langle \vec{S}_k \cdot \vec{S}_{-k} \rangle$

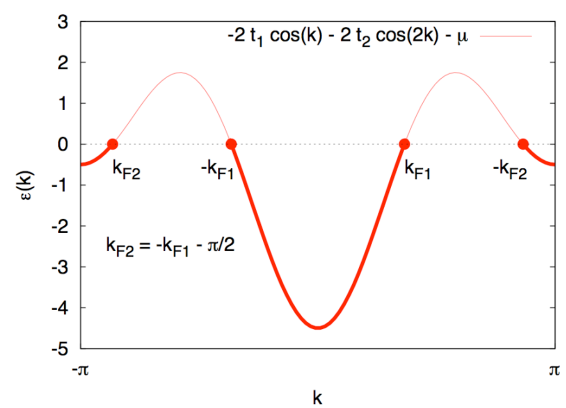


$\langle \vec{S}_k \cdot \vec{S}_{-k} \rangle$

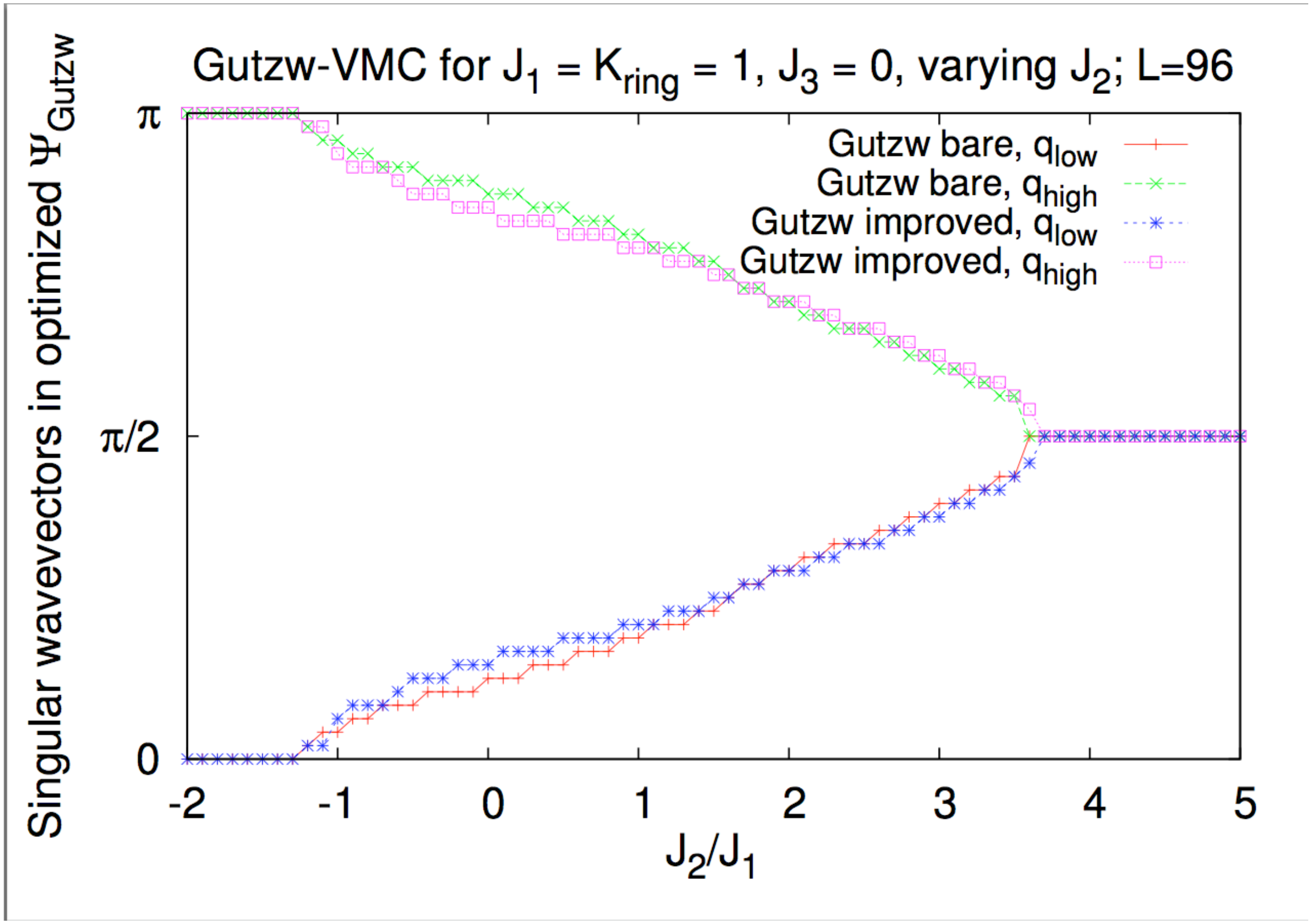


(Gutzwiller improved has 2 variational parameters)

