Dynamical cluster quantum Monte Carlo studies on square and triangular lattice Hubbard model

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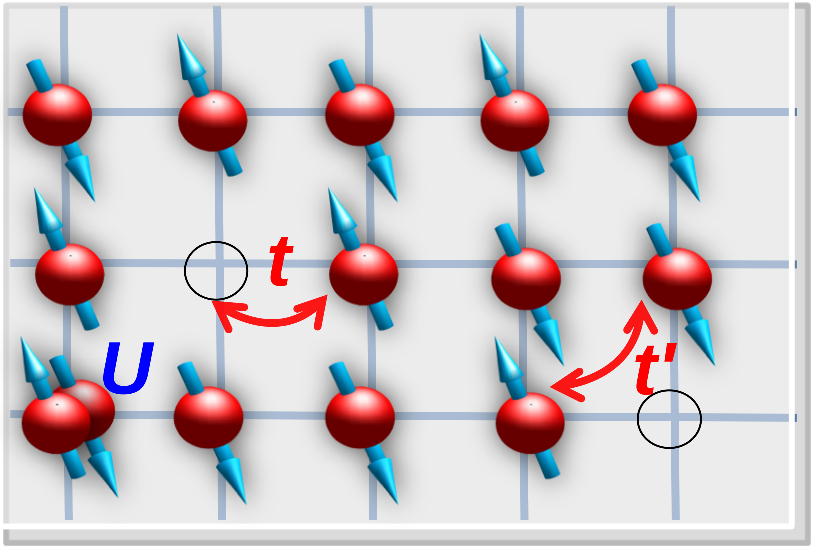
A tale of two strongly correlated Systems

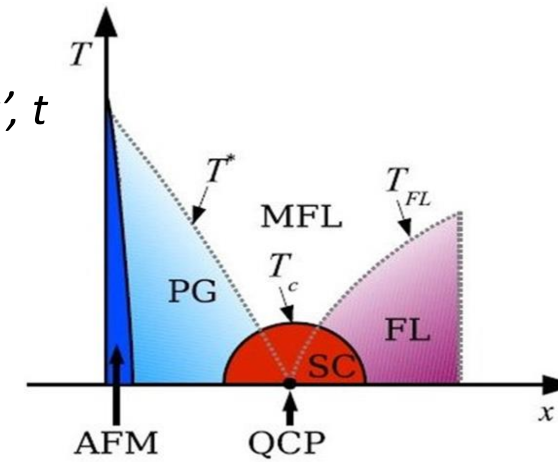


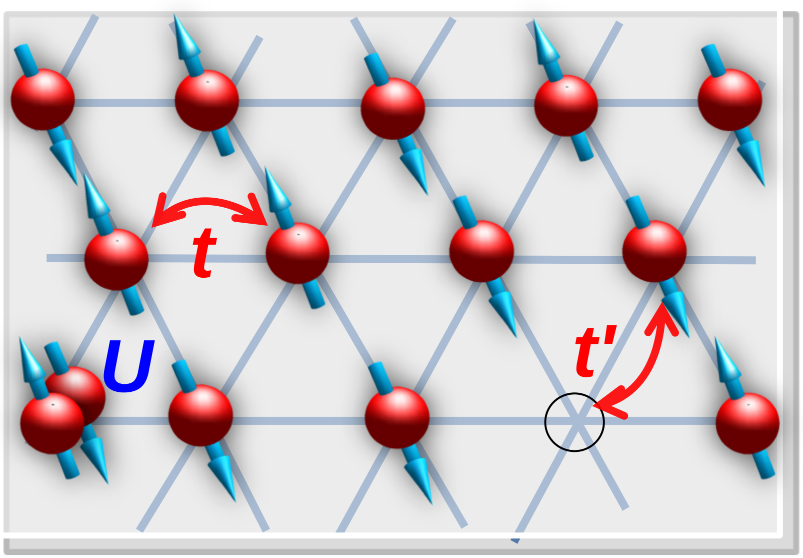
Hubbard model on square lattice

$$H = -t\sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma}c_{j,\sigma} - t'\sum_{\langle\langle i,j\rangle\rangle,\sigma} c^{\dagger}_{i,\sigma}c_{j,\sigma} + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow}$$

parameters:

