Mott quantum criticality in anisotropic Hubbard models

Fakher F. Assaad (KITP, August 28, 2015
New Phases and Emergent Phenomena in Correlated Materials with Strong Spin-Orbit Coupling)

Outline

- Model, motivation and methods
- Results from

  → Exact methods (BSS-QMC) (weakly coupled chains)
  → Cluster methods (CDMFT/VCA) (full phase diagram)

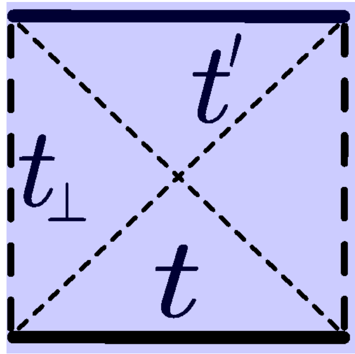
- Conclusions

Marcin Raczkowski (Uni. Würzburg)
Lode Pollet (LMU)
Thomas Pruschke (Göttingen)
Benjamin Lenz (Göttingen)
Salvatore Manmana (Göttingen)

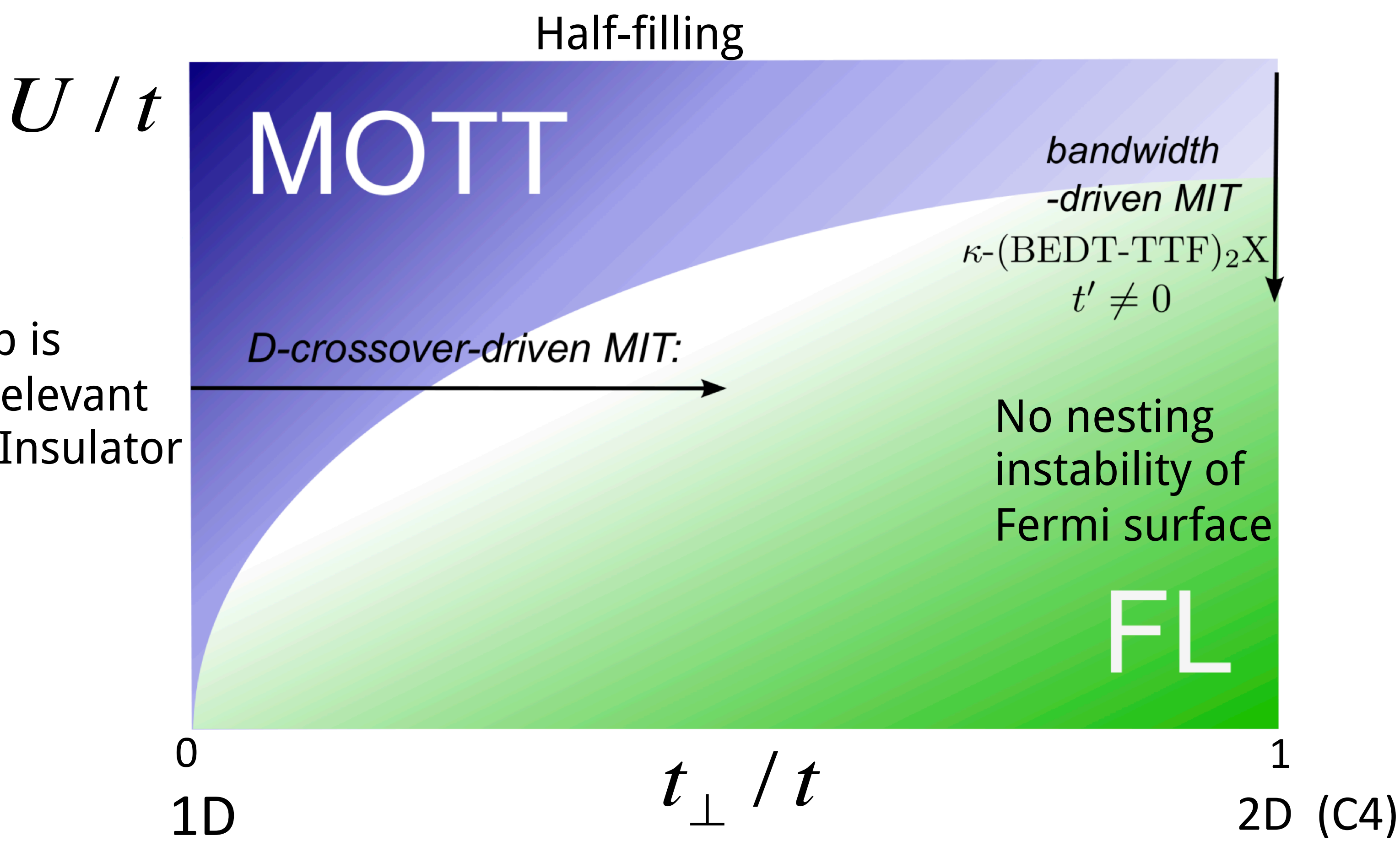
B. Lenz, M. Raczkowski, S. Manmana, T. Pruschke, FFA in preparation
M. Raczkowski, FFA, L. Pollet, FFA, Phys. Rev. B 91, 045137 (2015)
M. Raczkowski, FFA, Phys. Rev. B 88, 085120 (2013)
M. Raczkowski, FFA, Phys. Rev. Lett. **109**, 126404 (2012)

Model

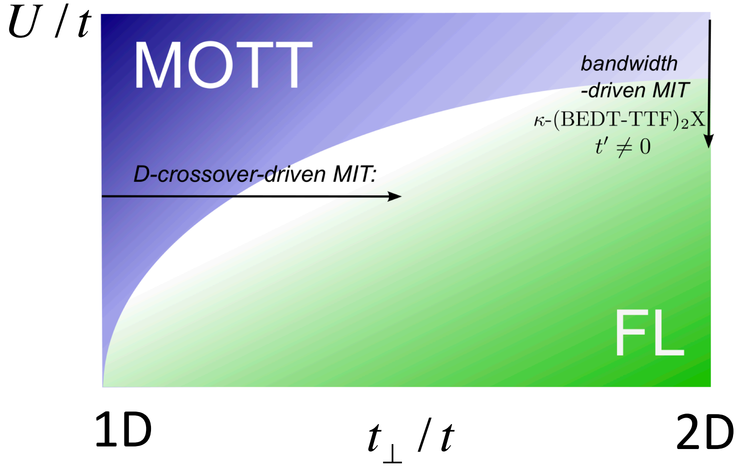
$$H = -\sum_{\mathbf{i},\mathbf{j},\sigma} t_{\mathbf{i},\mathbf{j}} c^{\dagger}_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i},\uparrow} n_{\mathbf{i},\downarrow} - \mu \sum_{\mathbf{i}} n_{\mathbf{i},\sigma}$$



$t' = -t_\perp / 4$



1D
Umklapp is
always relevant
→ Mott Insulator



3D band width controlled MIT: V_2O_3

Universality and Critical Behavior at the Mott Transition

P. Limelette,[1*] A. Georges,[1,2] D. Jérome,[1] P. Wzietek,[1]
P. Metcalf,[3] J. M. Honig[3]

Science 302, 89 (2003).

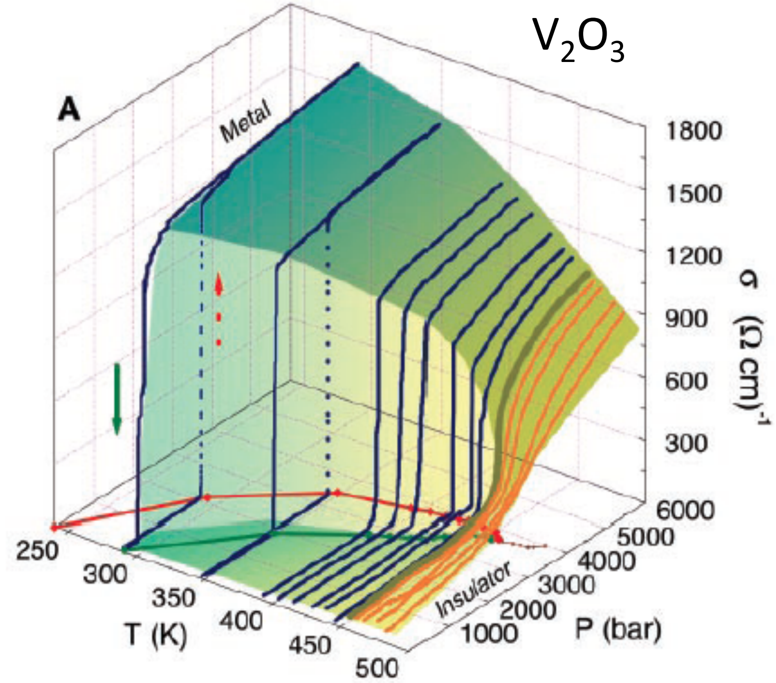
First order
Critical endpoint
$T_c = 457.5K$

$$\sigma(T,P_c)-\sigma_c \sim (T_c - T)^{\beta}$$

$$\sigma(T_c,P)-\sigma_c \sim (P - P_c)^{1/\delta}$$

$$\left.\frac{d\sigma(T,P)}{dP}\right|_{P=P_c} \sim (T_c - T)^{\gamma}$$

Order parameter:
double occupancy =
scalar local field →
Ising universality



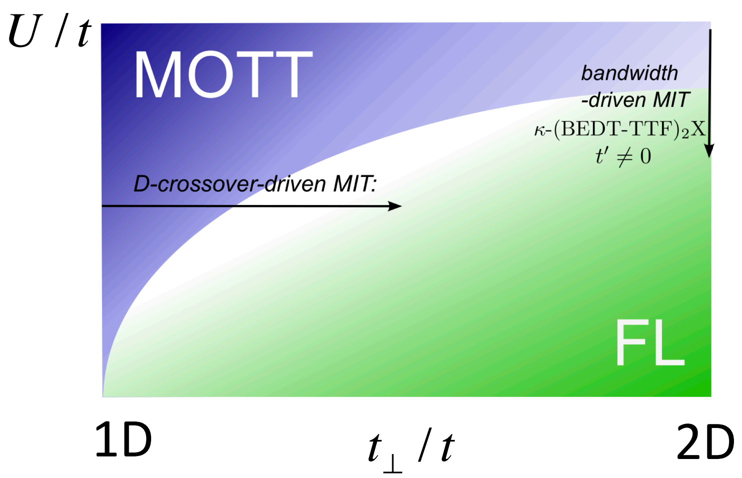
Data consistent with mean-field over wide T range

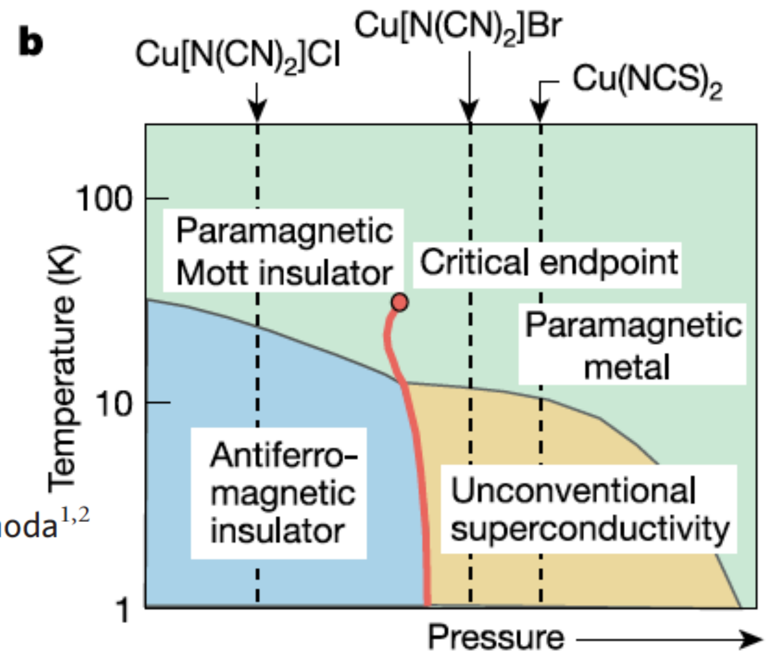
$(\beta, \delta, \gamma) = (0.5,\ 3,\ 1)$ → DMFT

Very close to transition crossover to 3D Ising:

$(\beta, \delta, \gamma) = (0.31,\ 5,\ 1.25)$

2D band width controlled MIT





First order Critical endpoint T_c =39.7K

F. Kagawa[1], K. Miyagawa[1,2] & K. Kanoda[1,2]

nature Vol 436|28 July 2005

$$\sigma(T,P_c)-\sigma_c \sim (T_c-T)^{\beta}$$

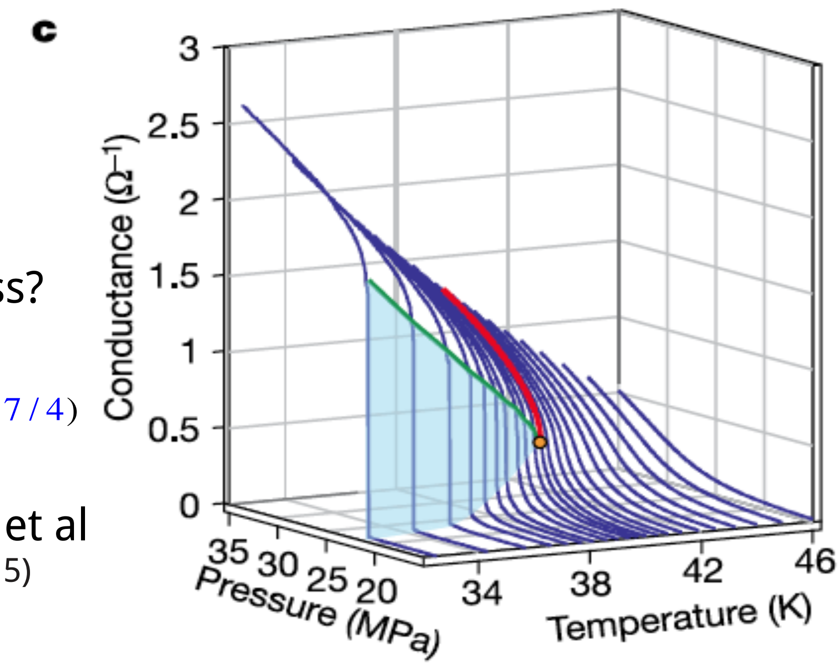
$$\sigma(T_c,P)-\sigma_c \sim (P-P_c)^{1/\delta}$$

$$\left.\frac{d\sigma(T,P)}{dP}\right|_{P=P_c} \sim (T_c-T)^{\gamma}$$

Universality class?