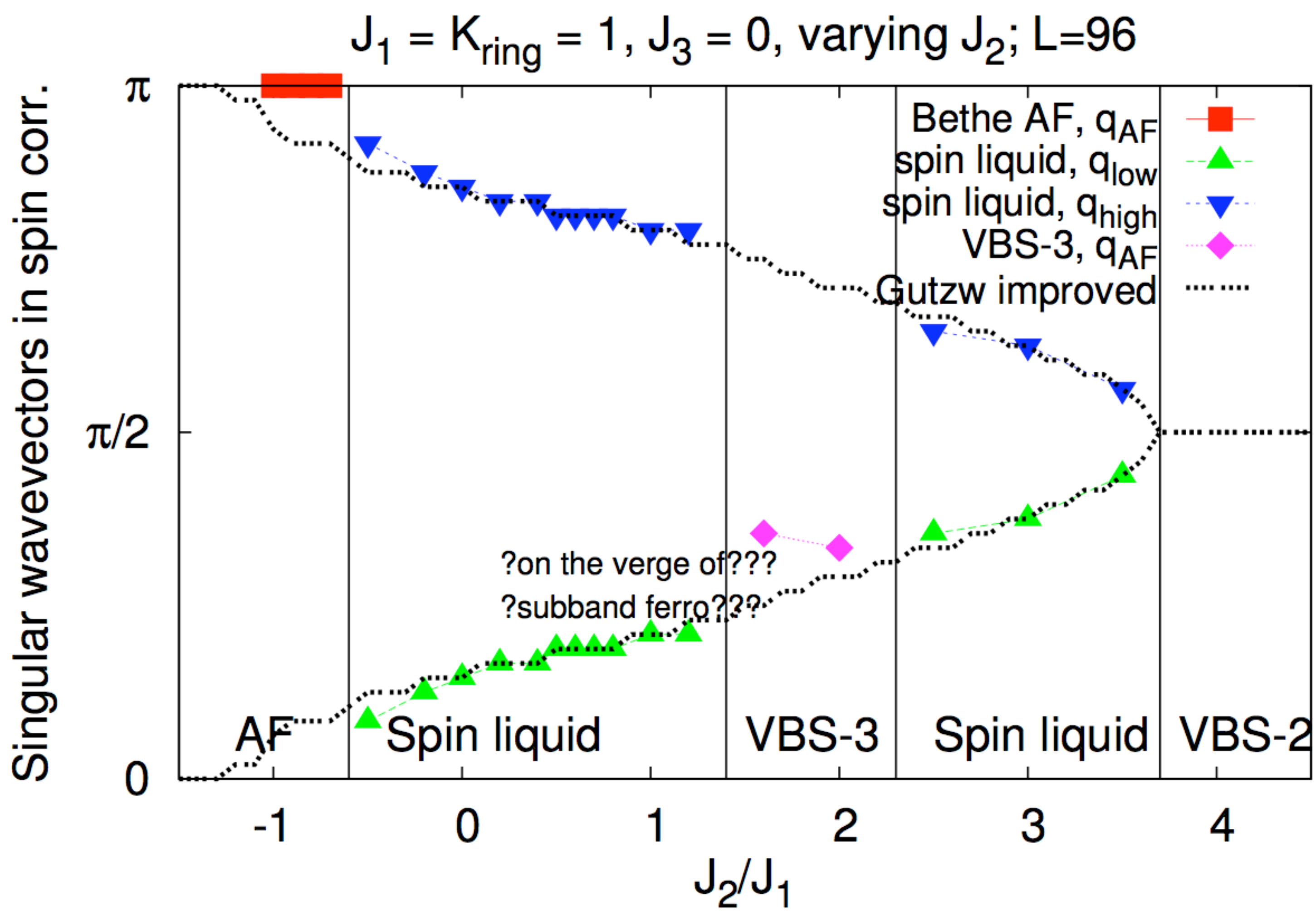
Singular momenta can be identified with $2k_{F1}$, $2k_{F2}$ which enter into Gutzwiller wavefunction!



