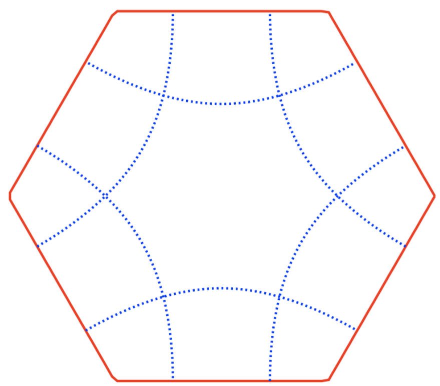
Mott Metal to Spin-Liquid Transition

MPA Fisher (with **O. Motrunich, Ryan Mishmash**, Matt Block, Ivan Gonzalez, Donna Sheng, **Roger Melko**)

KITP Conference on Exotic Phases of Frustrated Magnets 10/7/12

Mott metal-insulator transition in 2d

- **Can the Mott transition be a 2^{nd} order T=0 quantum phase transition?**
- **If yes, what is nature of the insulating phase?**
- **What is the nature of the quantum critical point?**



- Here, seek to address using controlled numerical calculations in quasi-1d systems (DMRG, VMC, bosonization of gauge theory)
- Next talk by Senthil – Analytic field theories and scaling approach to 2d Mott transition

(Some) References

Theory of a continuous Mott transition in two dimensions
T. Senthil, PRB (2008).

Mott transition between a spin-liquid insulator and a metal in three dimensions
D. Podolsky, A. Paramekanti, Yong Baek Kim, **T. Senthil**, PRL (2009).

A controlled expansion for certain non-Fermi liquid metals
D. F. Mross, J. McGreevy, H. Liu, **T. Senthil**, PRB (2010)

Decohering the Fermi liquid: A dual approach to the Mott Transition
D. F. Mross, **T. Senthil**, PRB (2011)

Universal transport near a quantum critical Mott transition in two dimensions
W. Witczak-Krempa, P. Ghaemi, **T. Senth**il, Y.B. Kim, arXiv:1206.3309

Spin Bose-Metal phase in a spin-1/2 model with ring exchange on a two-leg triangular strip,
D.N. Sheng, O.I. Motrunich, MPAF, PRB (2009)

Spin Bose-Metal and Valence Bond Solid phases in a spin-1/2 model with ring exchanges on a four-leg triangular ladder, M.S.Block, D.N. Sheng. O.I. Motrunich, MPAF, PRL (2011)

Mott metal to Spin Liquid transition in quasi-1d electron models,
R.V. Mishmash, I. Gonzalez, R. Melko, O. Motrunich, MPAF (in the works!)

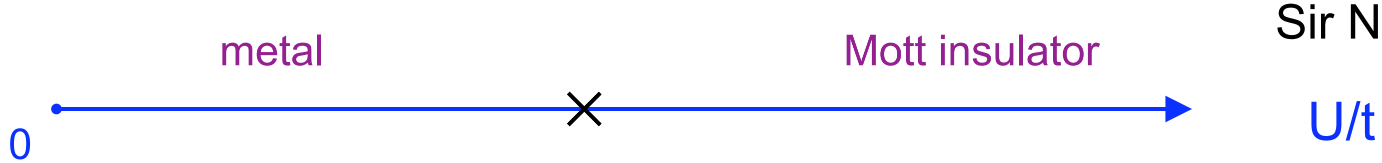
2d Metal and Mott insulator phases

2d Hubbard model, one electron/site:

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

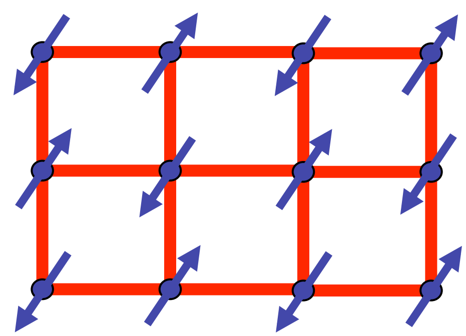
Metal for small U/t (band theory)
Mott insulator for large U/t, electrons localize

Sir Neville Mott



Mott Insulator --> effective spin Hamiltonian

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



(Almost!) Invariably the Spins order (AFM) in the Mott insulator

Mott metal-insulator ***transition***??

Nature of T=0 transition?

- First order, always possible
- 2nd order (continuous) is problematic

For continuous Metal to AFM insulator transition
need insulating behavior and magnetism to turn on *together*. ***Not generic!***

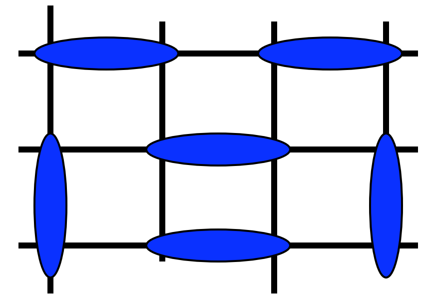
(Simplest scenario - intervening AFM ordered metal, between metal and AFM insulator)

But what if Mott insulator is in a ***Spin Liquid*** (no magnetic order)?

Is a 2nd order metal to spin-liquid Mott transition possible?
And if so, *which* spin-liquid?

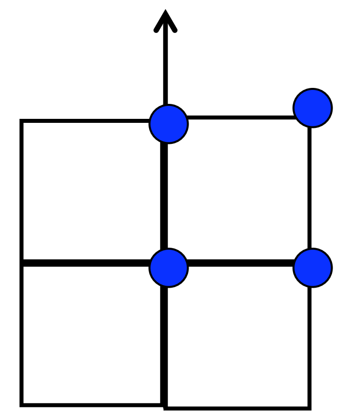
Not all 2d Spin liquids alike!

Topological Spin Liquids



- Fully gapped
- Fractionalized excitations, eg s=1/2 spinon

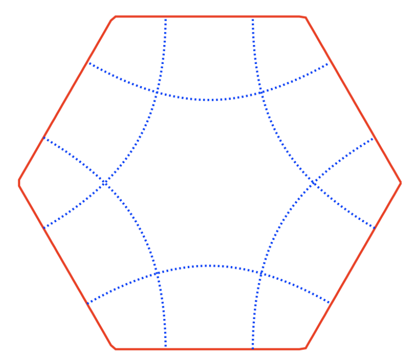
Algebraic Spin Liquids



- Stable gapless phase
- Power-law correlations at finite set of discrete momenta

“Spin Bose-Metals”

- Stable Gapless phase
- Spin correlations singular on ***surfaces*** in momentum space



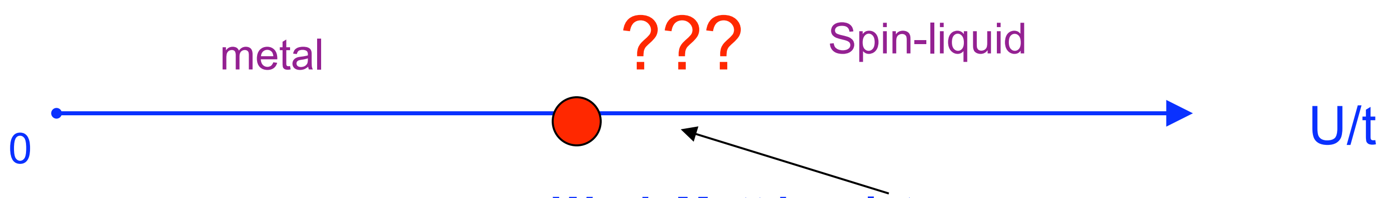
“Bose Surfaces”

Continous Mott transition: Into which Spin-liquid?