2D Ising:

$$(\beta,\delta,\gamma)=(1/8,\ 15,\ 7/4)$$



Data consistent with.

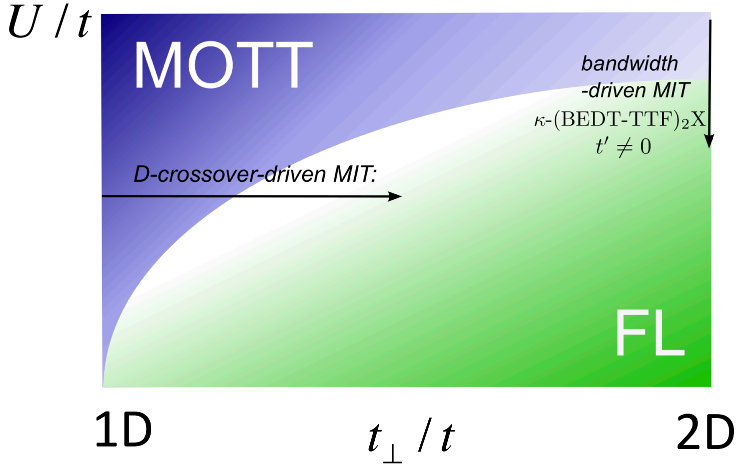
$$(\beta,\delta,\gamma)=(1,\ 2,\ 1)$$

Widom: $\beta(\delta-1)=\gamma$ ✓

M. Abdel-Jawad et al

PRL 114, 106401 (2015)

→ 2D Ising



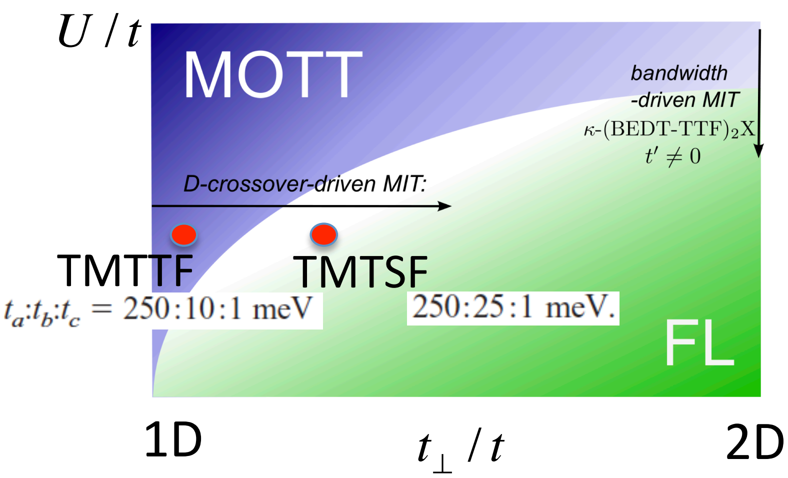
D< 2: Dimensional-driven MIT

Questions

a) Nature of the transition.
Quantum ($T_c = 0$) or classical ($T_c > 0$) ?

b) Nature of metallic state in the vicinity of the dimensional driven MIT?

D< 2: Dimensional-driven MIT



Questions

a) Nature of the transition.
   Quantum ($T_c = 0$) or classical ($T_c > 0$) ?

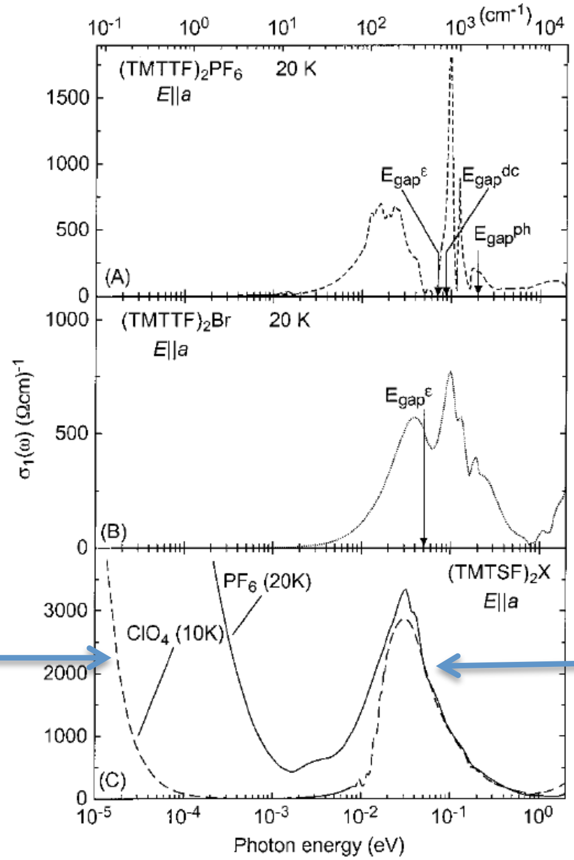
b) Nature of metallic state in the vicinity of the dimensional driven MIT?

Dimensionality-Driven Insulator-to-Metal Transition in the Bechgaard Salts

V. Vescoli, L. Degiorgi, W. Henderson, G. Grüner, K. P. Starkey, L. K. Montgomery

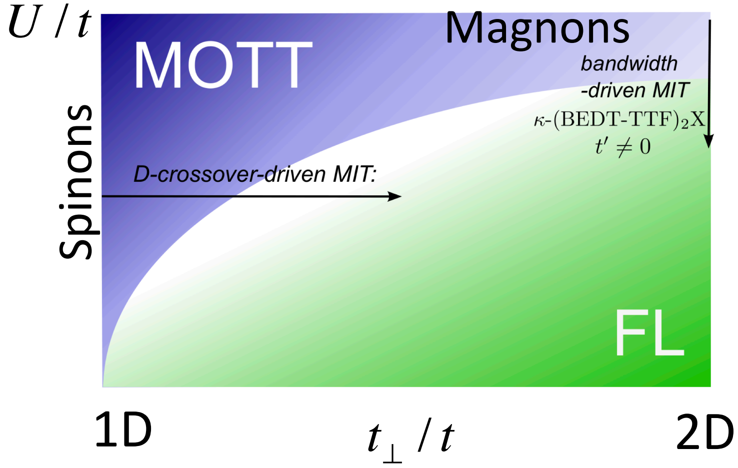
Science **281**, 1181 (1998)

2D *Fermi liquid*



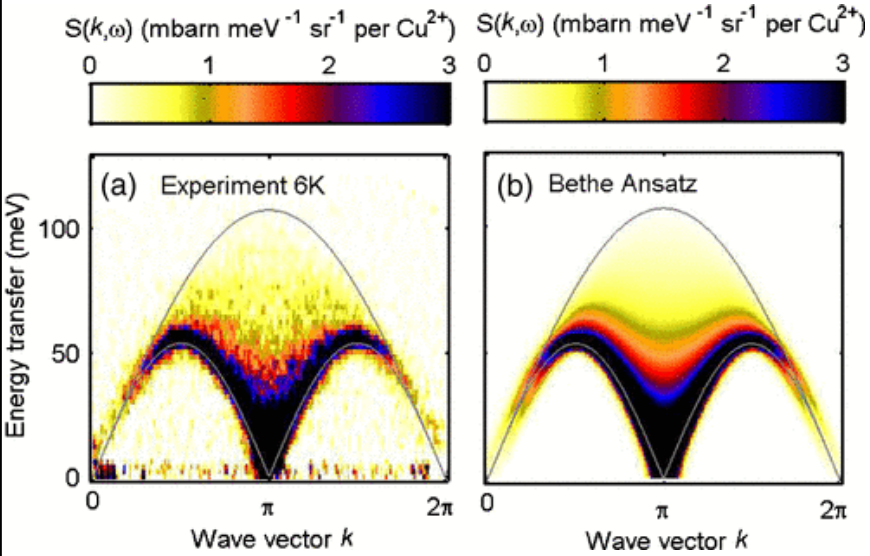
1D Chains.

D< 2: Dimensional-driven MIT
What about the spin degrees of freedom?



$$H_{Heis} = J\sum_{\mathbf{i}} \mathbf{S}_{\mathbf{i}} \cdot \mathbf{S}_{\mathbf{i}+\mathbf{a}_x} + \delta\, \mathbf{S}_{\mathbf{i}} \cdot \mathbf{S}_{\mathbf{i}+\mathbf{a}_y}, \quad \mathbf{S}_{\mathbf{i}} = \frac{1}{2}\sum_{s,s'} f^{\dagger}_{\mathbf{i},s}\, \sigma_{s,s'}\, f_{\mathbf{i},s'}, \quad \sum_{s} f^{\dagger}_{\mathbf{i},s} f_{\mathbf{i},s} = 1$$

δ=0



B. Lake et al. Phys. Rev. Lett. 111, 137205 (2013)

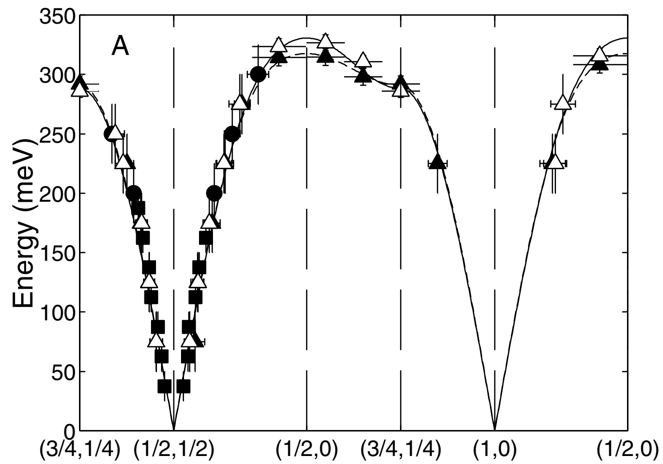
$KCuF_3$

Confinement

T=0, no frustration,
δ_c=0
(A. Sandvik. PRL 83, 1999)

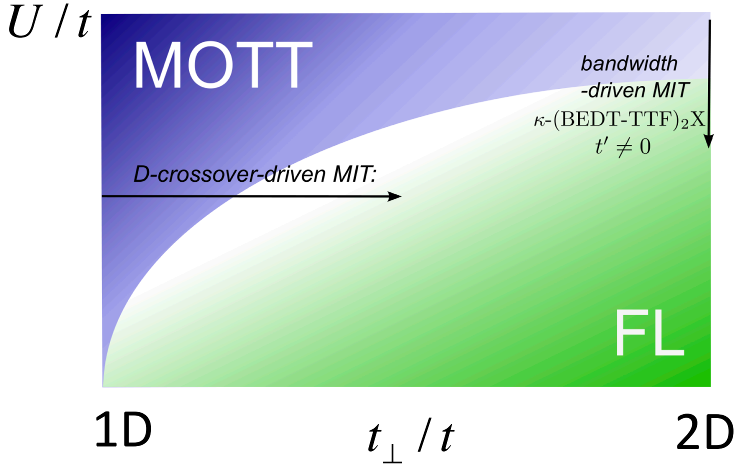
δ=1

La_2CuO_4



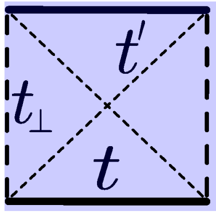
R. Coldea et al. Phys. Rev. Lett. 86, 5377 (2001)

With frustration?



Methods

$$H = -\sum_{\mathbf{i},\mathbf{j},\sigma} t_{\mathbf{i},\mathbf{j}} c^{\dagger}_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i},\uparrow} n_{\mathbf{i},\downarrow} - \mu \sum_{\mathbf{i}} n_{\mathbf{i},\sigma}$$



$t' = -t_{\perp}/4$

Exact BSS approach

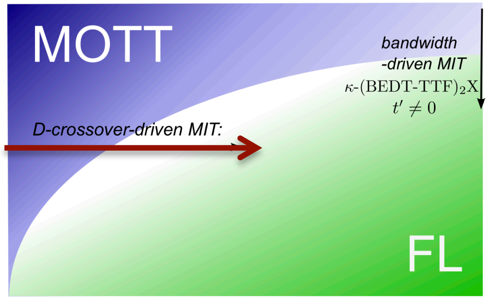
Exact evaluation of

$$\langle O \rangle = \frac{\mathrm{Tr}\left[e^{-\beta(H-\mu N)} O \right]}{\mathrm{Tr}\left[e^{-\beta(H-\mu N)} \right]}$$

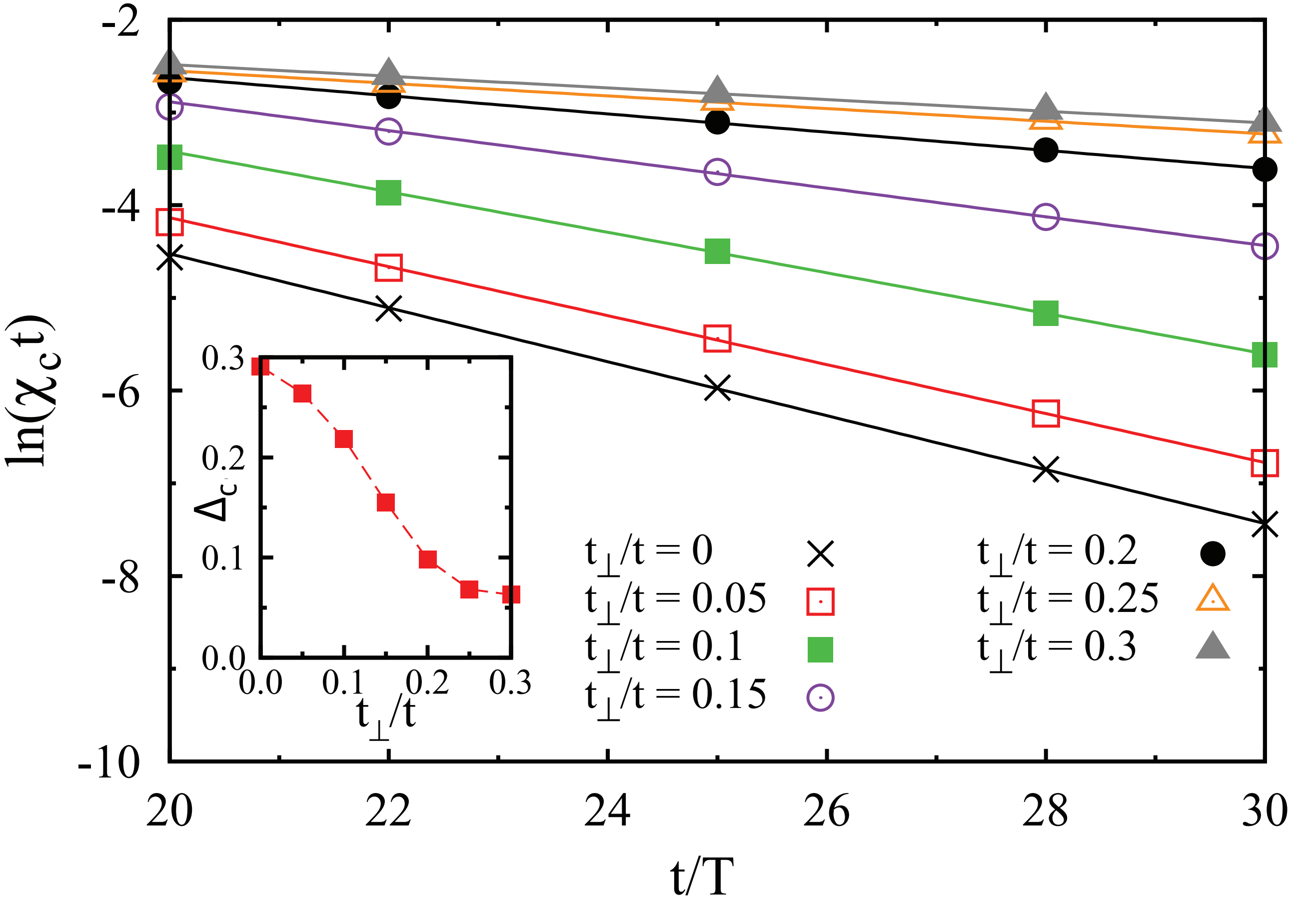
Advantage. Two particle quantities.
Spatial fluctuations.