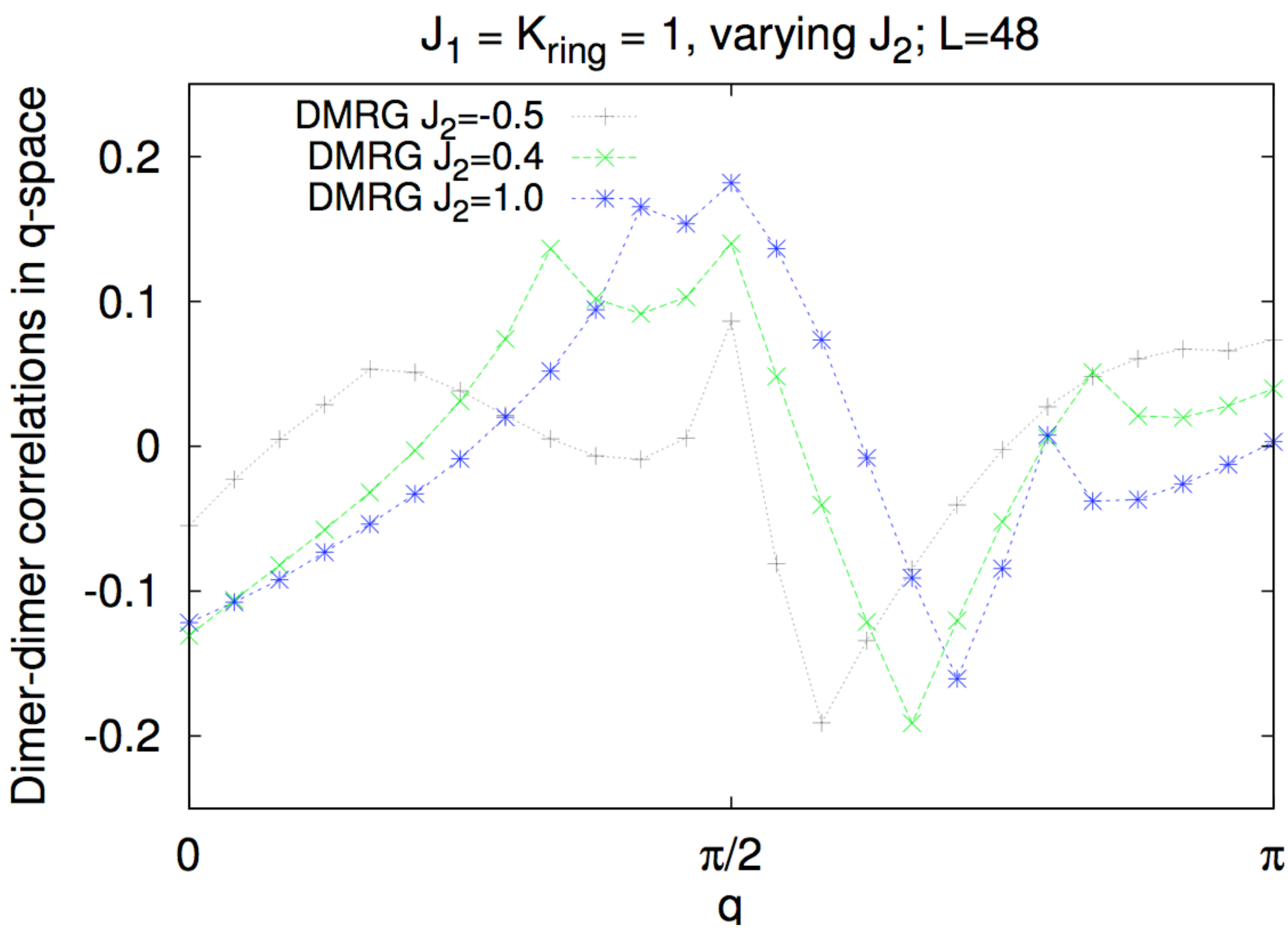
Singular momenta from VMC



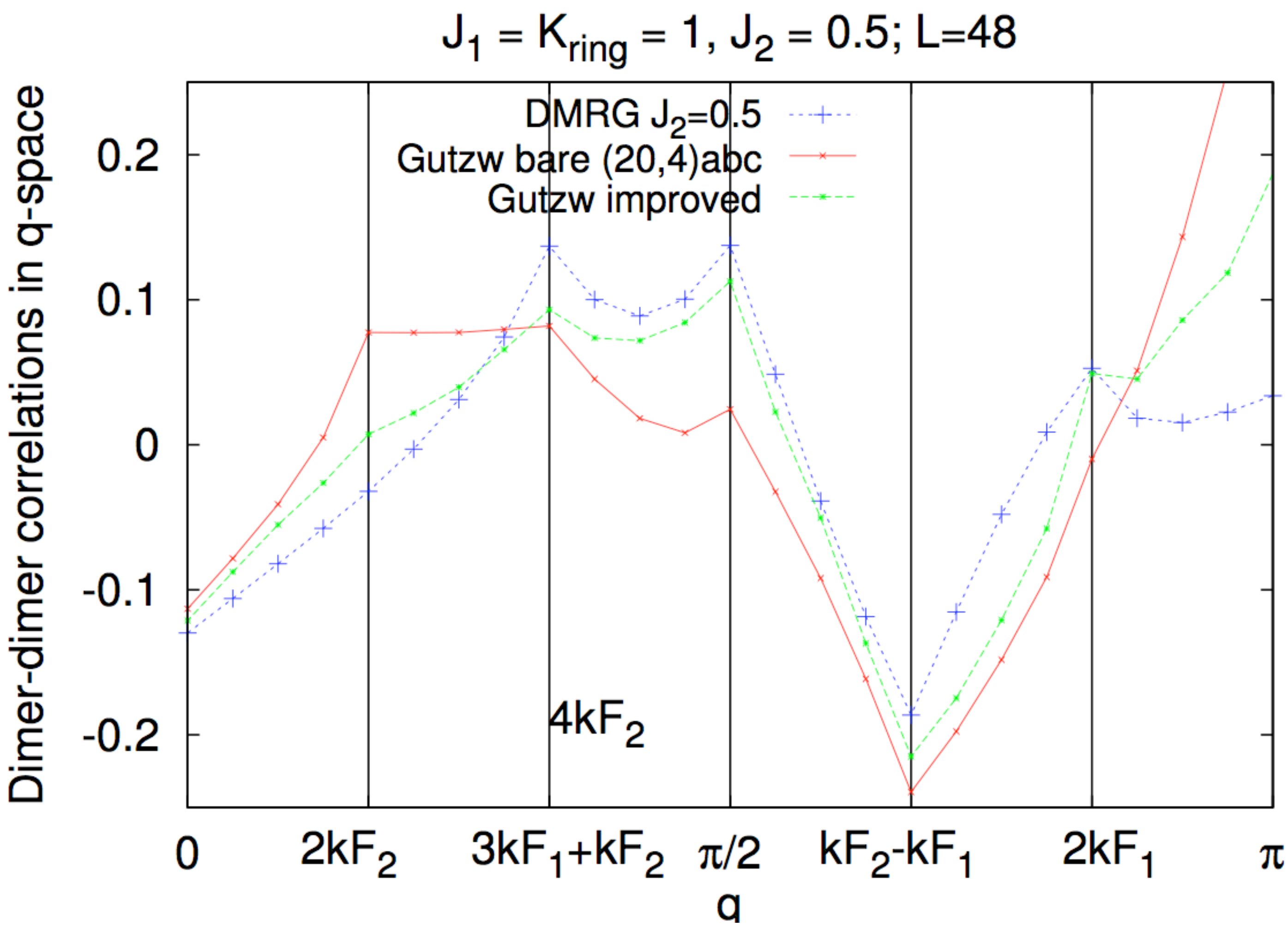
Compare Bose surface in DMRG and VMC



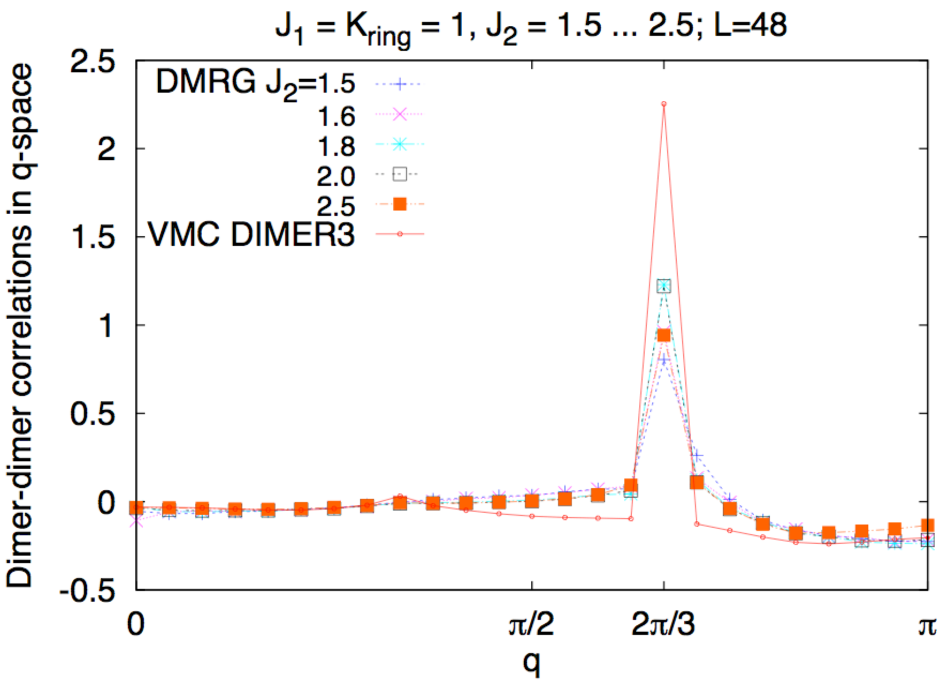
Dimer-dimer correlators in DMRG

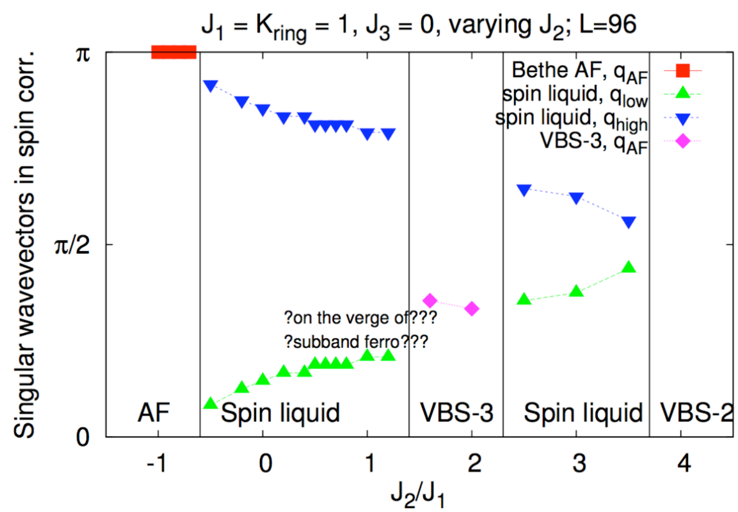


Dimer correlators in DMRG and VMC