- NN, NNN, hopping *t'*, *t*
- Interaction *U / t*
- Temperature *T / t*
- Hole doping



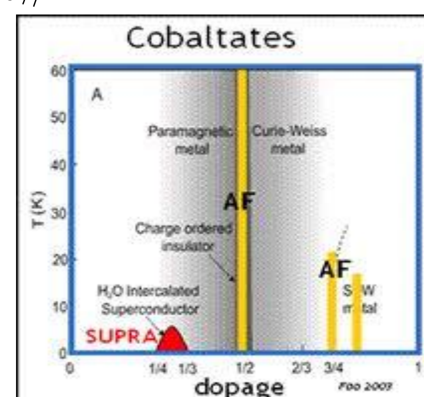


Hubbard model on triangular lattice

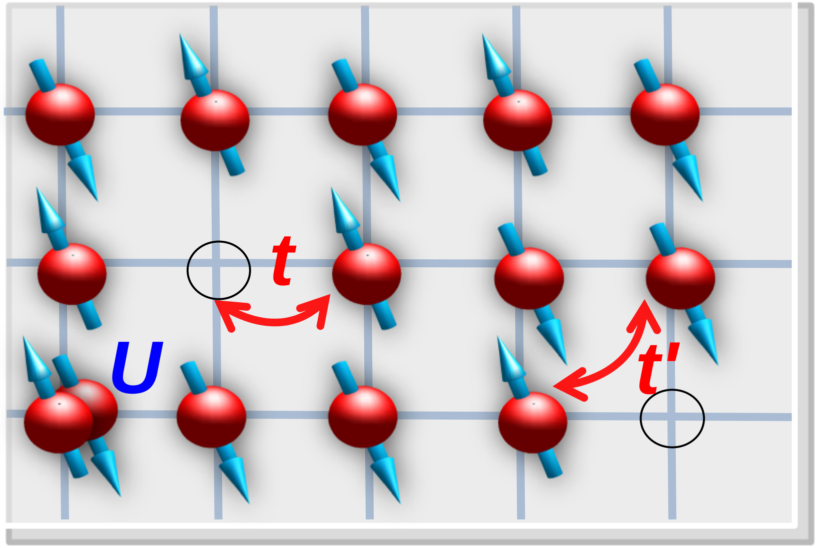
$$H = -t\sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma}c_{j,\sigma} - t'\sum_{\langle\langle i,j\rangle\rangle,\sigma} c^{\dagger}_{i,\sigma}c_{j,\sigma} + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow}$$

Phase diagram:

- Mott transition
- d+id chiral superconductivity



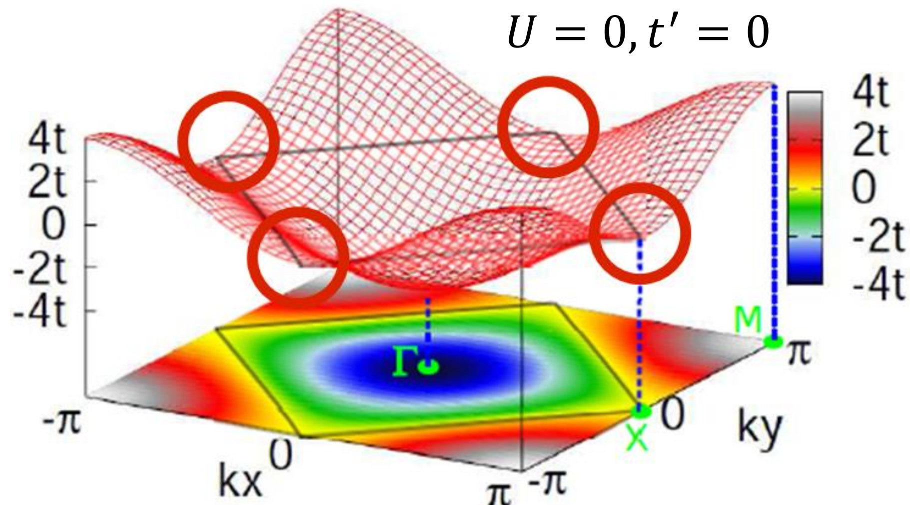
Hubbard Model on square Lattice

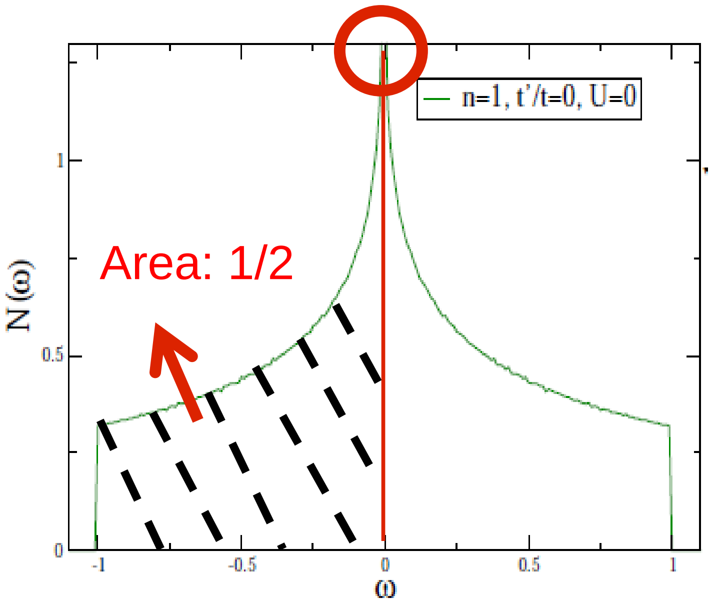


$$H = \sum_{\boldsymbol{k},\sigma} (\epsilon_{\boldsymbol{k}}^{0} - \mu)\, c_{\boldsymbol{k},\sigma}^{\dagger} c_{\boldsymbol{k},\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

$$\epsilon_{\boldsymbol{k}}^{0} = -2t(\cos k_x + \cos k_y) - 4t'(\cos k_x \cos k_y - 1)$$