If metal-insulator transition is 2nd order, then have a

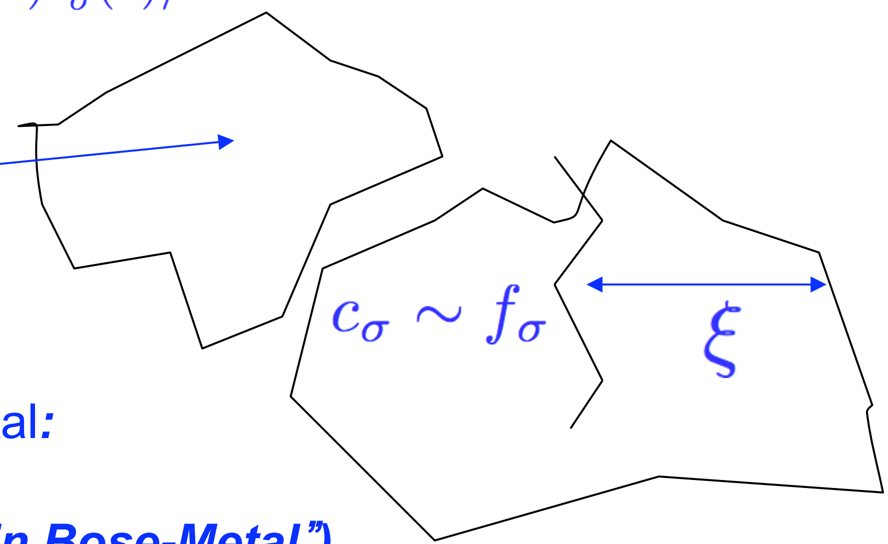
Weak Mott insulator

Long charge correlation length



$$\langle c_\sigma(x) c_\sigma^\dagger(0)\rangle \sim e^{-x/\xi} \qquad \xi >> a$$

Inside correlation region electrons do not "know" they are insulating



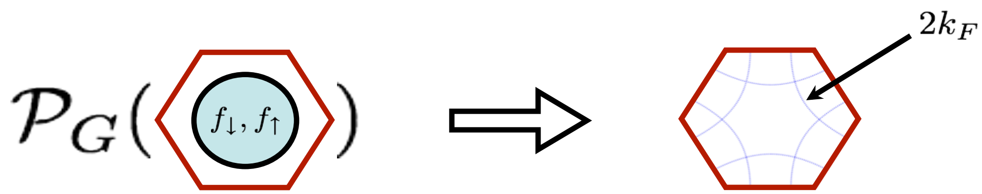
Candidate spin liquid that "resembles" a metal*:*

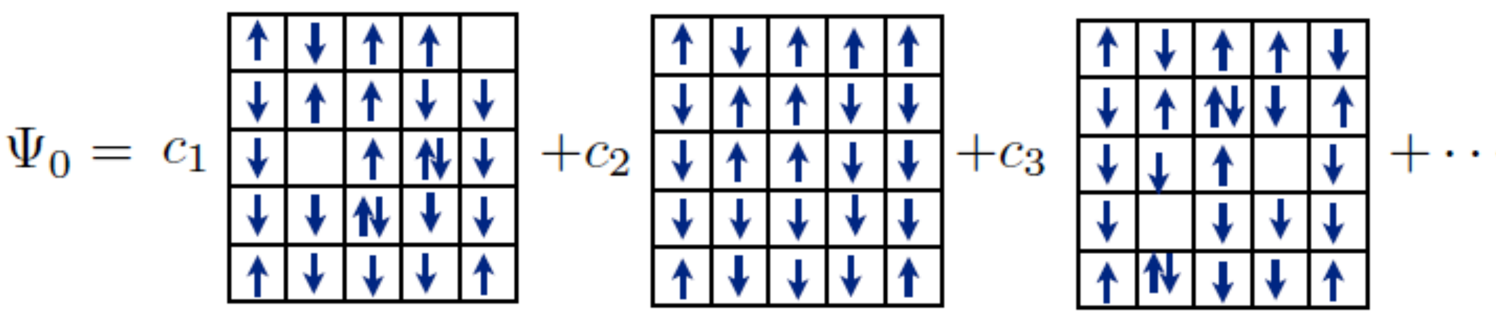
Gutzwiller projected Fermi sea (a "Spin Bose-Metal")

Motrunich, PRB (2005); S. Lee and P. A. Lee, PRL (2005)

Gutzwiller projected Fermi sea
(spin Bose-metal)

Construct spin-wavefunction from free Fermi gas with one Fermion/site





Gutzwiller projected Fermi sea
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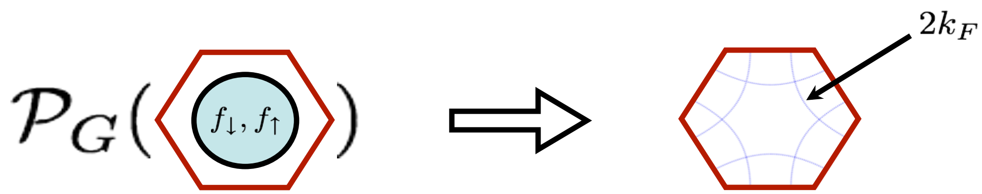
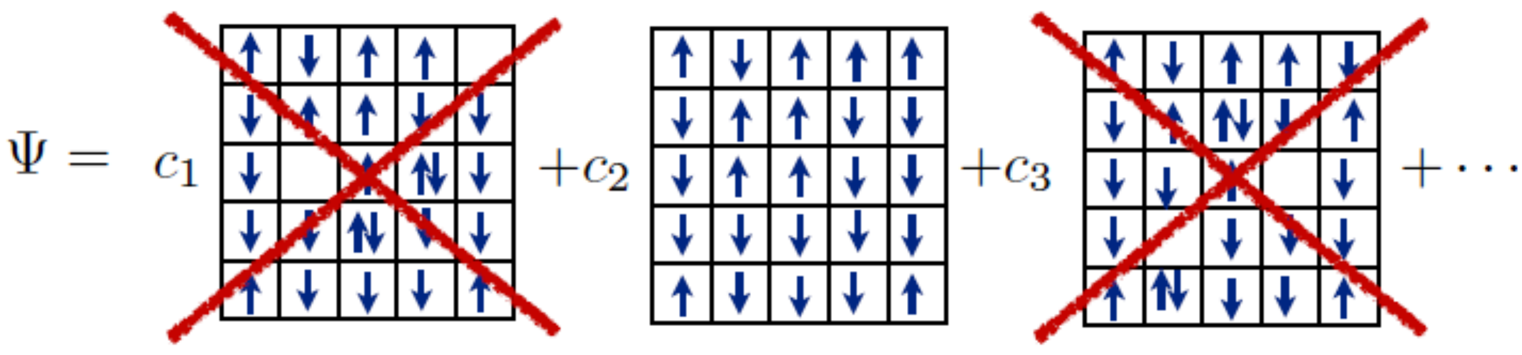
Construct spin-wavefunction from free Fermi gas with one Fermion/site





Quantum Spin Liquid Wavefunction

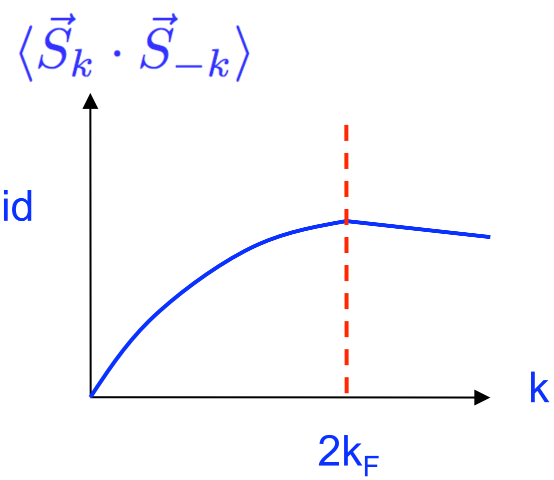
$\Psi = P_G \Psi_0$ Throw away all parts of wf with empty/doubly-occupied sites