Issues. Sign problem.
Sign problem is *mild* in a non-trivial portion of the phase diagram.
→ 20 X 20 lattices down to βt=30.

Charge susceptibility: 16x16 @ U/t = 2.3

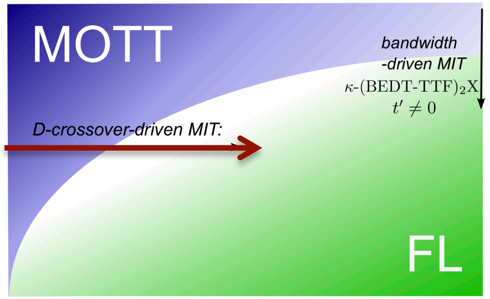


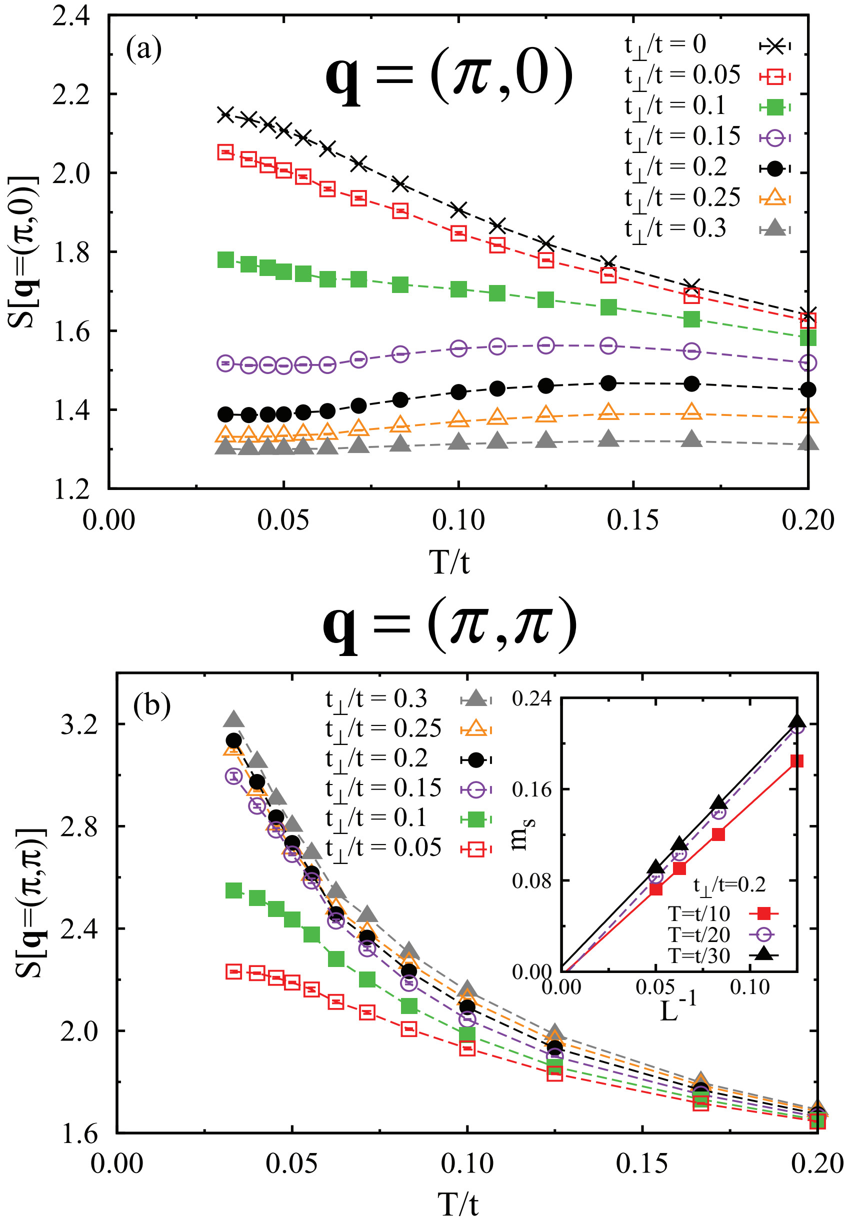
$$\chi_c = \beta\left(\langle N^2\rangle - \langle N\rangle^2\right)/L^2 \sim e^{-\Delta_c/T}$$

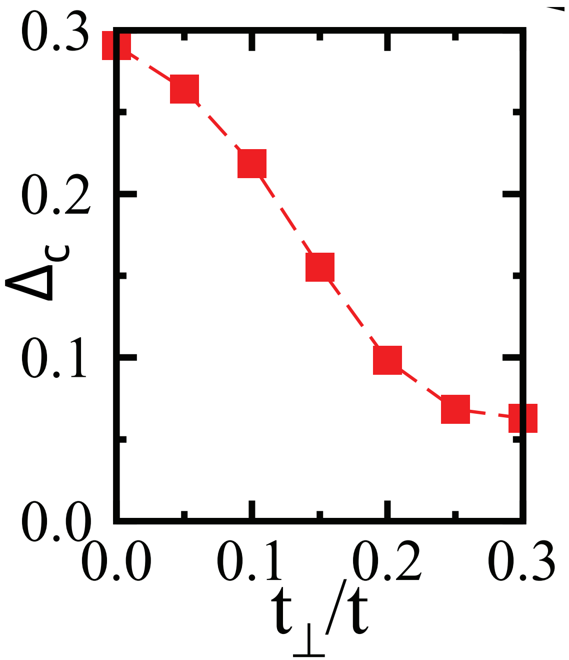


Origin of charge gap?

$$S(\mathbf{q}) = \sum_{\mathbf{r}} e^{i\mathbf{qr}} \left\langle \hat{S}_z(\mathbf{r}) \hat{S}_z(0) \right\rangle$$







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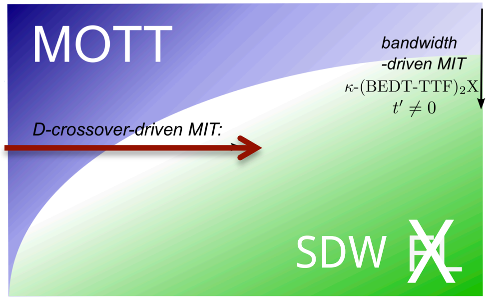
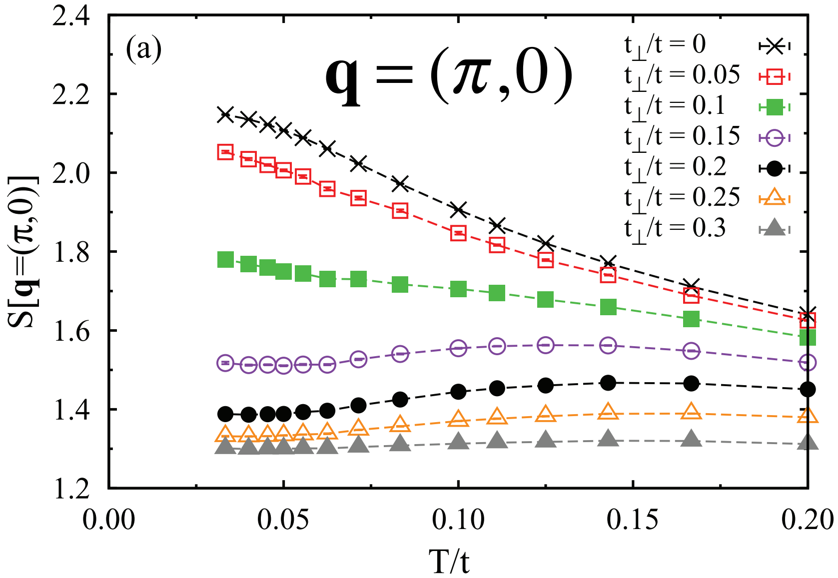
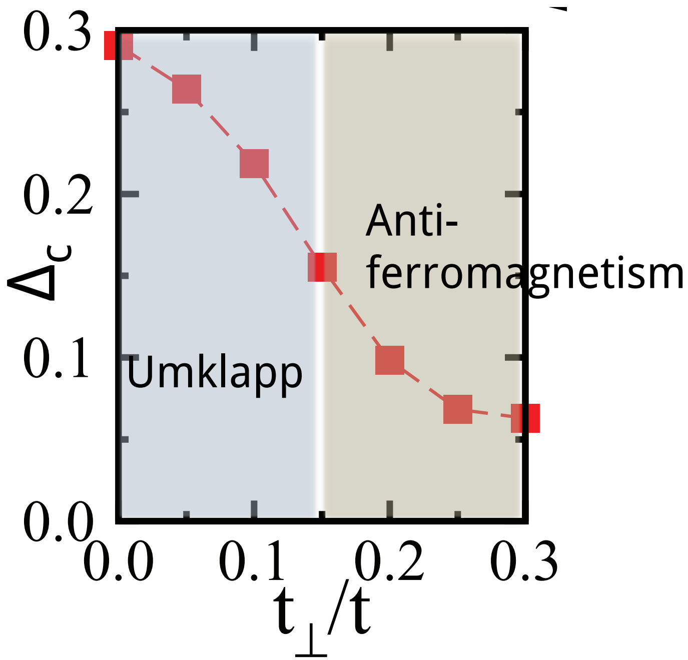
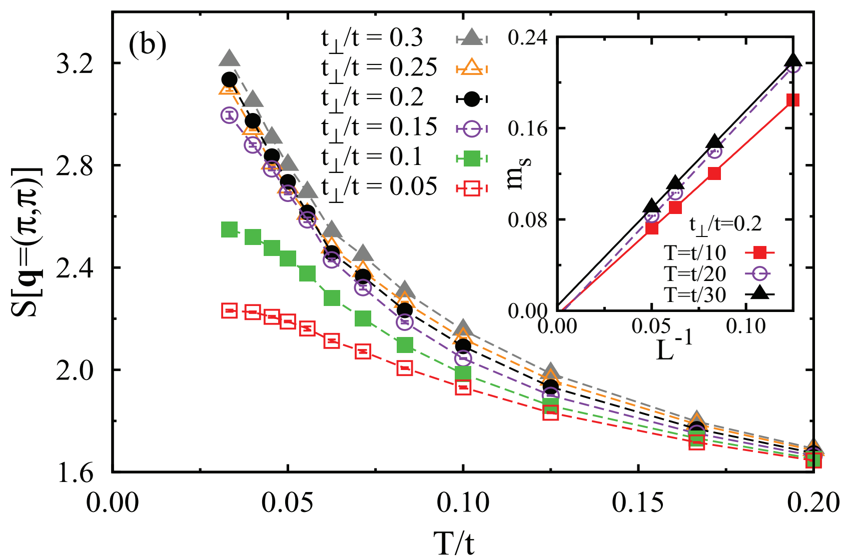




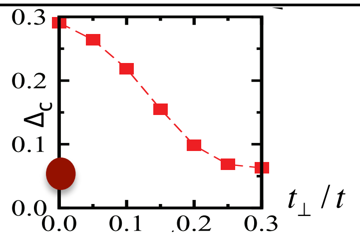
Frustration effects are not strong enough to guarantee FL-state down to low temperatures! $t' = -t_\perp / 4$

$\mathbf{q} = (\pi, \pi)$

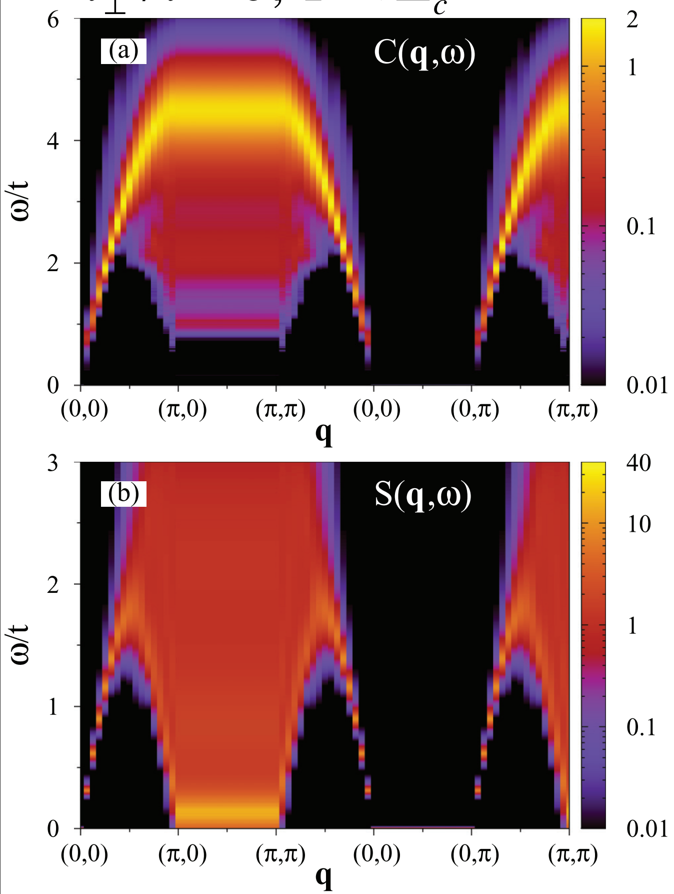




Spin and charge dynamics @ T= 1/20



$$t_\perp / t = 0,\ T < \Delta_c$$



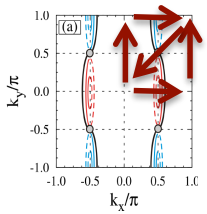
$$C(\mathbf{q},\omega) = \frac{\pi}{Z}\sum_{n,m} e^{-\beta E_n} \left|\langle m | N_{\mathbf{q}} | n\rangle\right|^2 \ \delta(E_m - E_n - \omega)$$

$$N_{\mathbf{q}} = \frac{1}{L}\sum_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k+q},\sigma} c_{\mathbf{k},\sigma}$$