$U = 0, t' = 0$

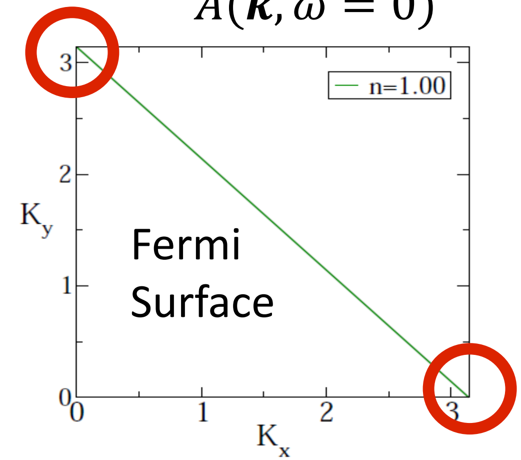




W=8t, 4t=1

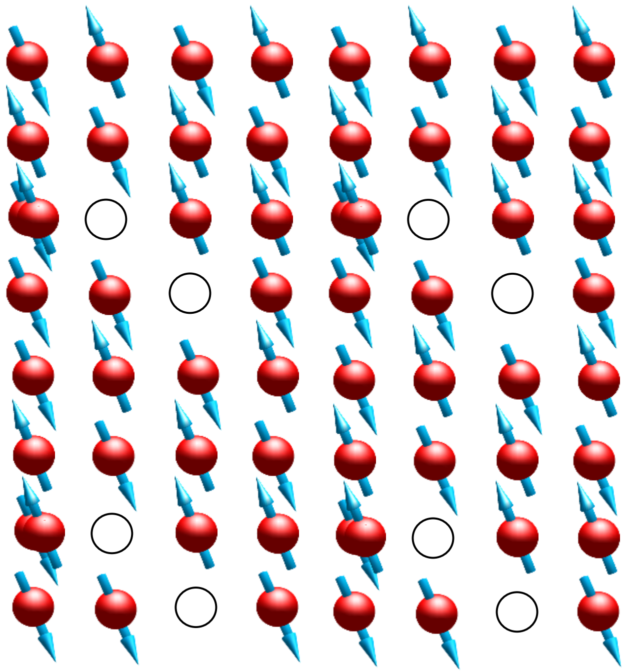
Van Hove Singularity

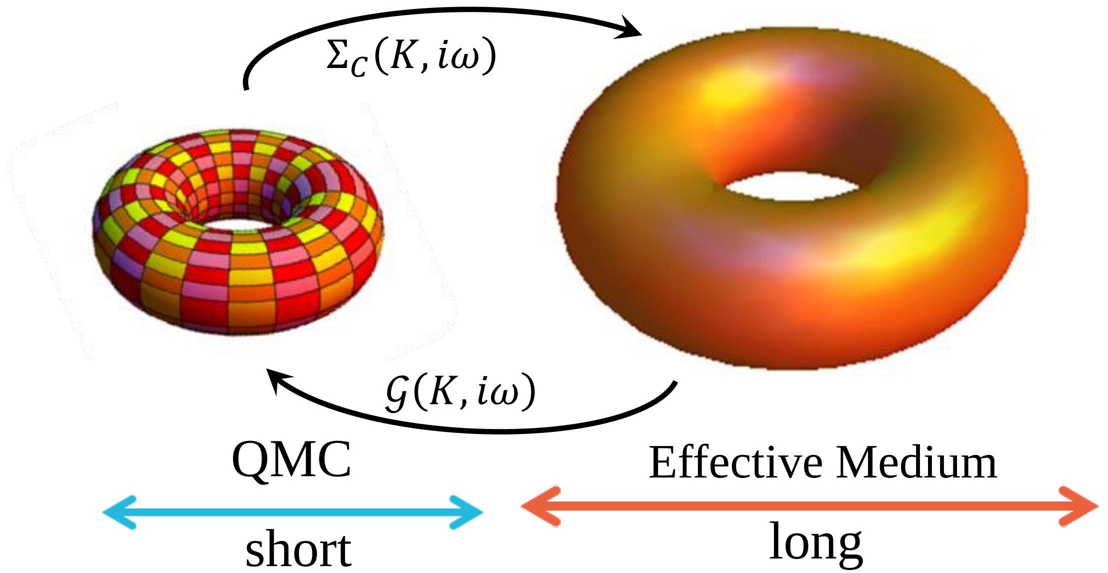
$A(\boldsymbol{k}, \omega = 0)$



Two length scale approach

Periodic Lattice





Th. Maier *et al.,* Rev. Mod. Phys. (2005)

- Short length scale physics within cluster treated explicitly.
- Long length scale physics treated at the mean field level.
- Obtain convergence self-consistently.
- Cluster solver is continuous time quantum Monte Carlo (CTQMC).

A. N. Rubtsov et. al, Phys. Rev. B 72, 035122 (2005)

Dynamical Cluster Approximation (DCA)

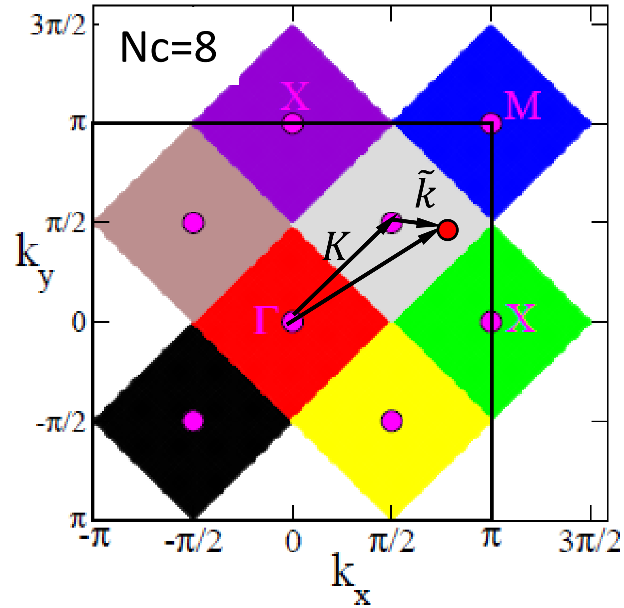
CTQMC
$G_C(K, i\omega), \chi_C(P, P', Q)$