Effective field theory: Fermionic spinons coupled to U(1) gauge field

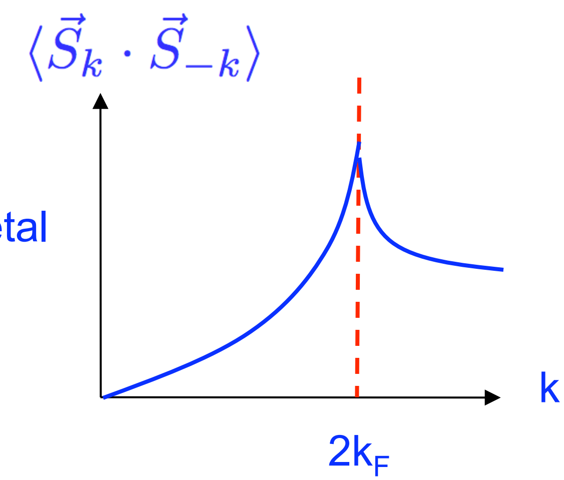
Phenomenology of Spin Bose-Metal
(from wf and Gauge theory)

Singular spin structure factor at "$2k_F$" in Spin Bose-Metal
(more singular than in Fermi liquid metal)

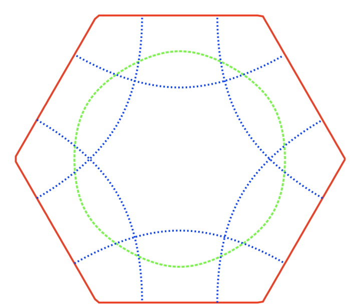
Fermi liquid



Spin Bose-metal



$2k_F$ "Bose surface" in
triangular lattice Spin Bose-Metal



Experimental candidate Spin Bose-Metals

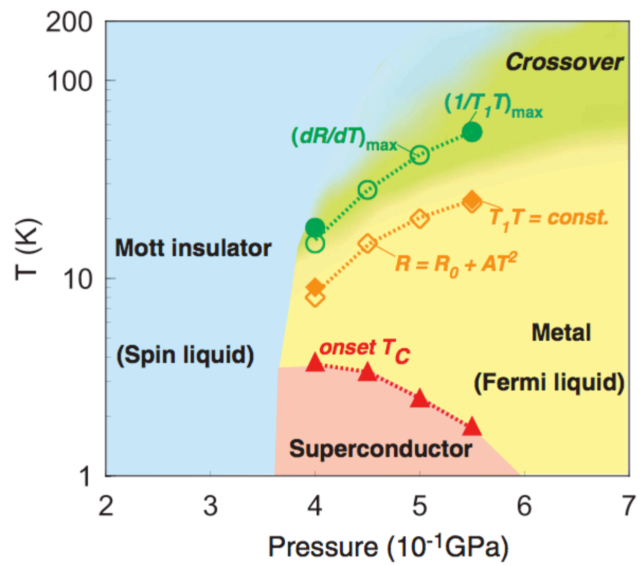
Organic triangular-lattice Mott materials

k-$(ET)_2Cu_2(CN)_3$ Kanoda et. al. PRL 91, 177001 (2005)

$EtMe_3Sb[Pd(dmit)_2]$ Itou, Kato et. al. PRB 77, 104413 (2008)

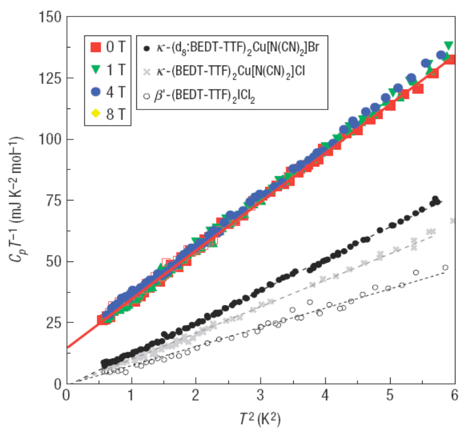
- Hubbard at half-filling
- Weak Mott insulator – metal under pressure
- No magnetic order for T << J
- Pauli spin susceptibility

Motrunich (2005) , S. Lee and P.A. Lee (2005)
"spinon Fermi sea" proposed



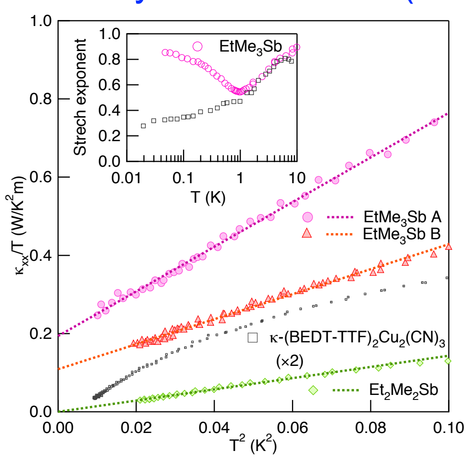
Metallic specific heat, C~T, Wilson ratio of order one

S. Yamashita et al
(2008)



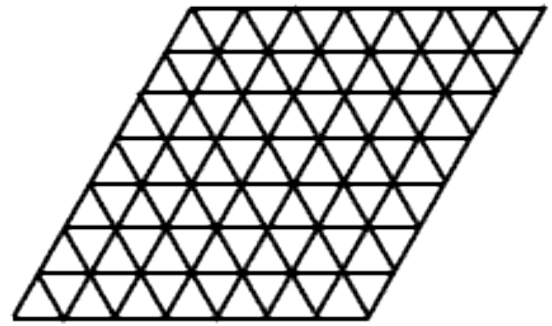
Thermal conductivity K/T ~ const in $(dmit)_2$

M. Yamashita et a
(2010)l

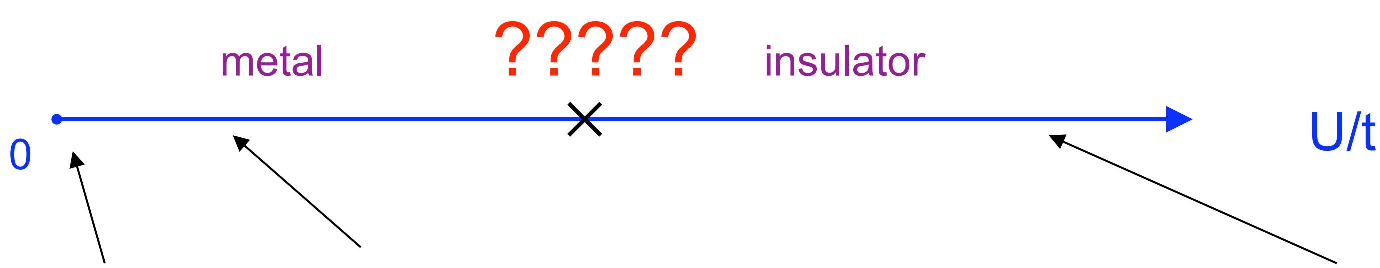


Hubbard model phase diagram on triangular lattice?

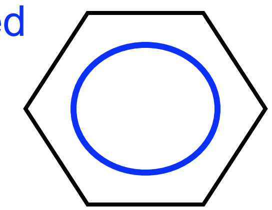
$$\mathcal{H} = -t \sum_{\langle ij \rangle} [c^\dagger_{i\alpha} c_{j\alpha} + h.c.] + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



Phase diagram at Half filling?