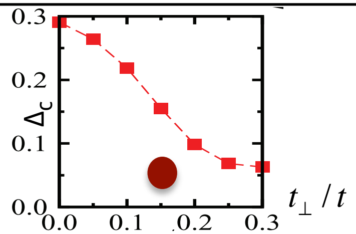
$$S(\mathbf{q},\omega) = \frac{\pi}{Z}\sum_{n,m} e^{-\beta E_n} \left|\langle m | S^{+}_{\mathbf{q}} | n\rangle\right|^2 \ \delta(E_m - E_n - \omega)$$

$$S^{+}_{\mathbf{q}} = \frac{1}{L}\sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k+q},\uparrow} c_{\mathbf{k},\downarrow}$$

One dimension
Two-spinon
continuum

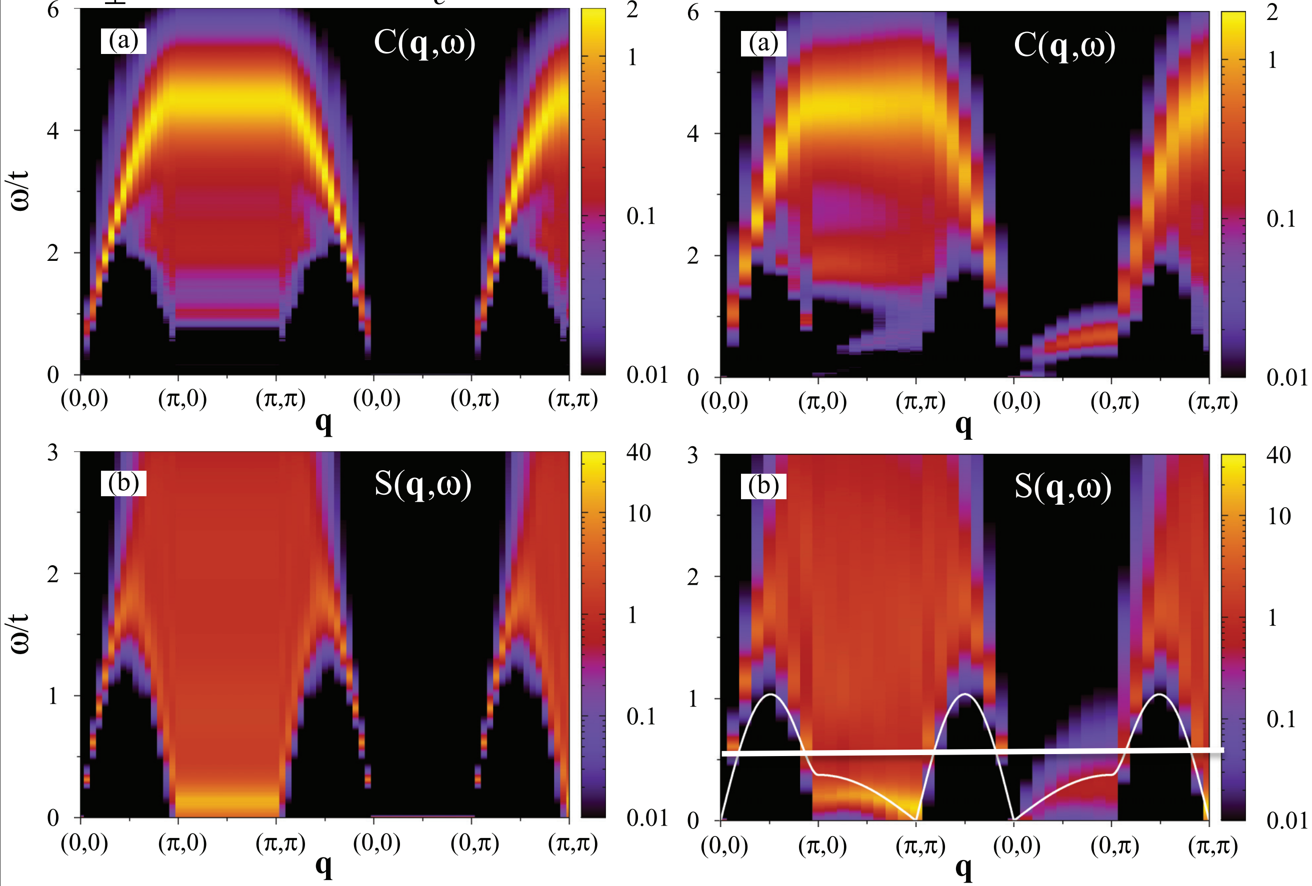


Spin and charge dynamics @ T= 1/20

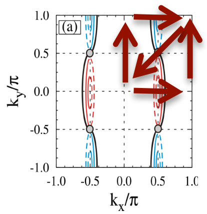


$t_\perp / t = 0,\ T < \Delta_c$

$t_\perp / t = 0.15, T < \Delta_c$

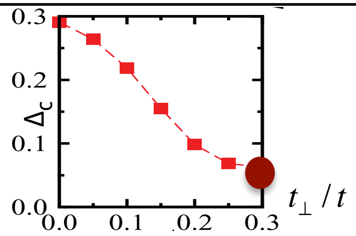


One dimension
Two-spinon continuum

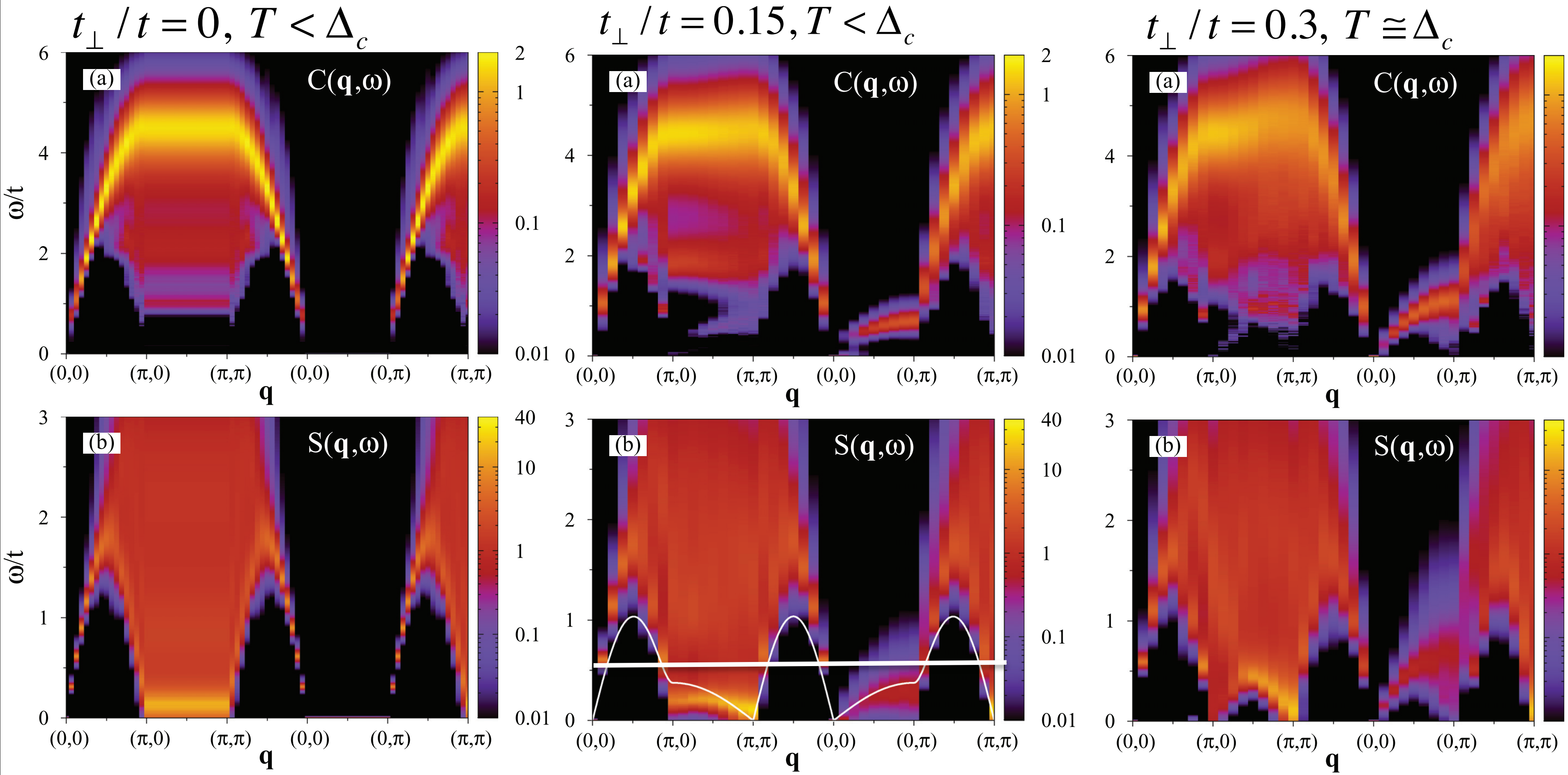


Low energy: spin-waves
High energy: 1D physics

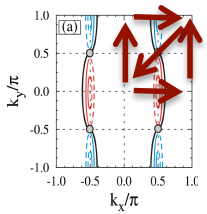
Spin waves decay into spinons



Spin and charge dynamics @ T= 1/20



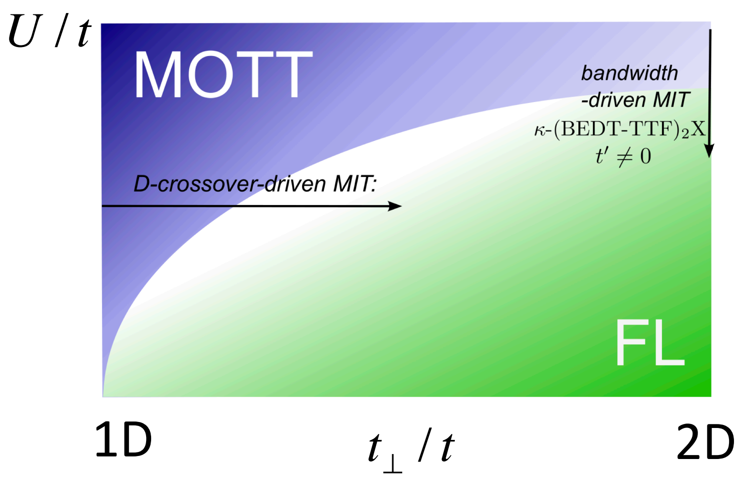
One dimension
Two-spinon
continuum



Low energy: spin-waves
High energy: 1D physics

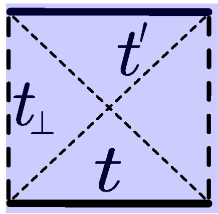
Spin waves decay into
spinons

Low energy: spin-waves
charge excitations
High energy: 1D physics
Spin waves decay into
particle-hole excitations



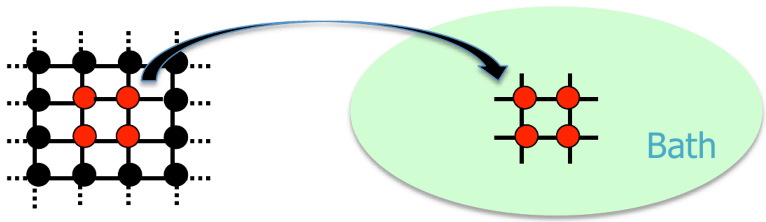
Methods

$$\boxed{H = -\sum_{\mathbf{i},\mathbf{j},\sigma} t_{\mathbf{i},\mathbf{j}}\, c^{\dagger}_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i},\uparrow} n_{\mathbf{i},\downarrow} - \mu \sum_{\mathbf{i}} n_{\mathbf{i},\sigma}}$$



$$t' = -t_{\perp}/4$$

CDMFT/VCA



Cluster sizes 8x2, 4x4, 2x2, Hirsch-Fye and ED solvers

Advantage. Mild sign problem → CPU $(\beta V)^3$
Paramagnetic phase

Issues. Cluster size.
Real space fluctuations.
Lattice two-particle quantities.

Chain-DMFT. S. Biermann, A. Georges, A. Lichtenstein, and T. Giamarchi, PRL **87**, 276405 (2001).