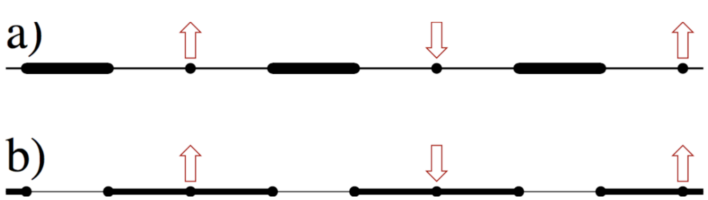


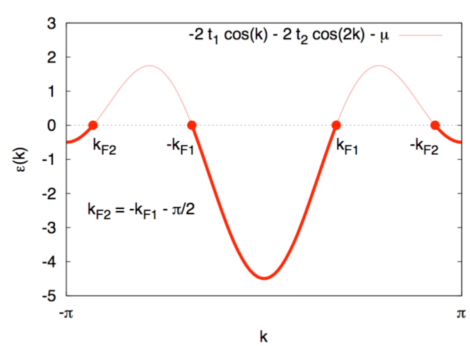
“VBS-3” Phase





$2k_{F1}$ = 2 pi/3 instability in gauge theory, gaps out the first spinon band, leaving second band gapless like a Bethe chain

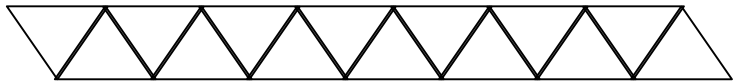




Summary & Outlook

- "Spin-Metals" are 2d gapless spin liquids with singular "Bose" surfaces
- Every 2d spin-metal has distinct quasi-1d descendents which should be numerically accessible
- The Heisenberg plus ring exchange Hamiltonian on the zigzag strip has a novel spin liquid ground state which is the quasi-1d descendent of the triangular lattice spinon-Fermi-surface spin liquid