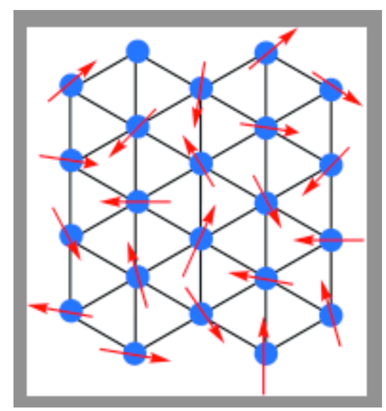
Free Fermi gas,
un-nested



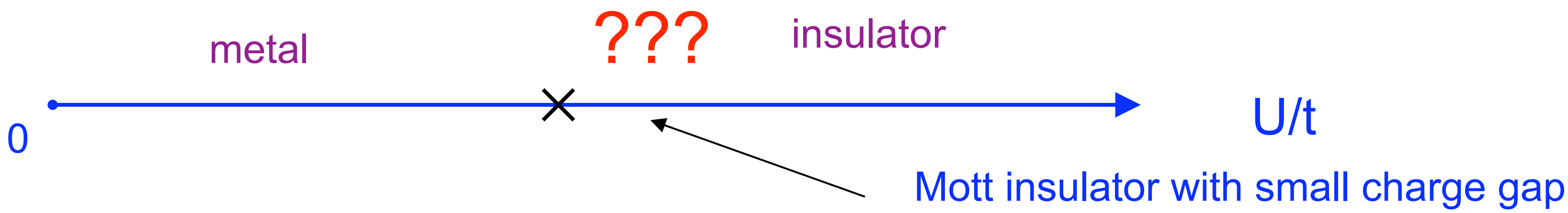
Fermi liquid

Heisenberg n.n. AFM
3-sublattice Neel state

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

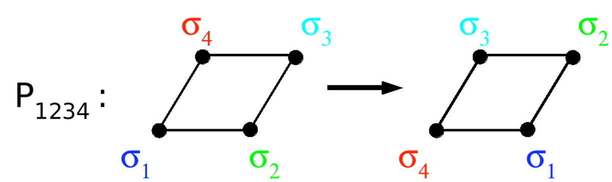


“Weak” Mott insulator on triangular lattice - Ring exchange



Expansion in t/U from Hubbard: spin model with ring exchange (mimics charge fluctuations)

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



Triangular Lattice Heisenberg Model with ring exchange

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

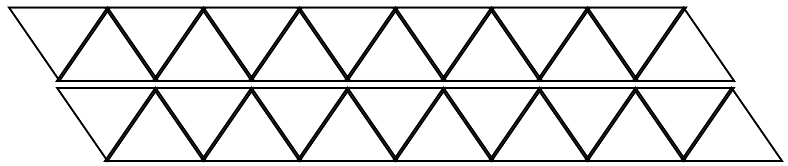
Is ground state a spin-liquid?   A projected Fermi sea state?

VMC suggests yes for $J_4/J_2 > 0.3$, O. Motrunich - 2005

But, VMC is biassed,
QMC has a sign problem,
DMRG is problematic in 2d .....   so we have a quandry ....

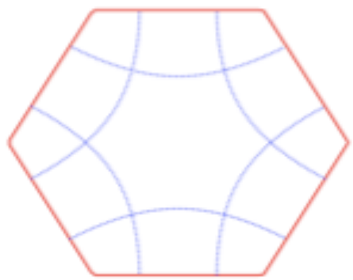
Quasi-1d route to "Spin Bose-Metals"

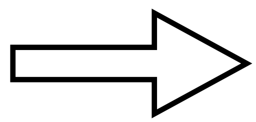
Triangular strips:

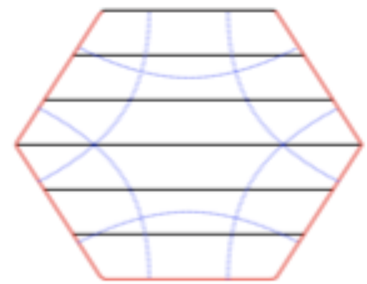


2d

Quasi-1d ladders







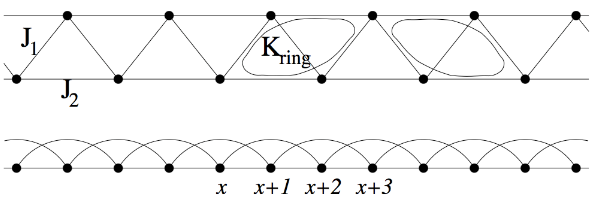
Singular $2k_F$ surface
in spin correlators
("Bose surface")

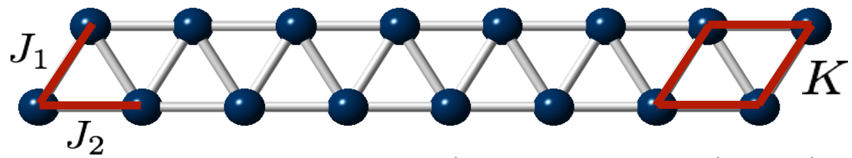
Fingerprint of 2d singular surface
on ladders - many gapless 1d modes,
of order N

2d Spin Bose-Metal should have quasi-1d descendent states

2-leg zigzag strip: SBM Descendent states?

View as 1d model





$$P_{1234}|\sigma_1, \sigma_2, \sigma_3, \sigma_4\rangle \to |\sigma_4, \sigma_1, \sigma_2, \sigma_3\rangle$$

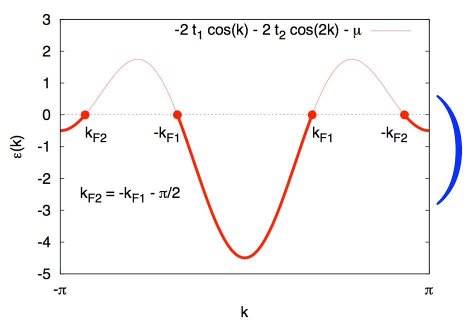
$$H_{\text{Heis}} + H_{\text{ring}} = \sum_x [2J_1 \mathbf{S}(x) \cdot \mathbf{S}(x+1) + 2J_2 \mathbf{S}(x) \cdot \mathbf{S}(x+2) + K(P_{x,x+2,x+3,x+1} + \text{h.c.})]$$

Analysis of J_1-J_2-K model on zigzag strip D.N. Sheng, O.I. Motrunich, MPAF, PRB (2009)