Exact BSS approach

Exact evaluation of

$$\langle O \rangle = \frac{\mathrm{Tr}\left[e^{-\beta(H-\mu N)} O \right]}{\mathrm{Tr}\left[e^{-\beta(H-\mu N)} \right]}$$

Advantage. Two particle quantities.
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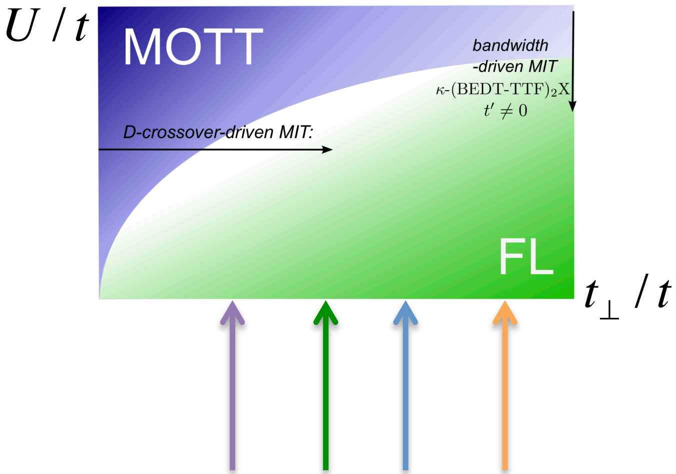
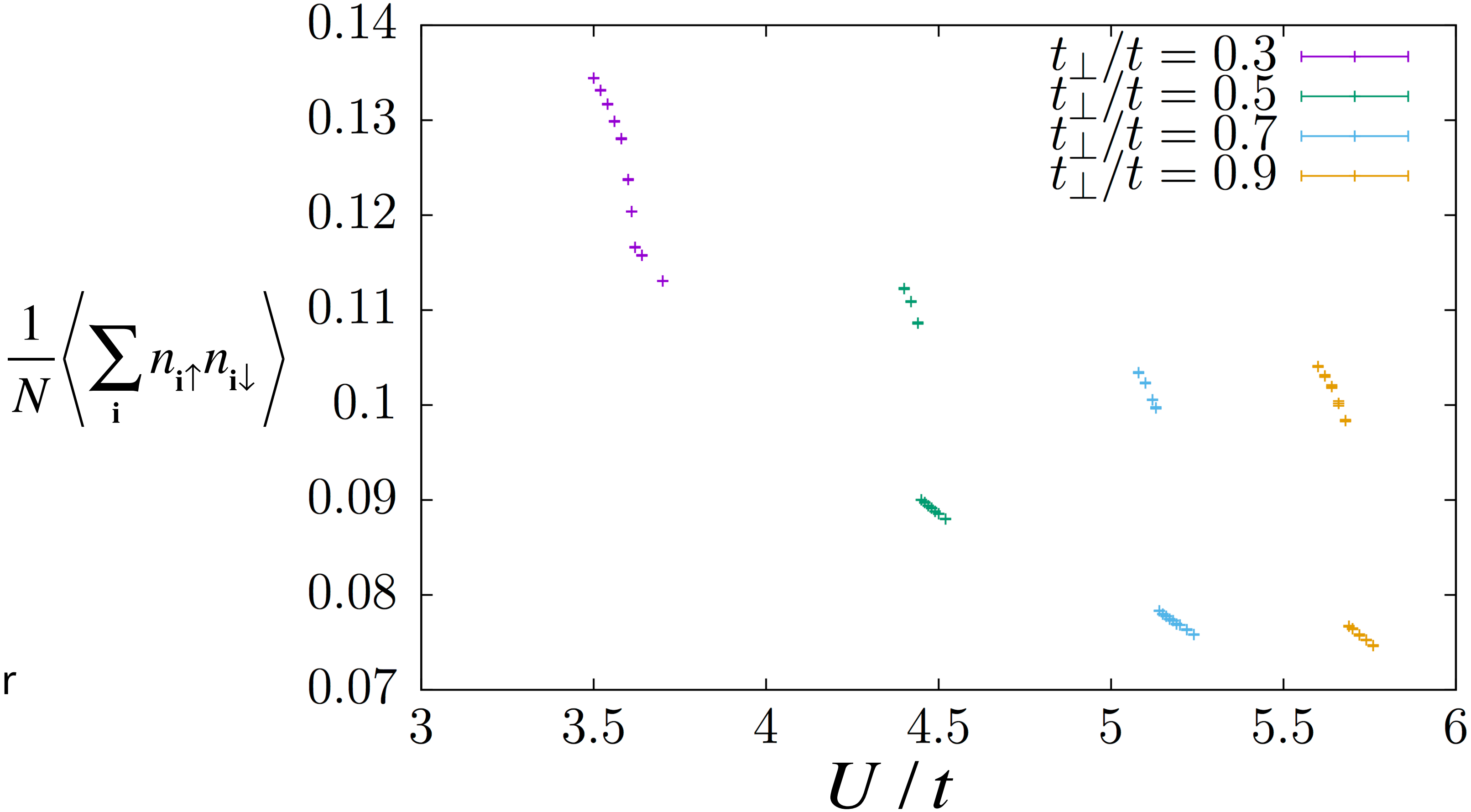
Sign problem is *mild* in a non-trivial portion of the phase diagram.
→ 20 X 20 lattices down to βt=30.



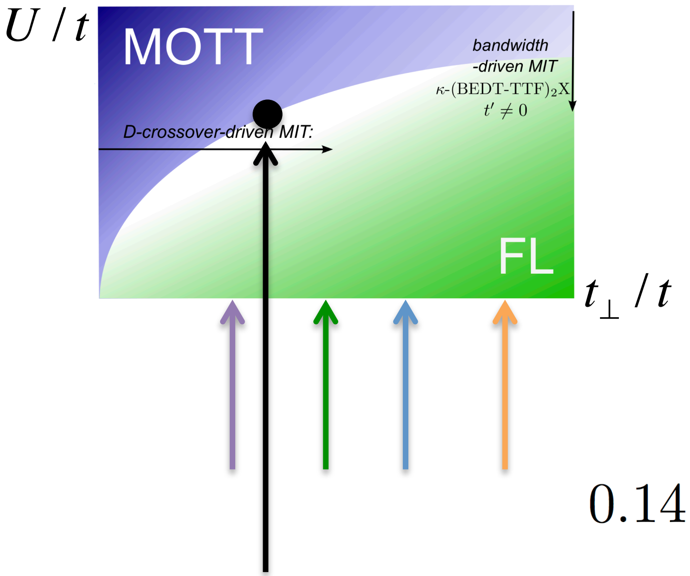
Nature of the transition

$$\frac{1}{N}\frac{\partial F}{\partial U} = \frac{1}{N}\left\langle \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \right\rangle$$



CDMFT
2x2 Cluster
$\beta t = 40$

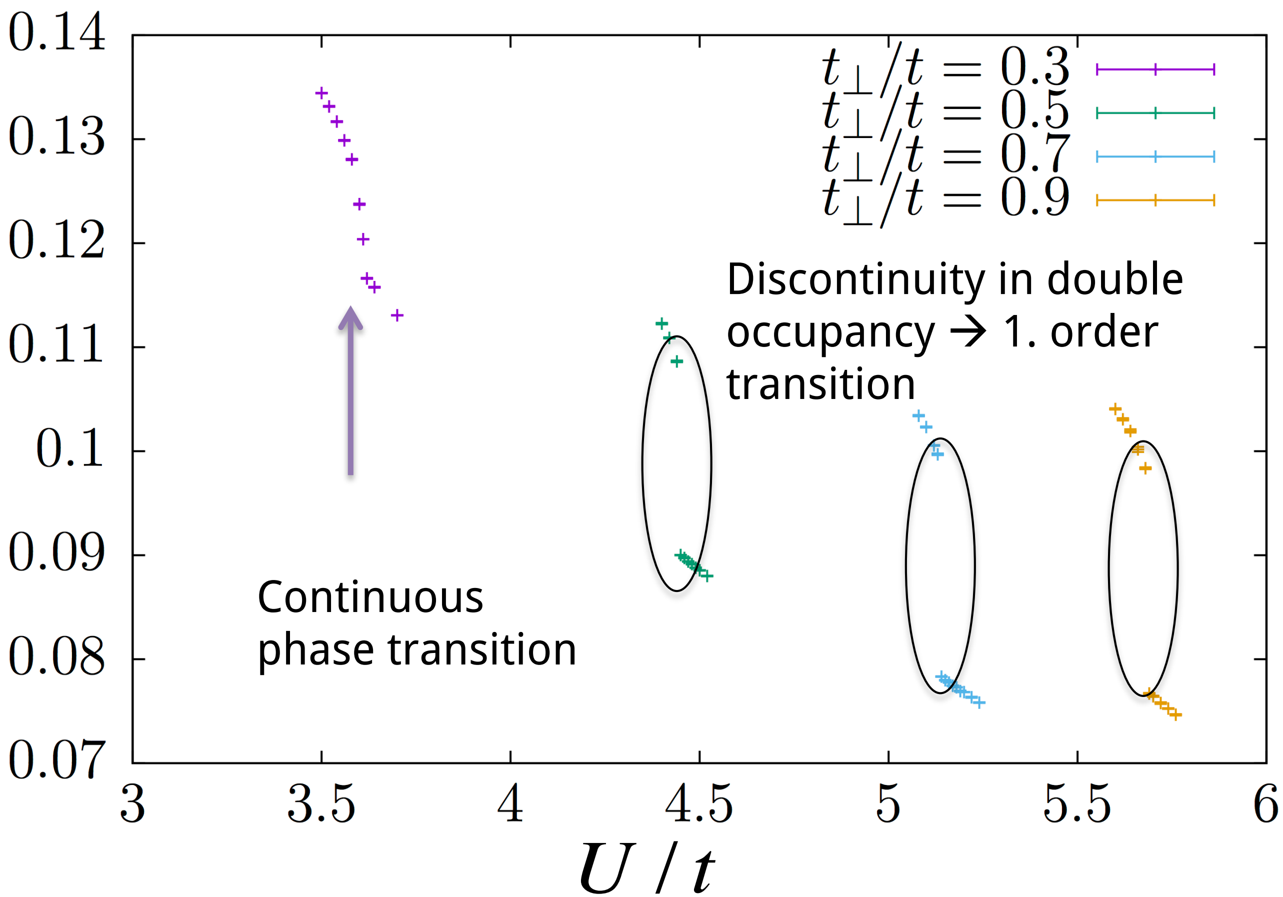
Nature of the transition, D



QCP at which T_c vanishes

$$\frac{1}{N}\frac{\partial F}{\partial U} = \frac{1}{N}\left\langle \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \right\rangle$$

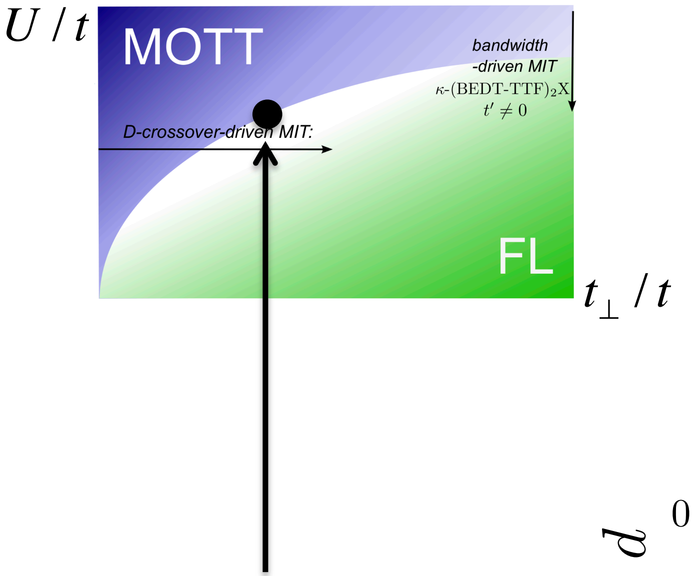
$$\frac{1}{N}\left\langle \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \right\rangle$$



Discontinuity in double occupancy → 1. order transition

Continuous phase transition

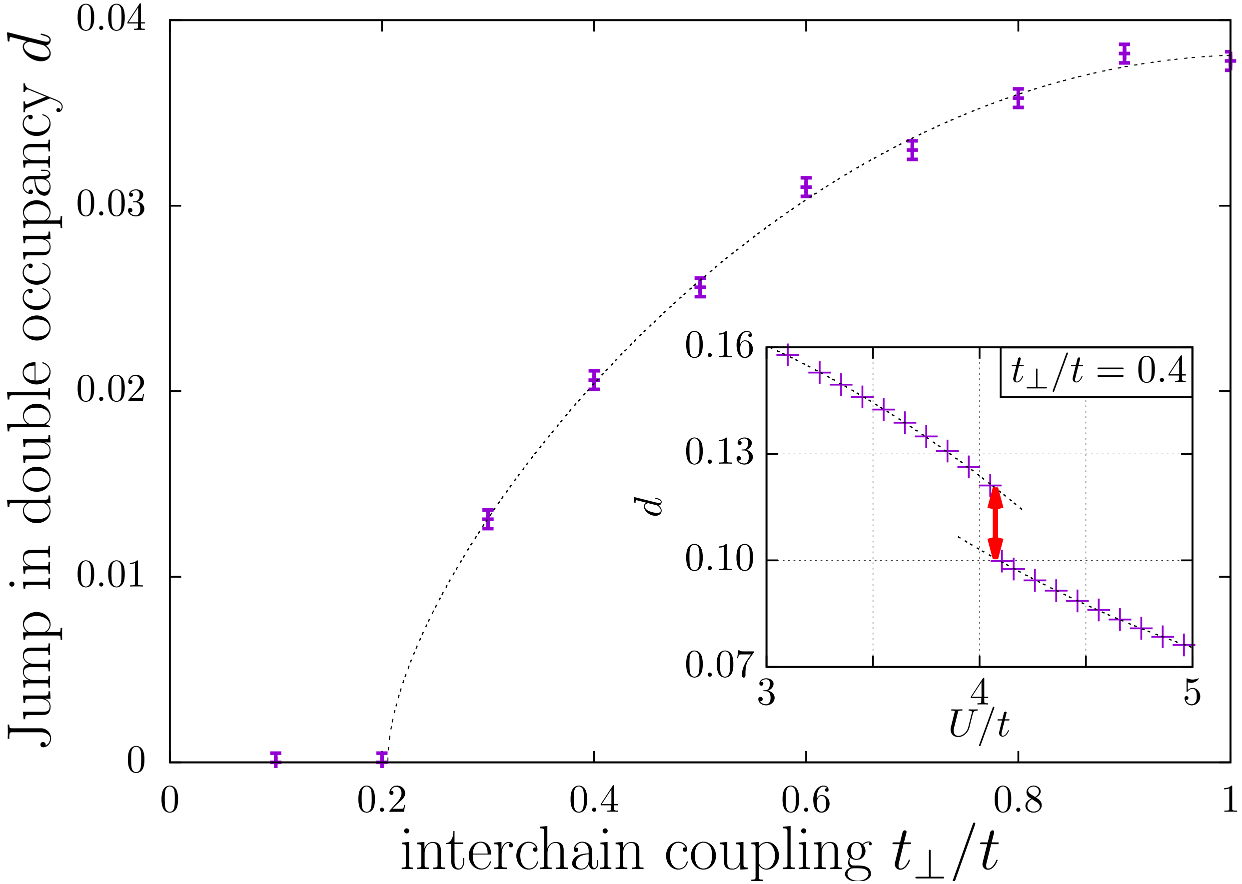
CDMFT
2x2 Cluster
$\beta t = 40$



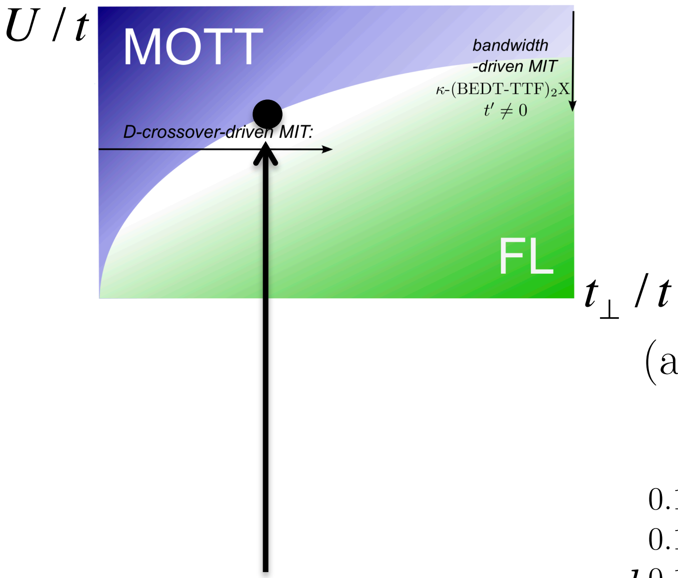
QCP at which T_c vanishes

Nature of the transition, D

$$\frac{1}{N}\frac{\partial F}{\partial U} = \frac{1}{N}\left\langle \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \right\rangle$$