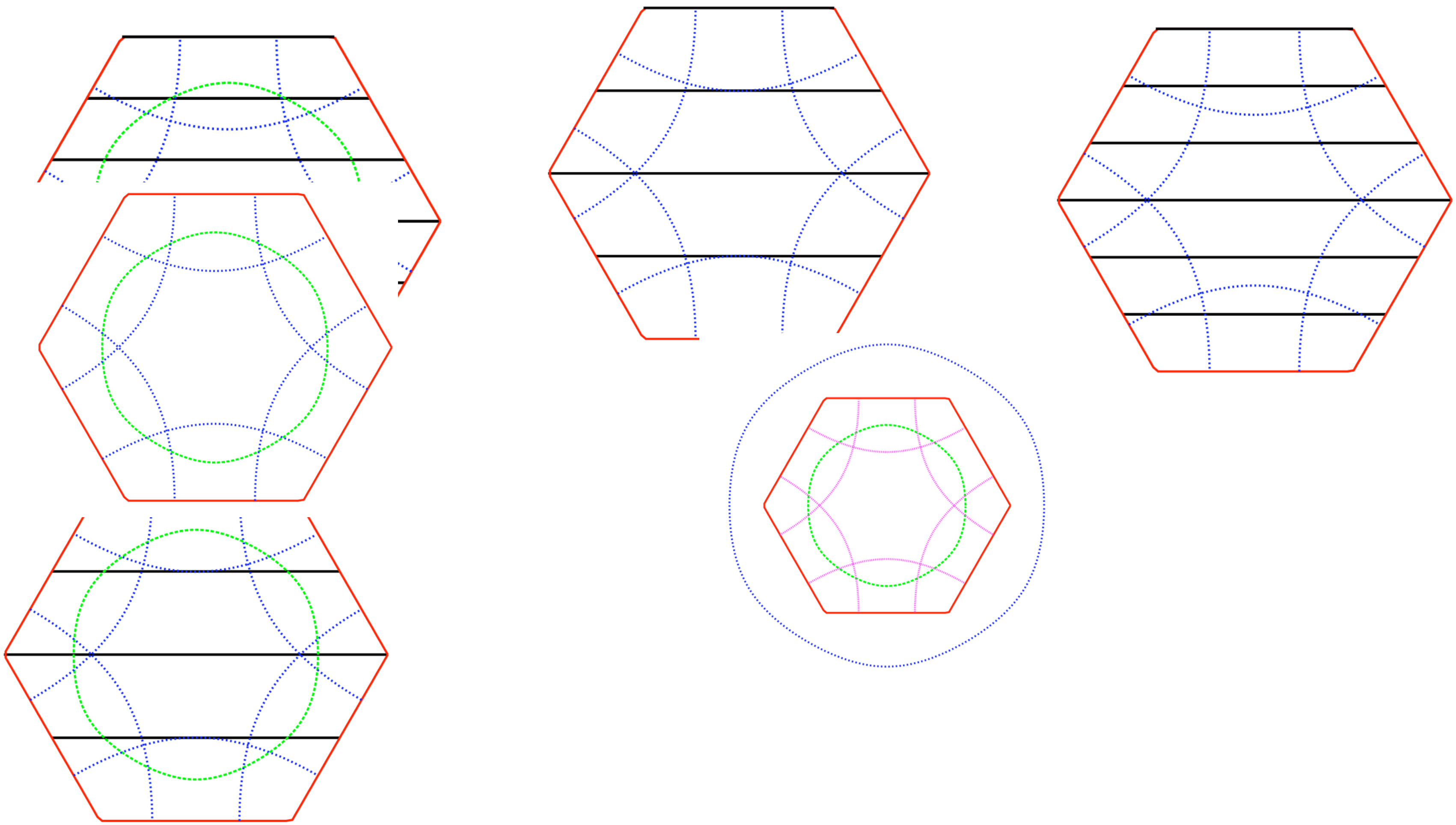
$$\mathcal{H}_\Delta = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + K \sum_{\langle 1234 \rangle} [\mathcal{P}_{1234} + \mathcal{P}_{1234}^{-1}]$$



Future generalizations (DMRG, VMC, gauge theory):

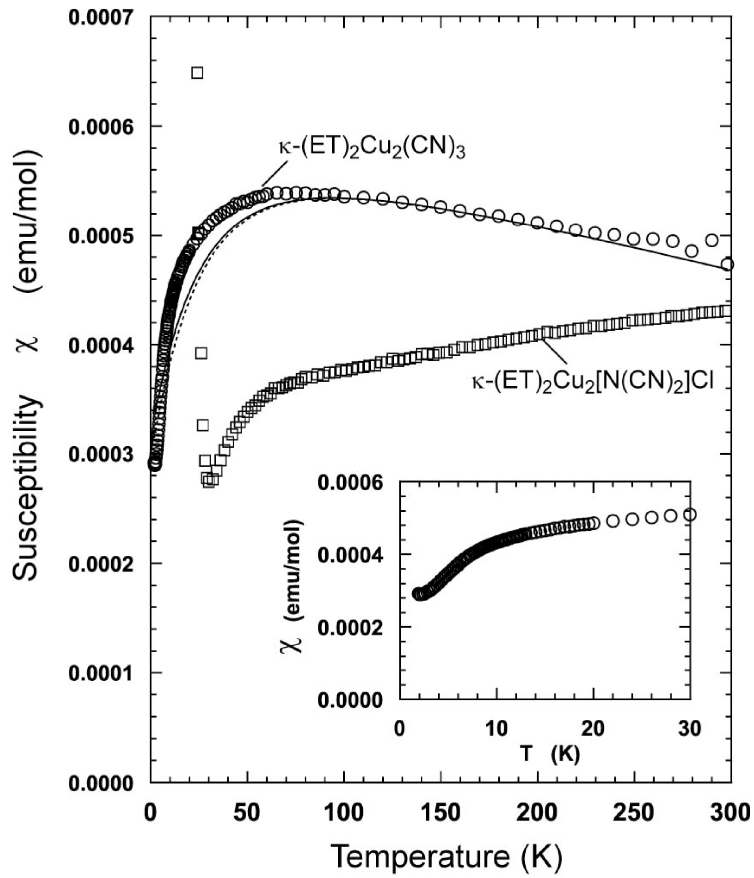
- Hubbard model on the zigzag strip
- Ring exchange model on 4-leg triangular strip
- XY boson ring model and the D-wave Bose liquid on n-leg ladders
- Quasi-1d descendents of 2d non-Fermi liquids of itinerant electrons?
- Non-Fermi liquid D-Wave Metal on the n-leg ladder?