- DMRG
- Bosonization of gauge theory

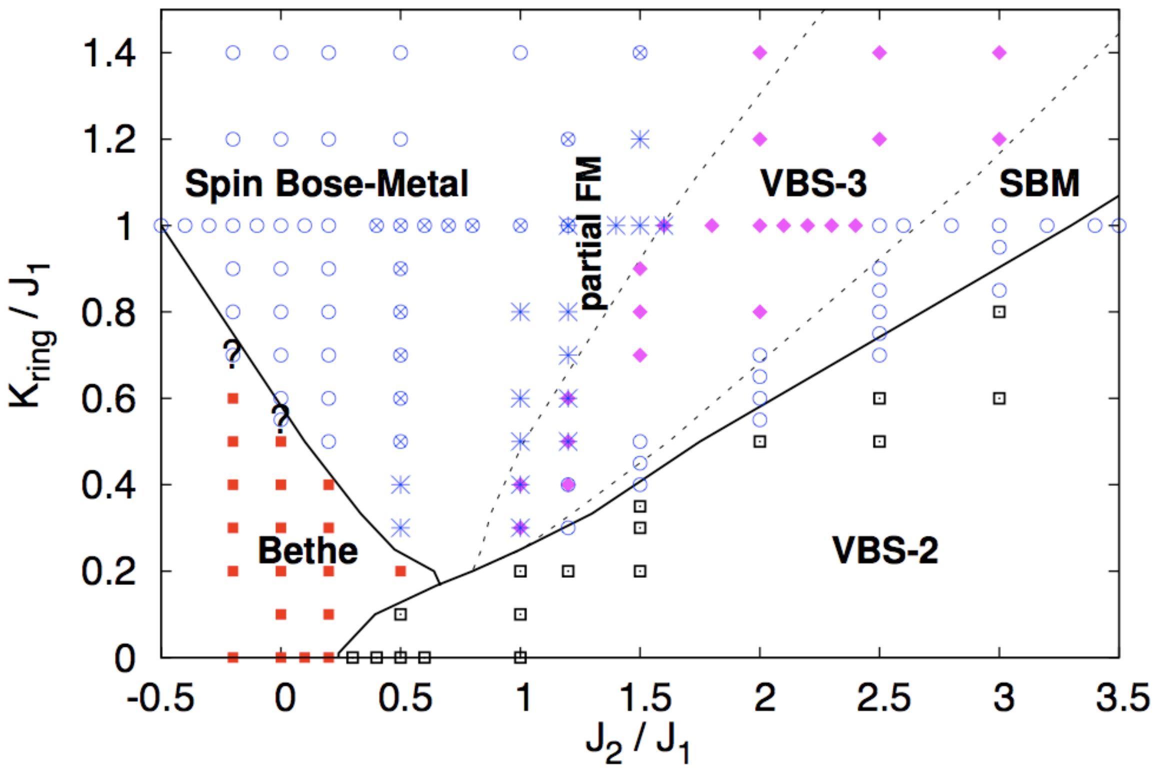
- Gutzwiller wavefunctions: study with VMC

$$\Psi_{VMC} = \mathcal{P}_G\Big(\quad \Big)$$



Single Variational parameter,
size of 2^{nd} Fermi sea

DMRG Phase Diagram of 2-leg zigzag ring model



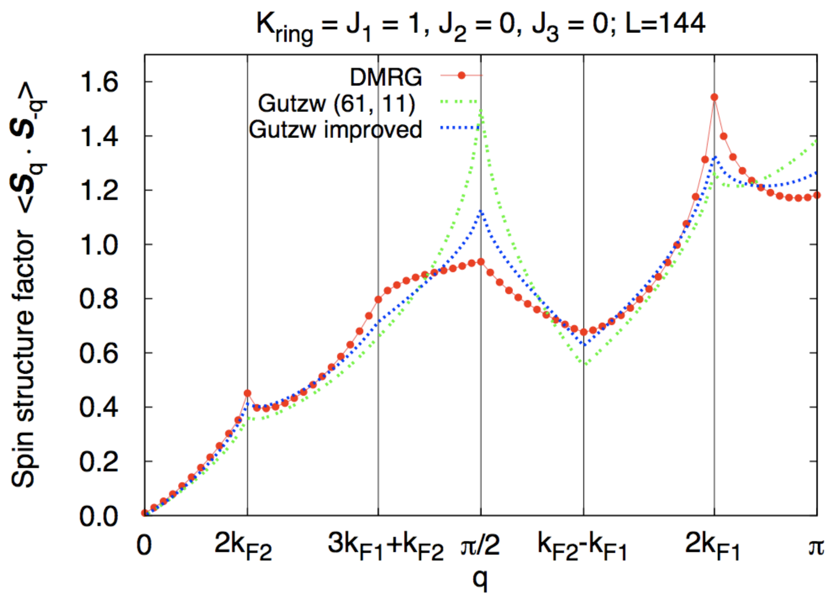
Spin-Bose-Metal phase (Gutzwiller projected Fermi sea) over large region

D.N. Sheng, O.I. Motrunich and MPAF, PRB (2009)

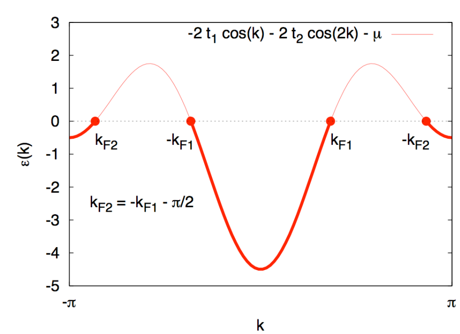
Spin Structure Factor in Spin Bose-Metal

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

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

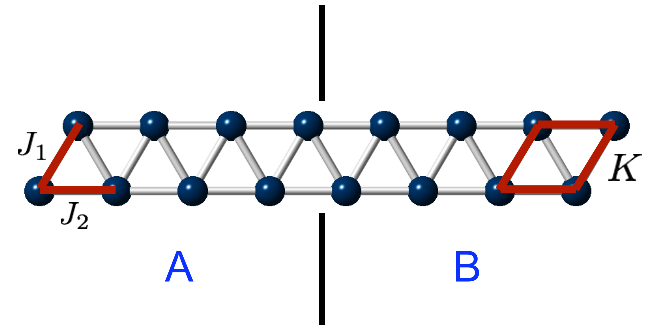


Singular momenta can be identified with $2k_{F1}$, $2k_{F2}$ which enter into Gutzwiller wavefunction



Entanglement in SBM

Reduced density matrix for sub-system A $\rho_A = Tr_B[\rho]$



Entanglement entropy $S_A = -Tr_A[\rho_A \ln \rho_A]$

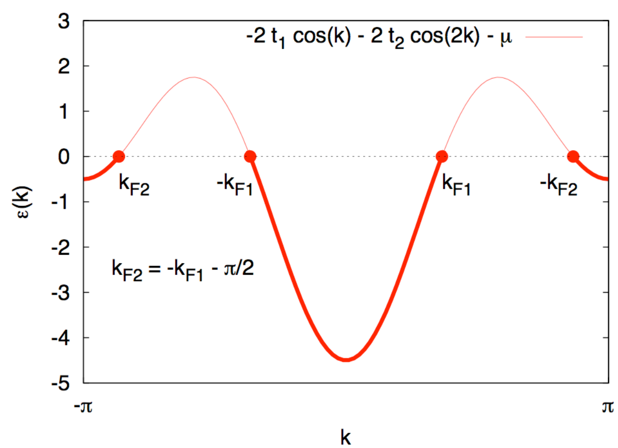
1d Gapless system (Conformal field theory, CFT) $S(X) = \frac{c}{3} \ln(X)$

c = central charge

Quasi-1d Gauge Theory for SBM

Two Fermi points - 2 charge and 2 spin modes

Gauge projection; Kills overall charge mode, 3 modes remain



Zigzag Spin Bose-Metal

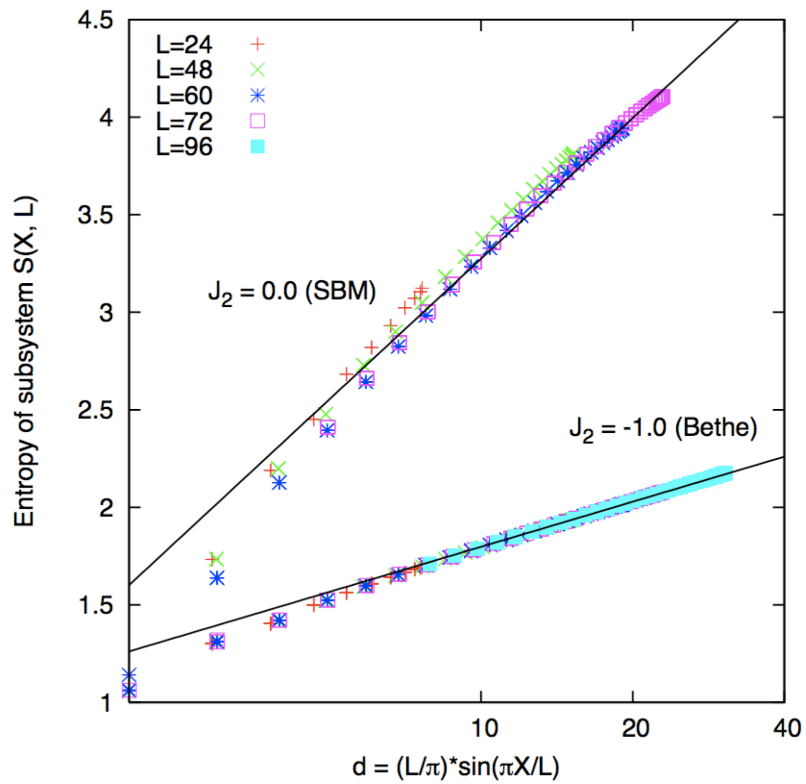
Two gapless spin modes and one gapless spin-chirality mode:
Central charge c=3 predicted