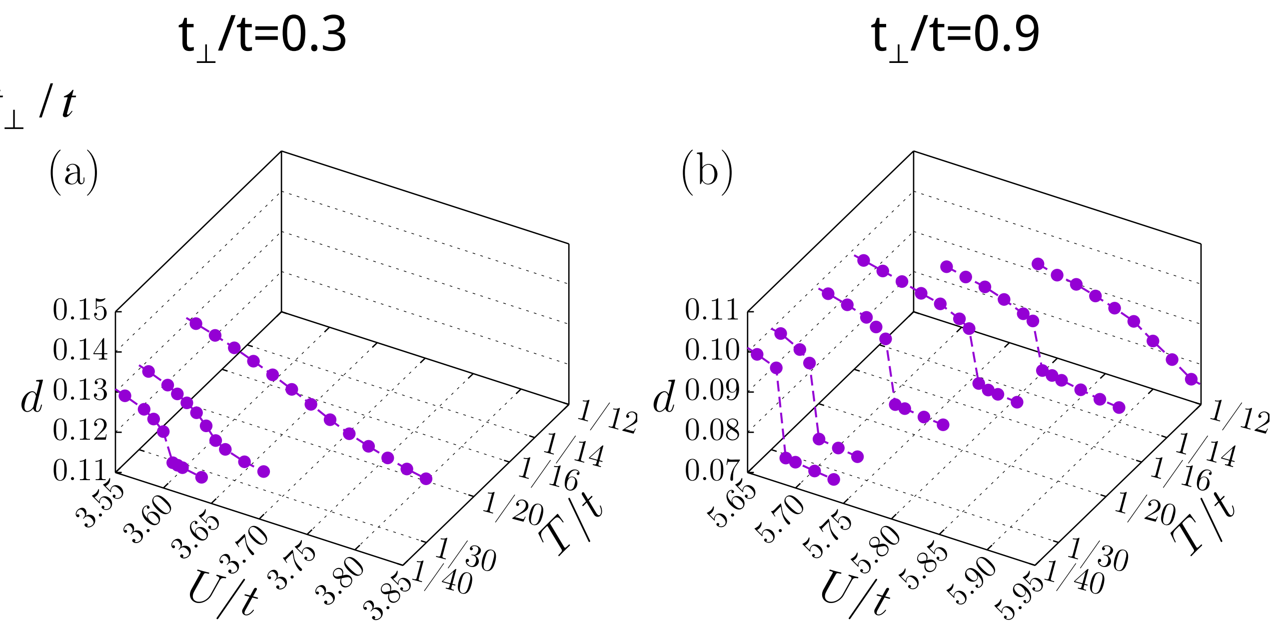


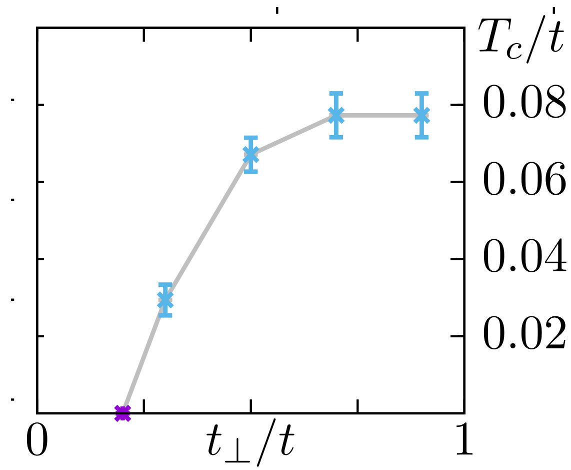
VCA (T=0)
2x2 Cluster
with 4 bath sites



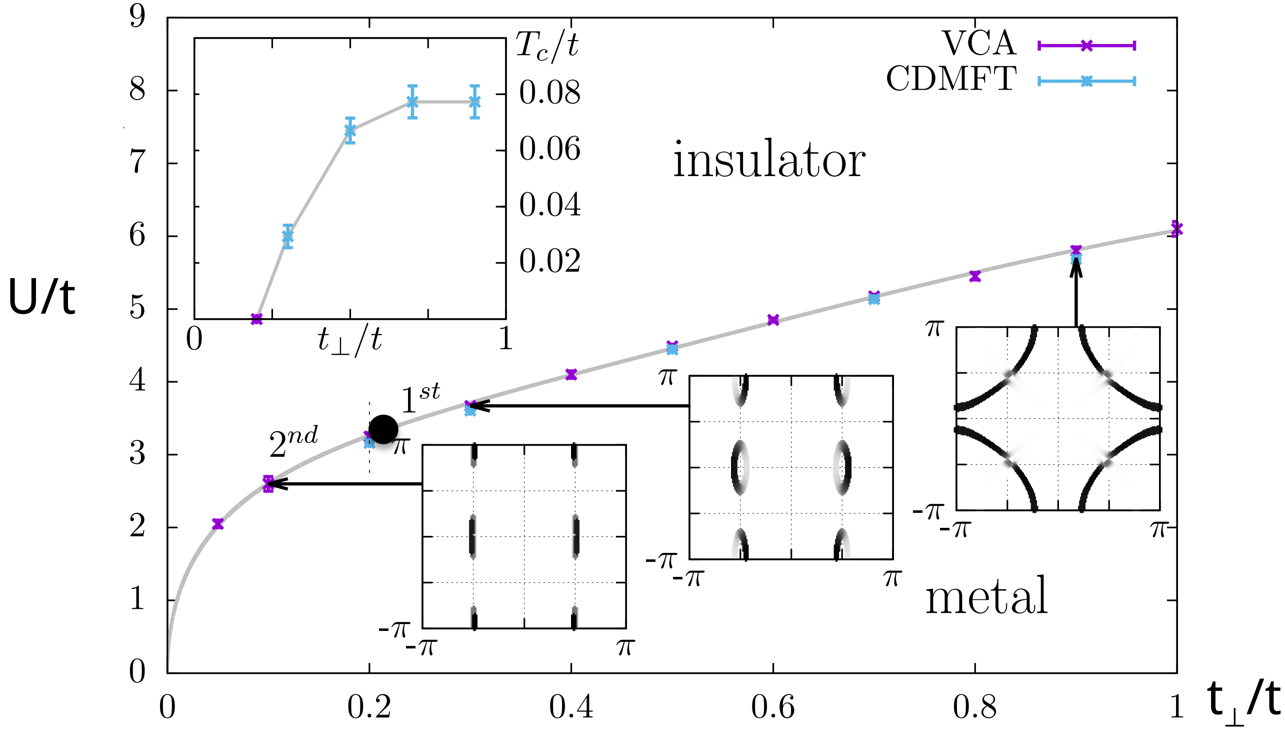
QCP at which T_c vanishes

Nature of the transition, T_c





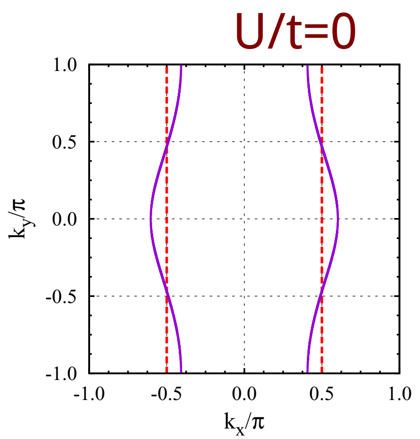
CDMFT
2x2 Cluster

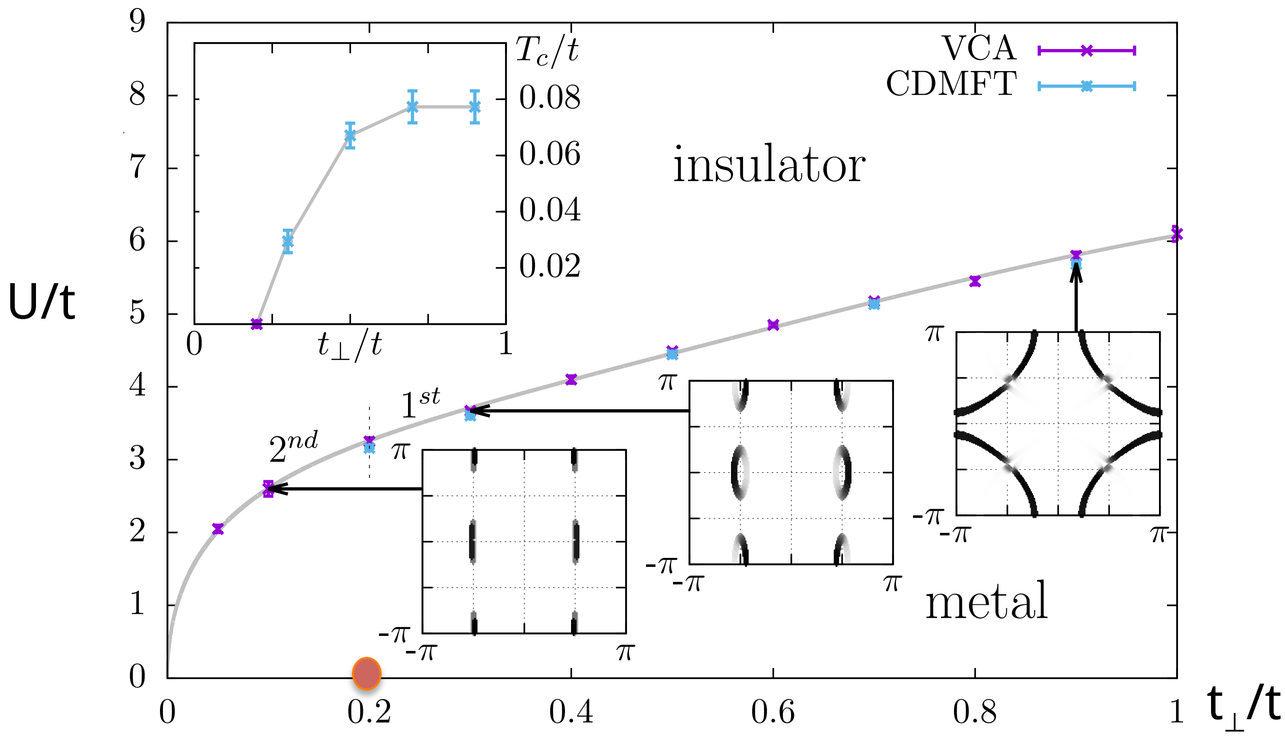


U/t
t⊥/t
VCA
CDMFT
insulator
metal
1st
2nd
Tc/t

Fermi surface topology

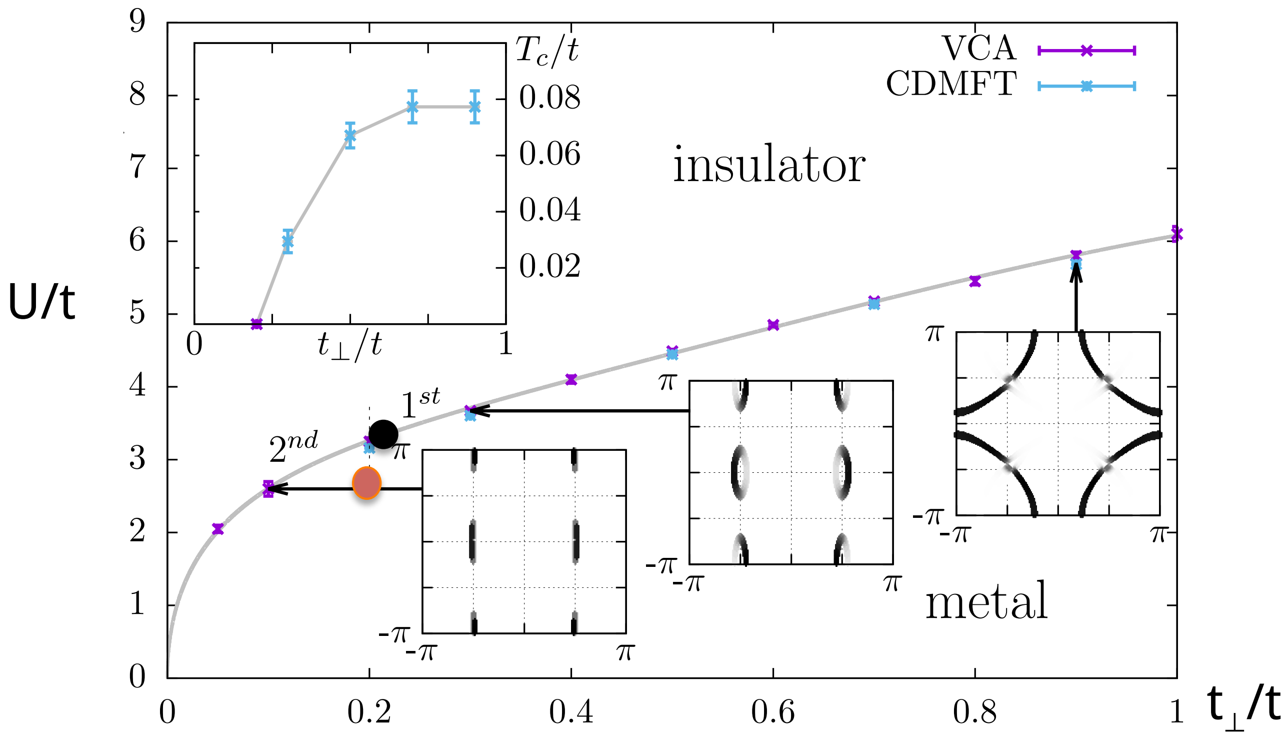
@ $t_{\perp}/t$ = 0.2 as a function of U/t



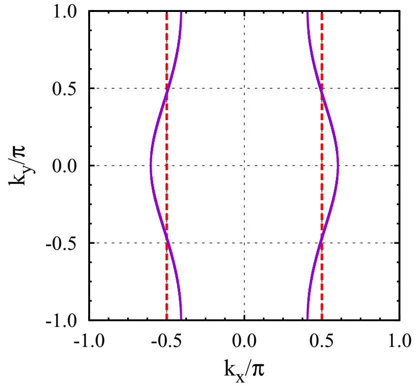


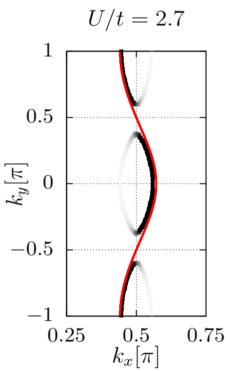
Fermi surface topology

@ $t_\perp/t$ = 0.2 as a function of U/t

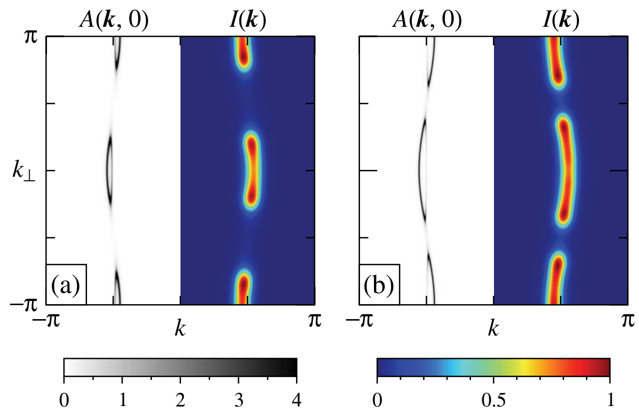


U/t=0





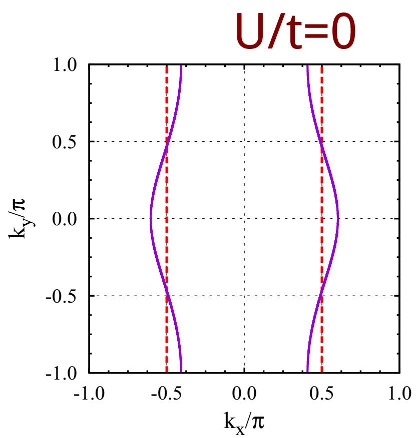
FS breaks up into electron and hole pockets.