4-leg and 6-leg cuts



κ–$(ET)_2Cu_2(CN)_3$ material facts

Spin susceptibility



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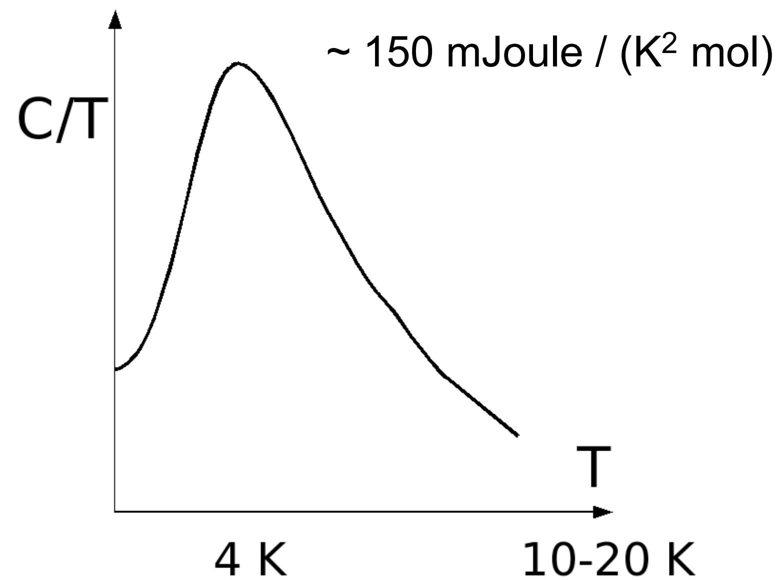
Specific heat