Entanglement Entropy from DMRG?

$$S(X,L) = \frac{c}{3}\log\left(\frac{L}{\pi}\sin\frac{\pi X}{L}\right) + .$$

nn 1d Heisenberg AFM
gives c=1, as expected

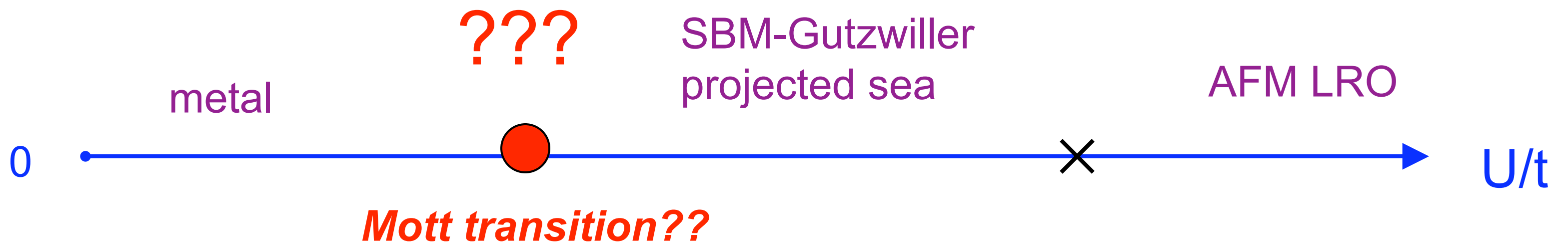
Spin Bose-Metal is
much more entangled



Entanglement entropy in SBM consistent with c=3

Metal to SBM Mott transition?

DMRG on 2-leg and 4-leg zigzag ladders - evidence for
SBM state in 2d triangular lattice



Can 2d metal to spin-Bose-metal Mott transition be 2nd order?

2d Effective field theories say yes! (see next talk, Senthil)

Electron split into s=1/2 fermionic (spinon) and charge 1 bosonic (``chargon”), coupled to a U(1) gauge field

$$c_\sigma = b f_\sigma$$

Mott transition driven by superfluid-insulator transition of b

Quantum Criticality of Mott Transition?

2d: Challenging spinon-chargon gauge theory

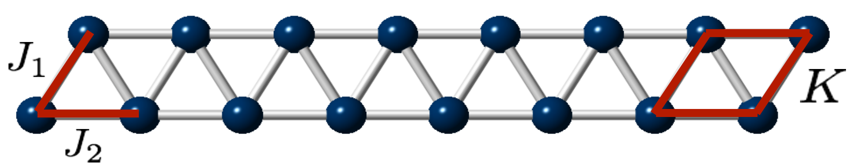
- Spinon fermi sea plus gauge field (SBM phase)

Mross, McGreevy, Liu and Senthil (2010)
and references therein

- Chargons/Spinons plus gauge field (Mott metal-SBM transition)

T. Senthil (2008); Mross and Senthil (2011),
Witczak-Kremoa, Ghaemi, Senthil, Kim, cond-mat:1206.3309

Toy Problem: Metal to Spin-Bose-metal transition on 2-leg zigzag

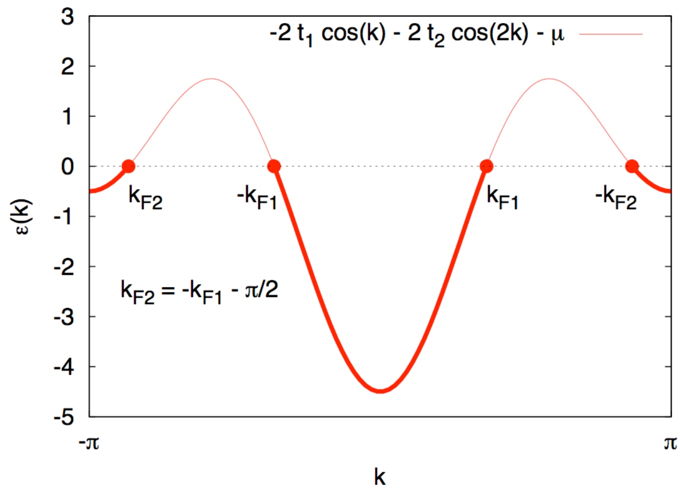


(I) Bosonize Hubbard model on triangular strip:

(II) DMRG solution of Hubbard-type model on 2-leg zigzag

Bosonization of Metal-SBM transition on 2-leg zigzag

- Metal: 2 band Luttinger liquid (4 gapless modes)



- Eight fermion Umklapp drives transition into insulator (at strong coupling)

$$H_8 = v_8(c^\dagger_{R1\uparrow}c^\dagger_{R1\downarrow}c^\dagger_{R2\uparrow}c^\dagger_{R2\downarrow}c_{L1\uparrow}c_{L1\downarrow}c_{L2\uparrow}c_{L2\downarrow} + \text{H.c.}),$$

- Kosterlitz-Thouless transition gaps overall charge mode, leaving 3 mode SBM

- Universal signature of KT Mott transition, Density correlator: $\langle \delta n_q \delta n_{-q} \rangle = g_\rho (2q/\pi)$

$$g_\rho \geq 1/2; \quad metal \qquad (g_\rho = 1; \quad free\ fermions)$$

$$g_\rho = 0; \quad insulator$$

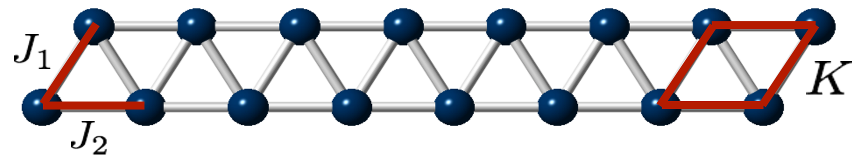
$$g^*_\rho = 1/2; \quad KT\ transition$$

DMRG for Metal-SBM transition on 2-leg zigzag

Kinetic energy: Electrons hopping on 2-leg zigzag

R.V. Mishmash, I. Gonzalez, R. Melko, O. Motrunich, MPAF (iunpublished)

$$\mathcal{H}_0 = -\sum_i [t c^\dagger_{i\sigma} c_{i+1\sigma} + t' c^\dagger_{i\sigma} c_{i+2\sigma} + h.c.]$$