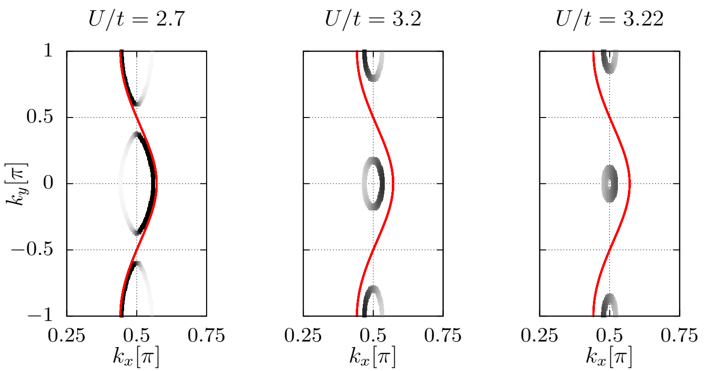


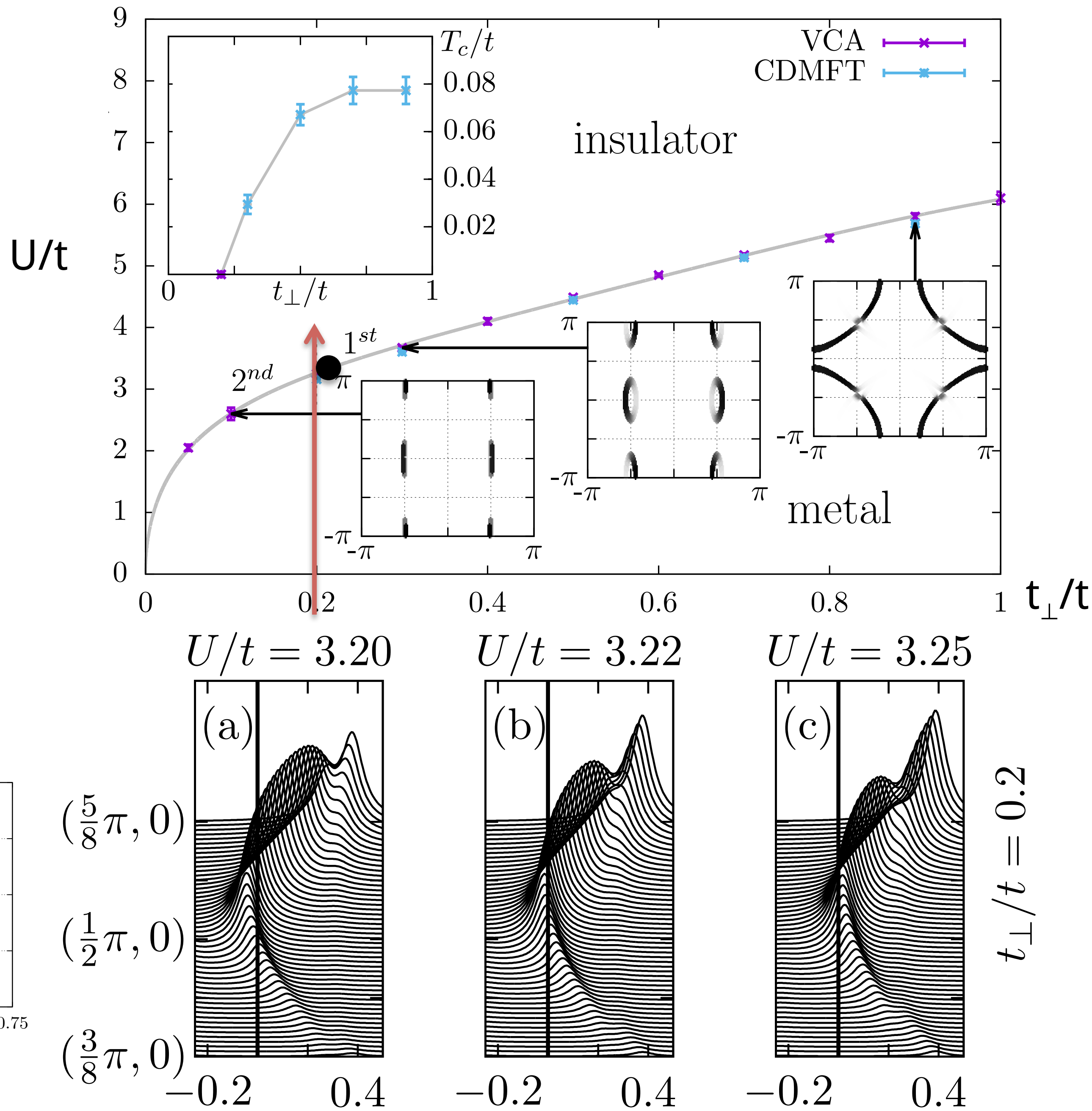
Spinless fermions:
C. Berthod, T. Giamarchi, S. Biermann, and A. Georges
Phys. Rev. Lett. 97, 136401 (2006)