$P = (K, i\omega)$

$\mathcal{G}^{-1}(K, i\omega) = \overline{G}^{-1} + \Sigma_C$

$\Sigma_C(K, i\omega) = \mathcal{G}^{-1} - G_C^{-1}$

$$\overline{G}(K, i\omega) = \frac{N_C}{N} \sum_{\tilde{k}} \left[i\omega - \varepsilon(K + \tilde{k}) + \mu - \Sigma_C(K, i\omega) \right]^{-1}$$



Single-particle quantities

CTQMC

$\Sigma_C(K, i\omega)$

MEM(Maximum Entropy Method)
Jarrell and Gubernatis, Phys. Rep. 269, 133 (1996)

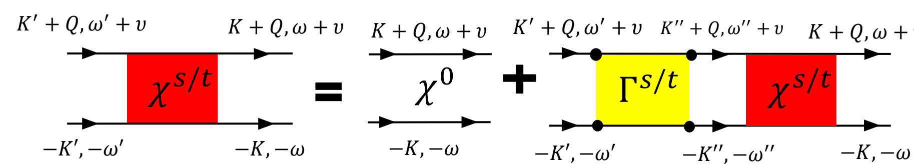
$\Sigma_C(K, \omega)$

Interpolation to lattice quantities

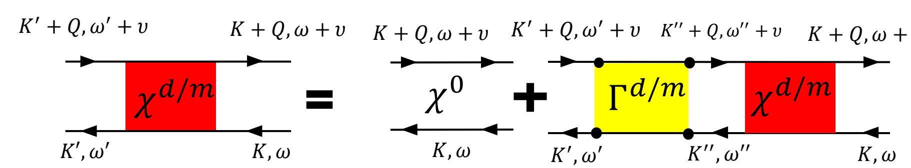
$\Sigma(k, \omega)$, $G(k, \omega)$, $A(k, \omega) = -\frac{1}{\pi}\mathrm{Im}(G(k, \omega))$, $N(\omega)$

Two-particle quantities

particle-particle: pairing



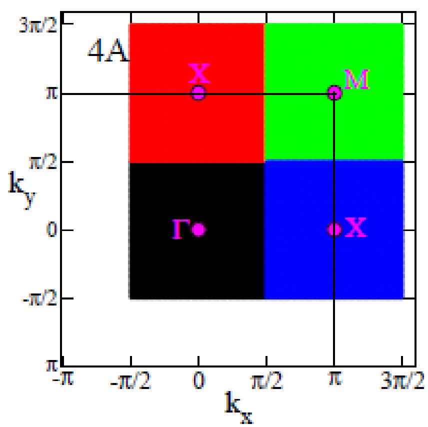
particle-hole: density (charge) & magnetic (spin)



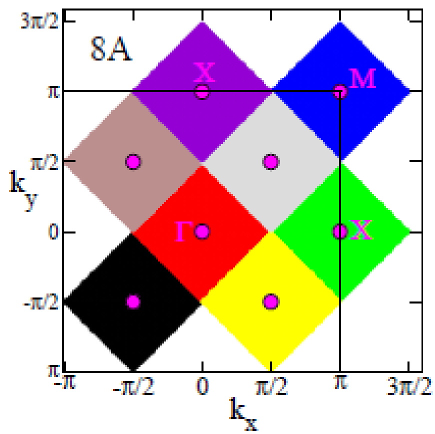
Dynamical Cluster Approximation (DCA)