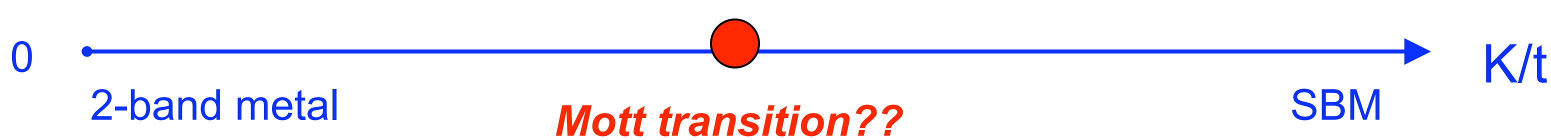


Interactions: 2 models

- Hubbard $\mathcal{H}_U = U \sum_i n_{i\uparrow} n_{i\downarrow}$
- 2-Spin and 4-spin ring exchanges

$$\mathcal{H}_{JK} = \sum_i [J_1 \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \vec{S}_i \cdot \vec{S}_{i+2}] + K(P_{i,i+2,i+3,i+1} + h.c.)$$

Here, we will fix K/J_1 =0, J_2/J_1=0, t'/t=0.75 and vary the single dimensionless parameter K/t:



DMRG for electron zigzag t-JK model

R.V. Mishmash, I. Gonzalez,
R. Melko, O. Motrunich,
MPAF (iunpublished)

Spin-spin and Density-density correlators

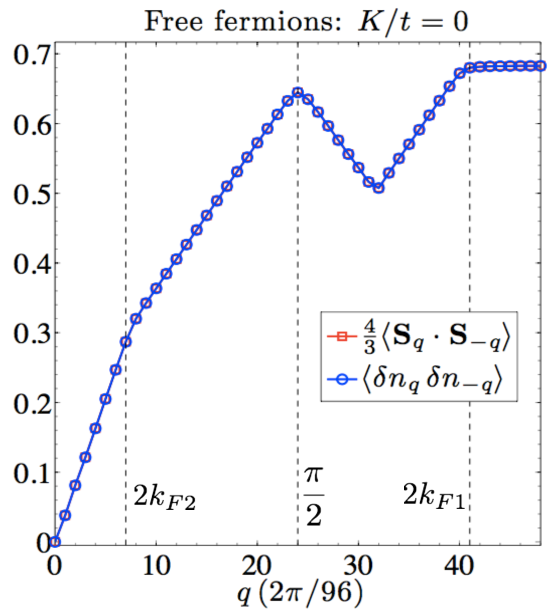
$$\langle \delta n_q \delta n_{-q} \rangle$$

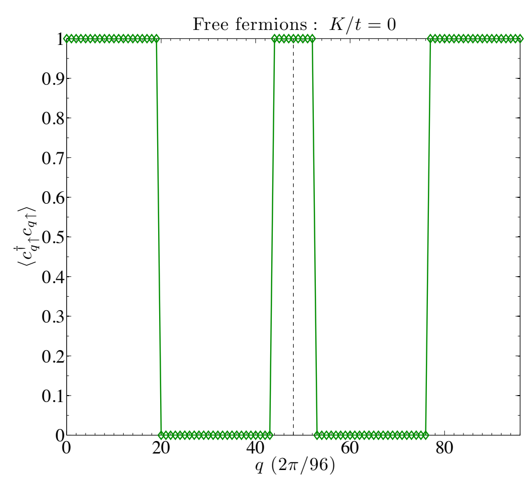
$$\langle \vec{S}_q \cdot \vec{S}_{-q} \rangle$$

Electron momentum distribution functions

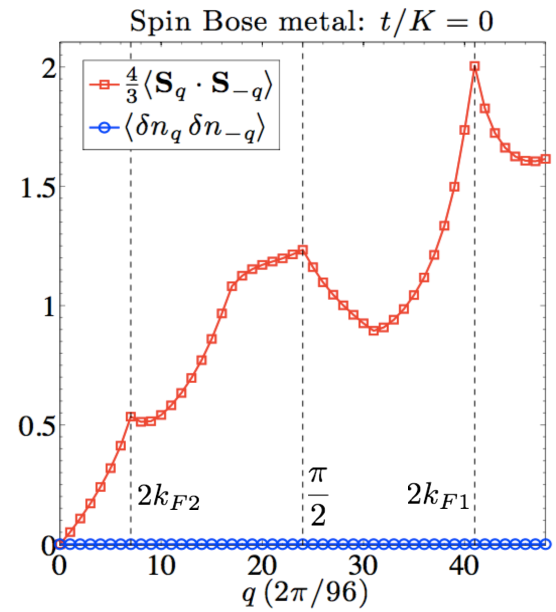
$$\langle c^\dagger_{q\uparrow} c_{q\uparrow} \rangle$$

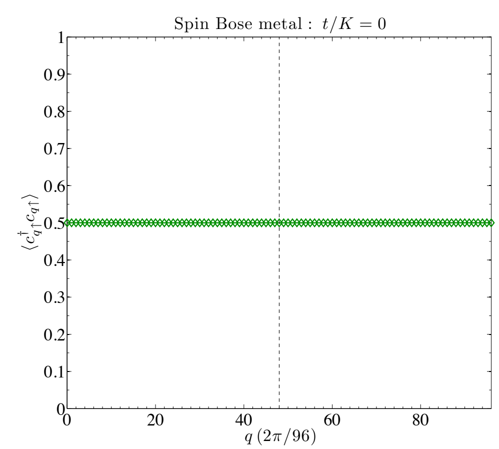
Free electron Metal: K/t=0





SBM Insulator: K/t = infinity





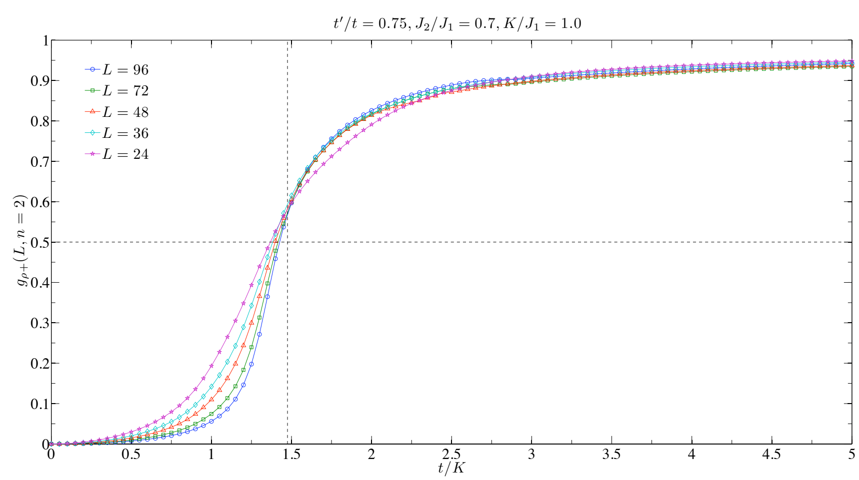
Quantum Criticality at Mott transition?

Evidence for Kosterlitz-Thouless from density-density structure factor

$$\langle \delta n_q \delta n_{-q} \rangle = g_\rho (2q/\pi)$$

KT Theory prediction:

$$g_\rho \geq 1/2; \quad metal \quad (g_\rho = 1; \; free\ fermions)$$
$$g_\rho = 0; \quad insulator$$
$$g_\rho^* = 1/2; \quad KT\ transition$$



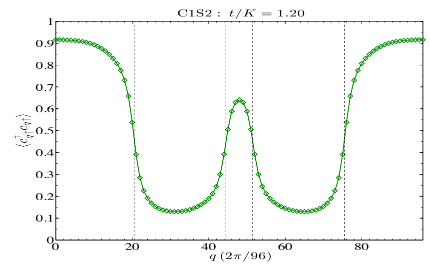
DMRG data for $L \to \infty$ consistent with $g_\rho = 0$ in insulator, and $g_\rho^* = 1/2$ at KT transition

Singular *charge-density* fluctuations in SBM Insulator!