Fermi surface topology

@ $t_\perp/t$ = 0.2 as a function of U/t



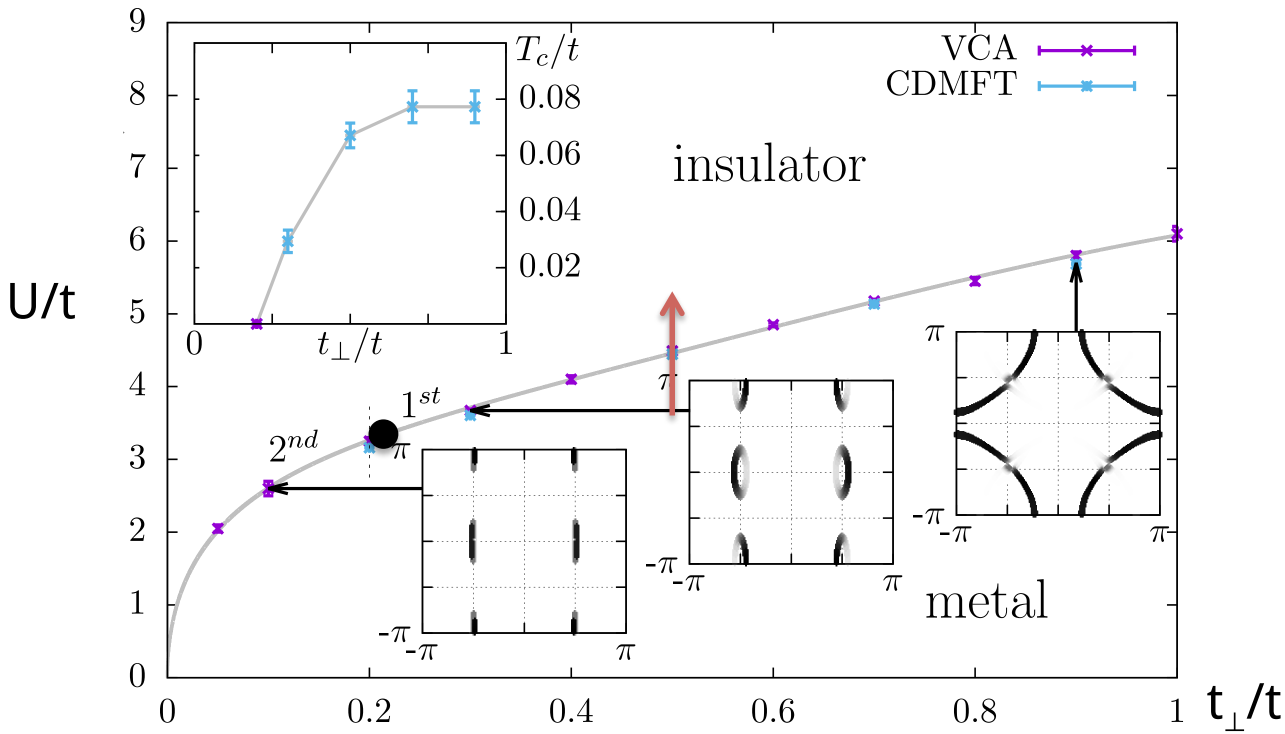


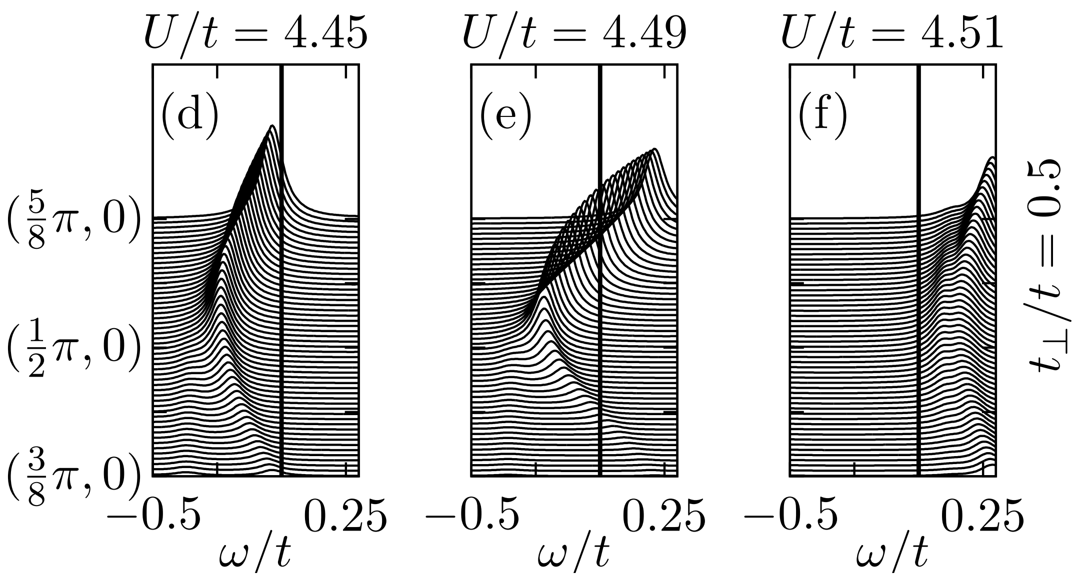


→ Volume of hole and electron pockets vanishes smoothly

Fermi surface topology

@ $t_\perp/t$ = 0.5 as a function of U/t

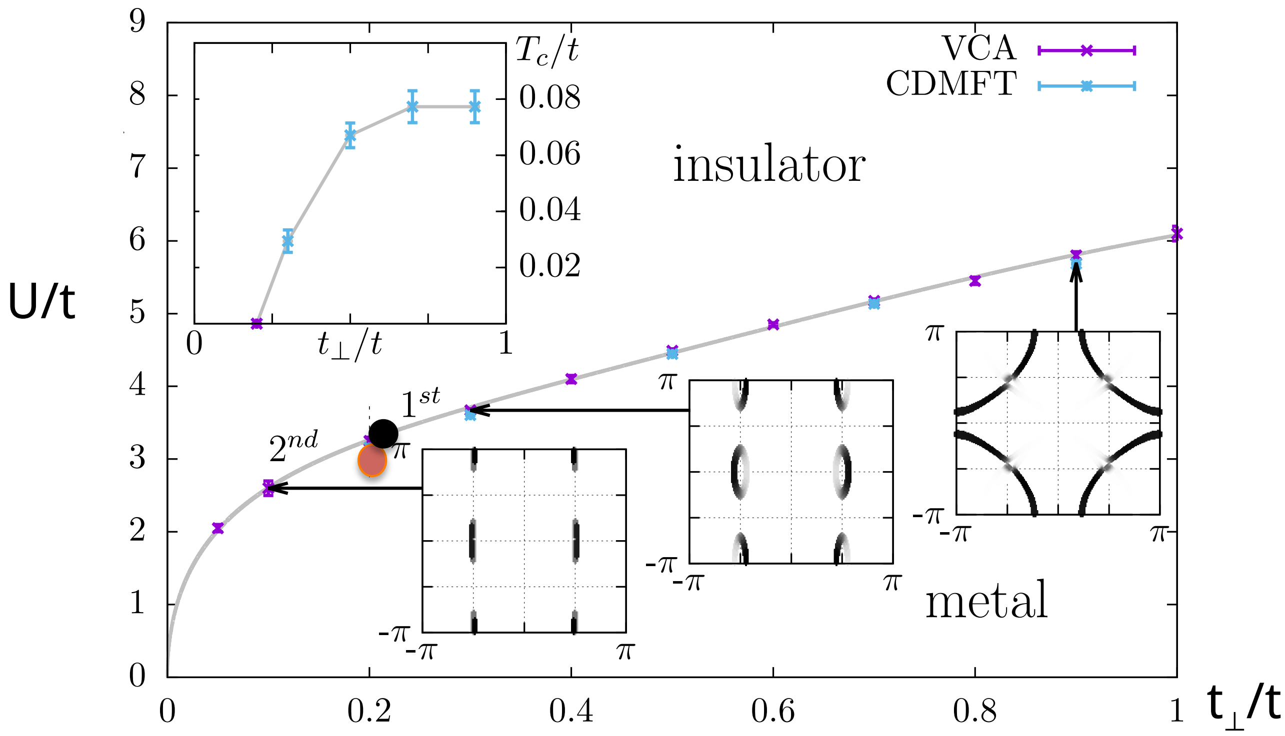




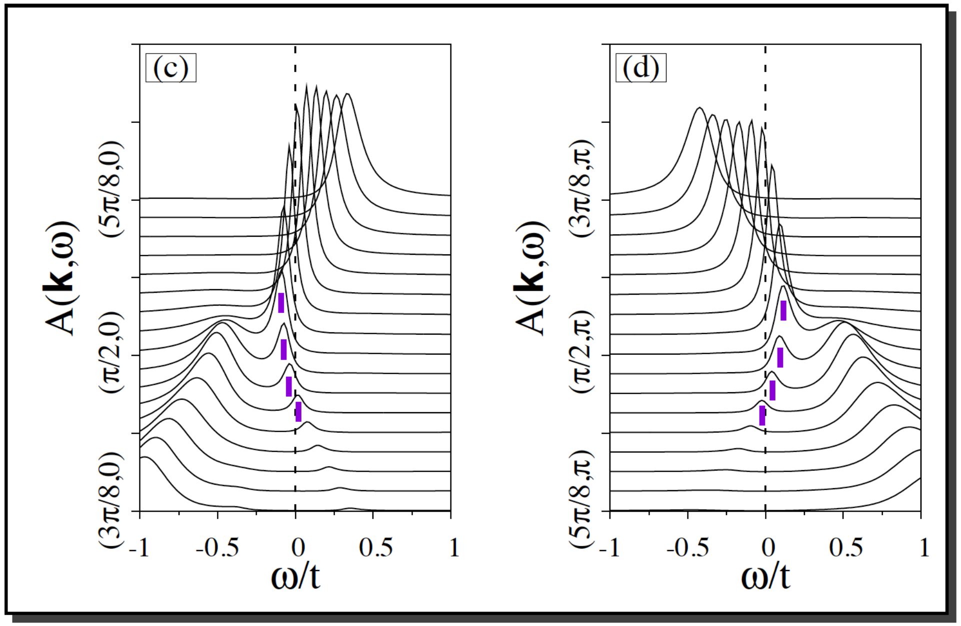
→ Jump in volume of hole and electron pockets across the transition

Fermi surface topology

Larger clusters

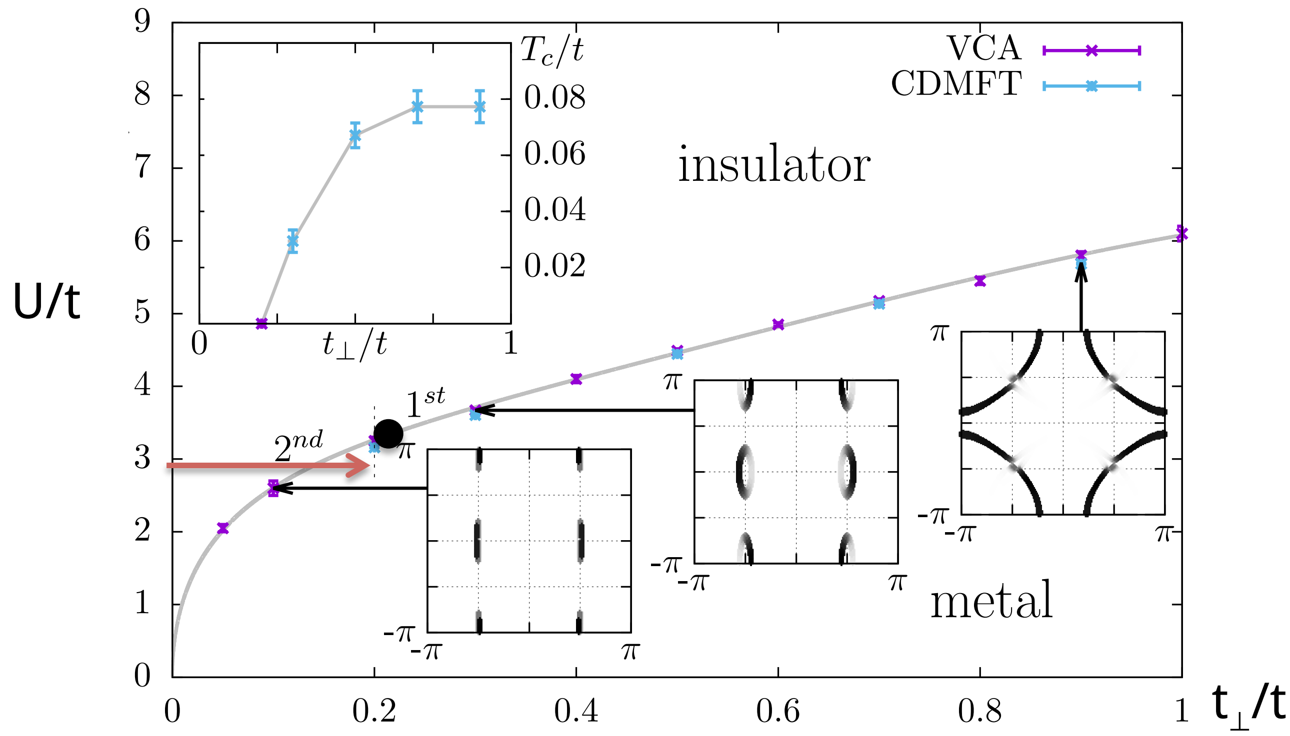


<u>U/t = 3, $t_\perp/t$ = 0.2, 4x4, βt = 30</u>



Fermi surface topology

Zeros and poles of the Green function.

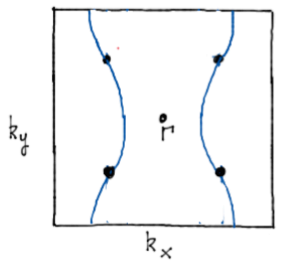


$$G(\mathbf{k},\omega)=\frac{1}{\omega-\varepsilon(\mathbf{k})-\Sigma'(\mathbf{k},\omega)-i\Sigma''(\mathbf{k},\omega)}$$

Poles $\omega-\varepsilon(\mathbf{k})-\Sigma'(\mathbf{k},\omega)=0 \rightarrow \omega_p(\mathbf{k})$

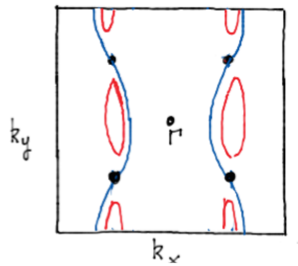
Zeros $\omega-\varepsilon(\mathbf{k})-\Sigma'(\mathbf{k},\omega)=\infty \rightarrow \omega_Z(\mathbf{k})$

Mott

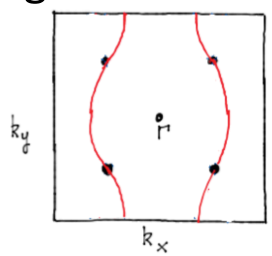


Pockets

Poles in the vicinity of zeros have small spectral weight.



Large Fermi surface



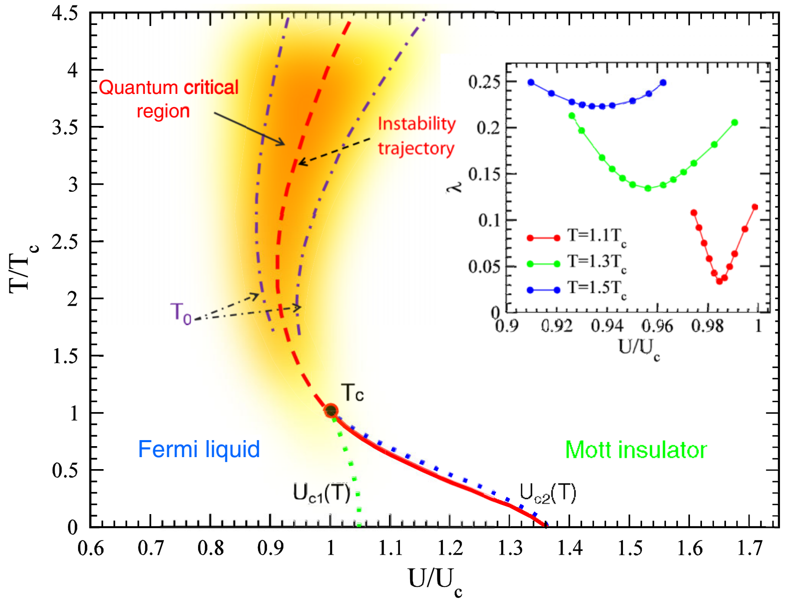
Sakai, Motome and Imada, PRL 2009.

Conclusion/outlook

PRL 107, 026401 (2011) PHYSICAL REVIEW LETTERS week ending 8 JULY 2011

Quantum Critical Transport near the Mott Transition

H. Terletska,[1] J. Vučičević,[2] D. Tanasković,[2] and V. Dobrosavljević[1]



Scaling Ansatz:

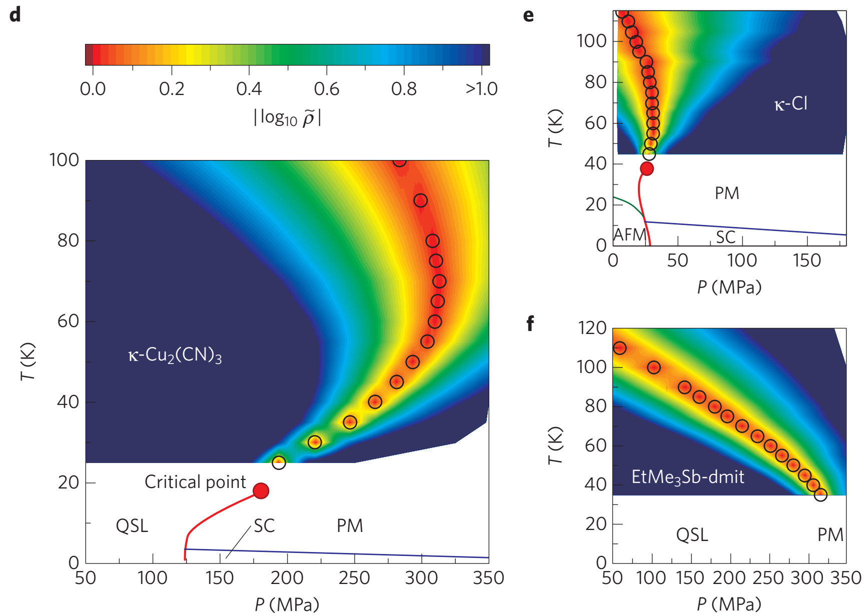
$$\rho(T,\delta U) = \rho(T,\delta U = 0)\, f(T/T_0)$$

$$\delta U = U - U^*(T),\ T_0 = c|\delta U|^{z\nu},\ z\nu \approx 0.56$$

nature physics LETTERS
PUBLISHED ONLINE: 9 FEBRUARY 2015 | DOI: 10.1038/NPHYS3235

Quantum criticality of Mott transition in organic materials

Tetsuya Furukawa[1]*, Kazuya Miyagawa[1], Hiromi Taniguchi[2], Reizo Kato[3] and Kazushi Kanoda[1]*



→ The $t_\perp/t$ axis drives T_c to zero and yields a model where the scaling Ansatz can be tested.

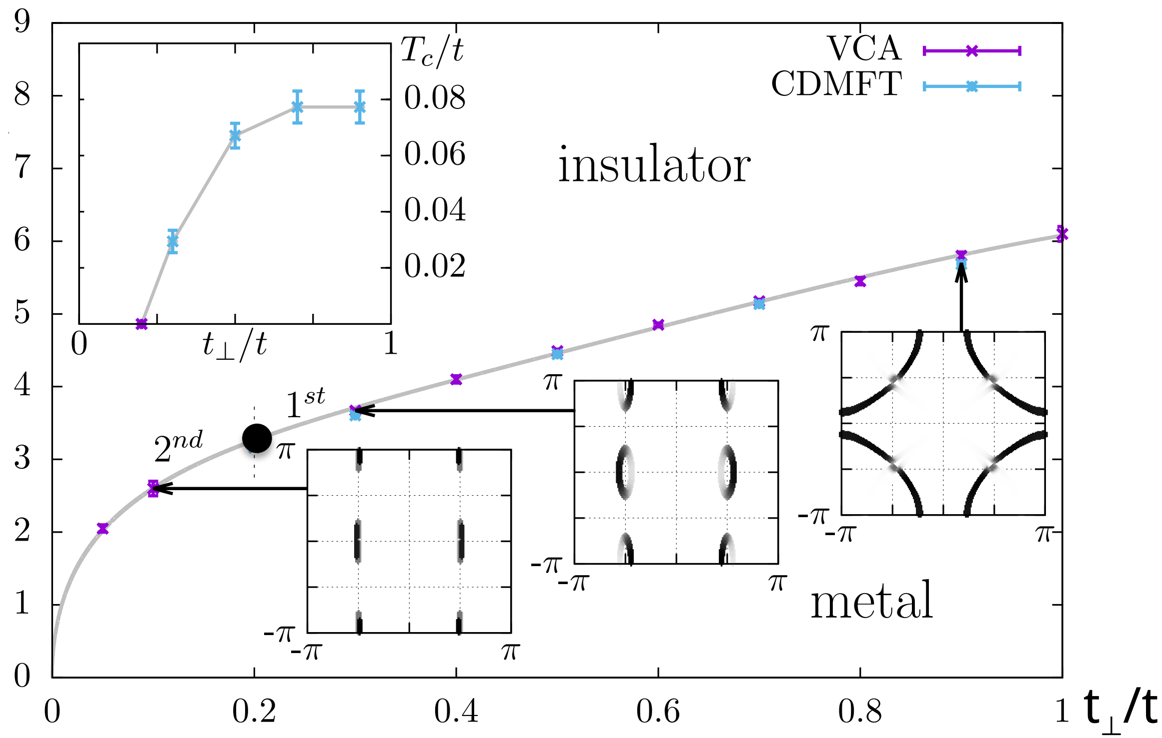
Conclusion/summary

Cluster methods.
(CDMFT + VCA)

T_c can be tuned to zero

Breakup of FS into electron and hole pockets

Below $t_\perp^c$ volume of electron and hole pockets vanishes continuously at U_c



Exact lattice methods (20x20)

Mott quantum phase transition is masked by magnetic ordering

Finite temperature crossover between Mott insulator and metallic state