Kanoda, APS March Meeting 2006

corr

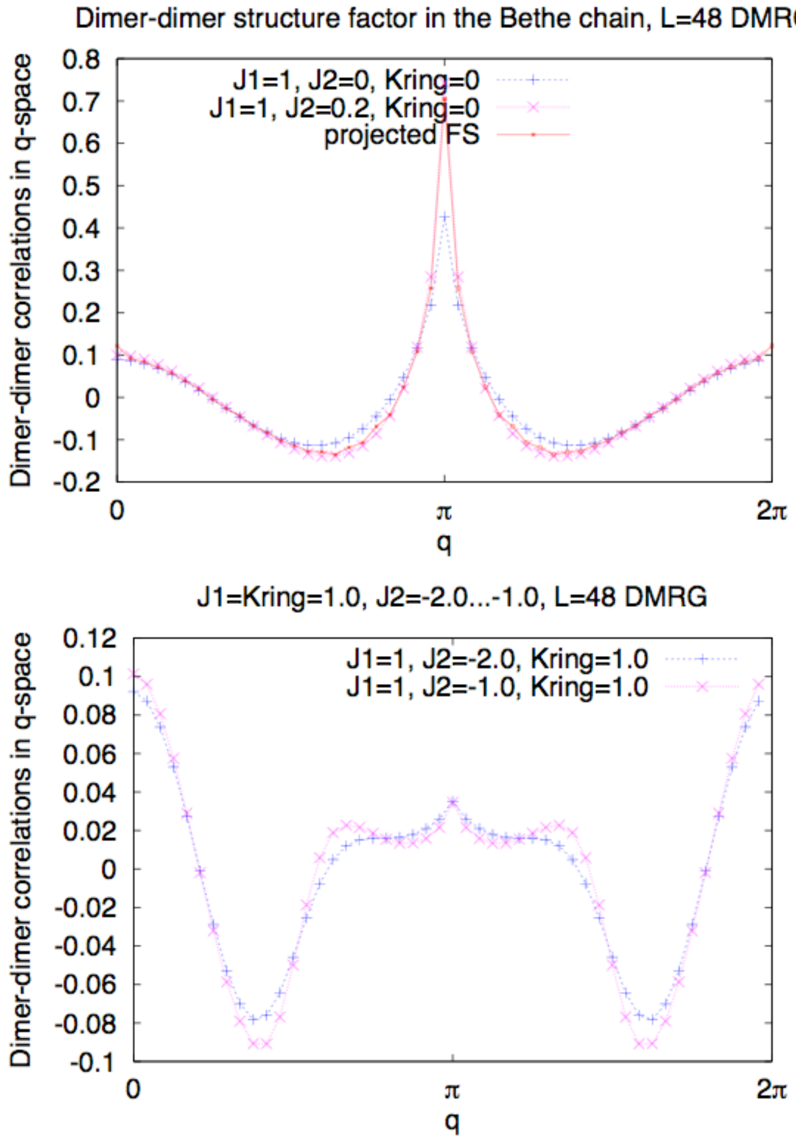


FIG. 1: Top panel: dimer-dimer struct.factor in the Bethe phase of the $J_1 - J_2$ chain with no ring exchanges. As we approach the transition point, $J_2 \approx 0.25$, the Gutzwiller-projected FS agrees better with the DMRG. Bottom panel: (the same as Donna's Fig.9) Bethe phase in the model with ring exchanges. The short-range correlations here are rather different (indeed the Gutzwiller wavefunction was rather poor), but the long-distance behavior should be the same, with the dimer-dimer correlations decaying as $\frac{(-1)^x}{x}$, just the amplitude is much smaller here. In Donna's Fig.8 in

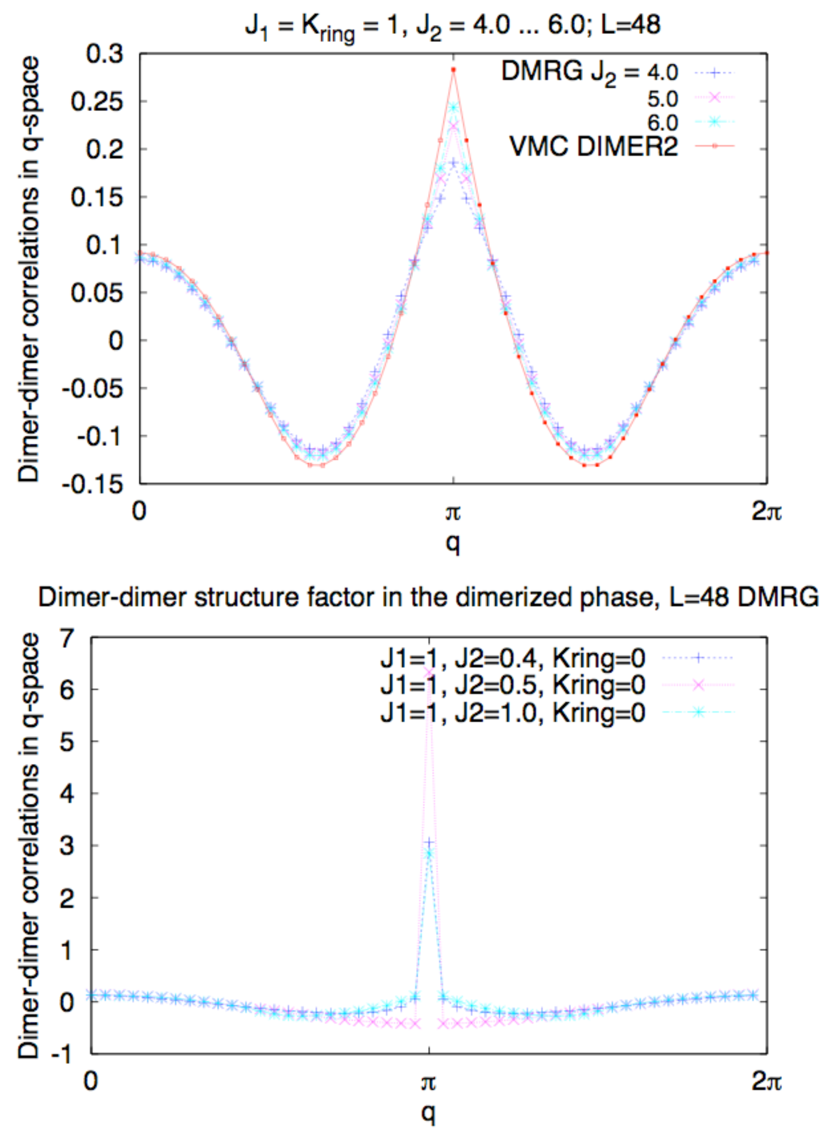


FIG. 6: Top: Dimer-dimer structure factor in the DIMER2 phase $J_2 >= 4.0$ in our ring model. Bottom pannel: Strongly dimerized phase in the $J_1 - J_2$ model near the Majumdar-Ghosh point $J_2 = 0.5$. Clearly the DIMER2 phase near our spin liquid is rather weak in comparison.