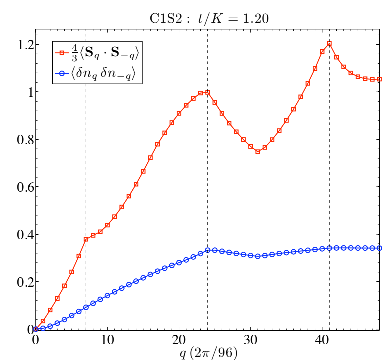
(Charge Friedel Oscillations in a Mott insulator: D.F. Mross and T. Senthil PRB (2011))

Electron gapped in insulator, smooth electron momentum distribution function

$$\langle c^\dagger_{q\uparrow} c_{q\uparrow} \rangle$$

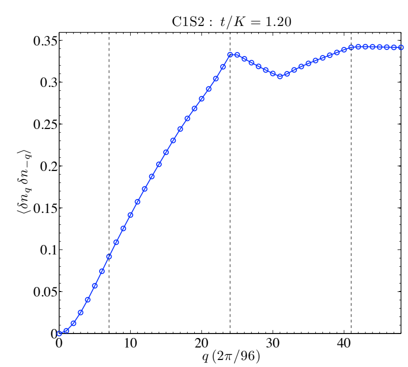


Spin structure factor singular at $2k_F$ (signature of "spinon Fermi-surface")



Density structure factor also singular at $2k_F$, despite being insulating

$$\langle \delta n_q \delta n_{-q} \rangle \sim q^2$$



DMRG for 2-leg zigzag Hubbard

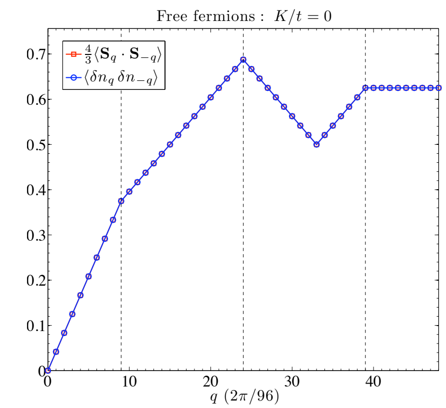
Free fermions U/t=0

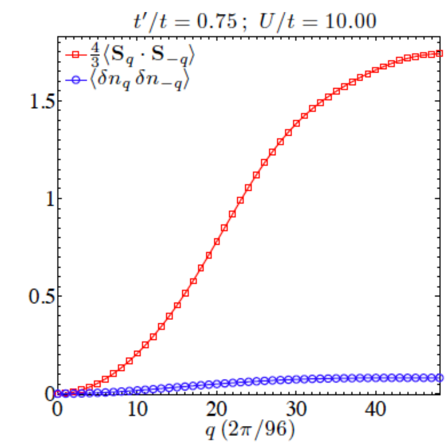
Insulator U/t=10

Spin-spin and Density-density correlators

$$\langle \delta n_q \delta n_{-q} \rangle$$

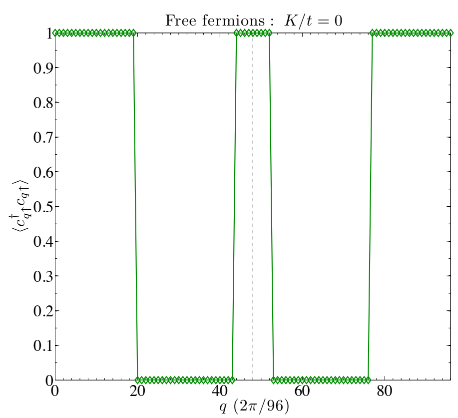
$$\langle \vec{S}_q \cdot \vec{S}_{-q} \rangle$$

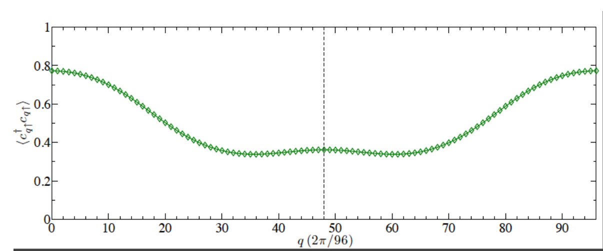




Electron momentum distribution functions

$$\langle c^\dagger_{q\uparrow} c_{q\uparrow} \rangle$$

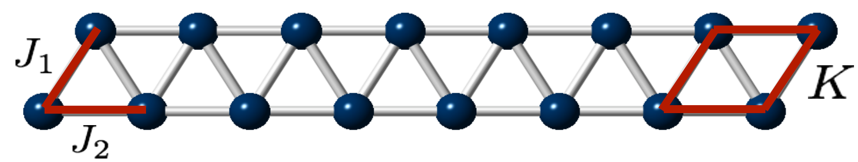




Summary and Outlook

- Continuous 2d Mott transition from metal to Spin-Bose-metal insulator (Gutzwiller projected Fermi sea state) is possible

- DMRG on 2-leg zigzag finds quasi-1d analog: Kosterlitz-Thouless transition from 2-band metal to quasi-1d SBM (Gutzwiller projected sea)



Numerics (DMRG)

- Continuous Mott transition on 2-leg zigzag Hubbard model?
- Mott transition accessible on multi-leg triangular lattice Hubbard model?
- Access 2d criticality?

Analytics: Field theory of 2^{nd} order 2d Mott metal-insulator transition (Senthil et. al.)

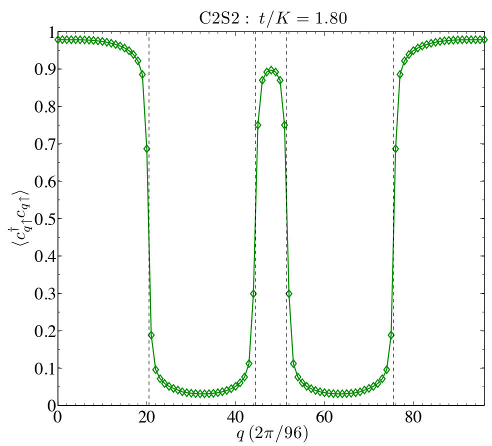
Experimental manifestation of continuous Mott transition?
(Organics, perhaps weak first order metal-insulator transition?)

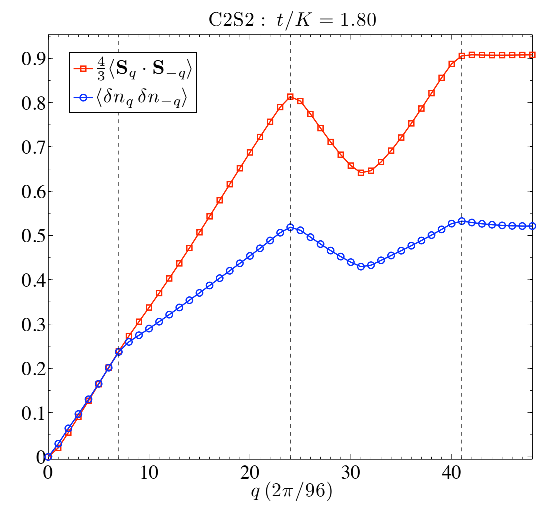
DMRG features

2-Band Luttinger liquid

Electron momentum distribution quite sharp despite O(1) interactions

Expected singular features in spin and density momentum structure factors





Evidence for Kosterlitz-Thouless Criticality at Mott transition

$$\langle \delta n_q \delta n_{-q} \rangle = g_\rho(2q/\pi)$$

$$L \to \infty, \quad \Delta g_\rho \approx 1/2$$