Square lattice clusters

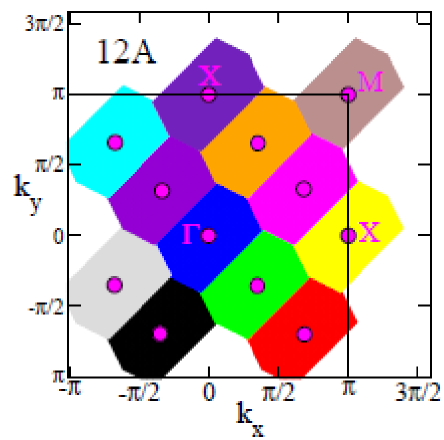
Nc=4



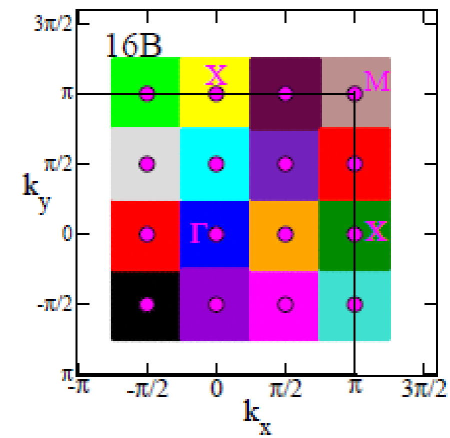
Nc=8



Nc=12

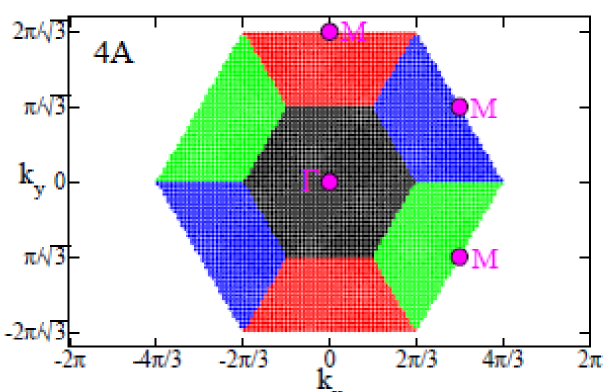


Nc=16

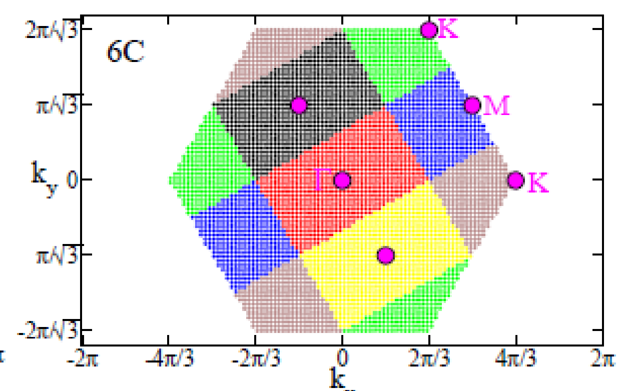


triangular lattice clusters

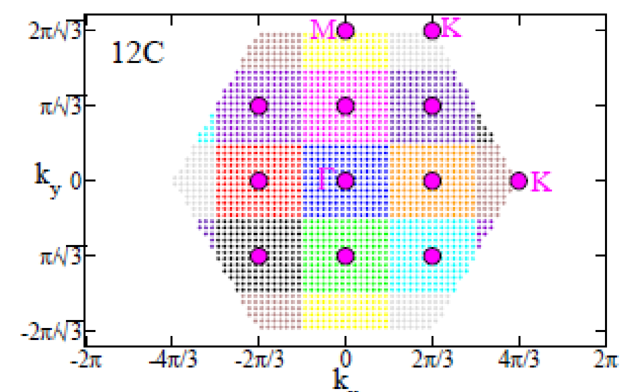
Nc=4



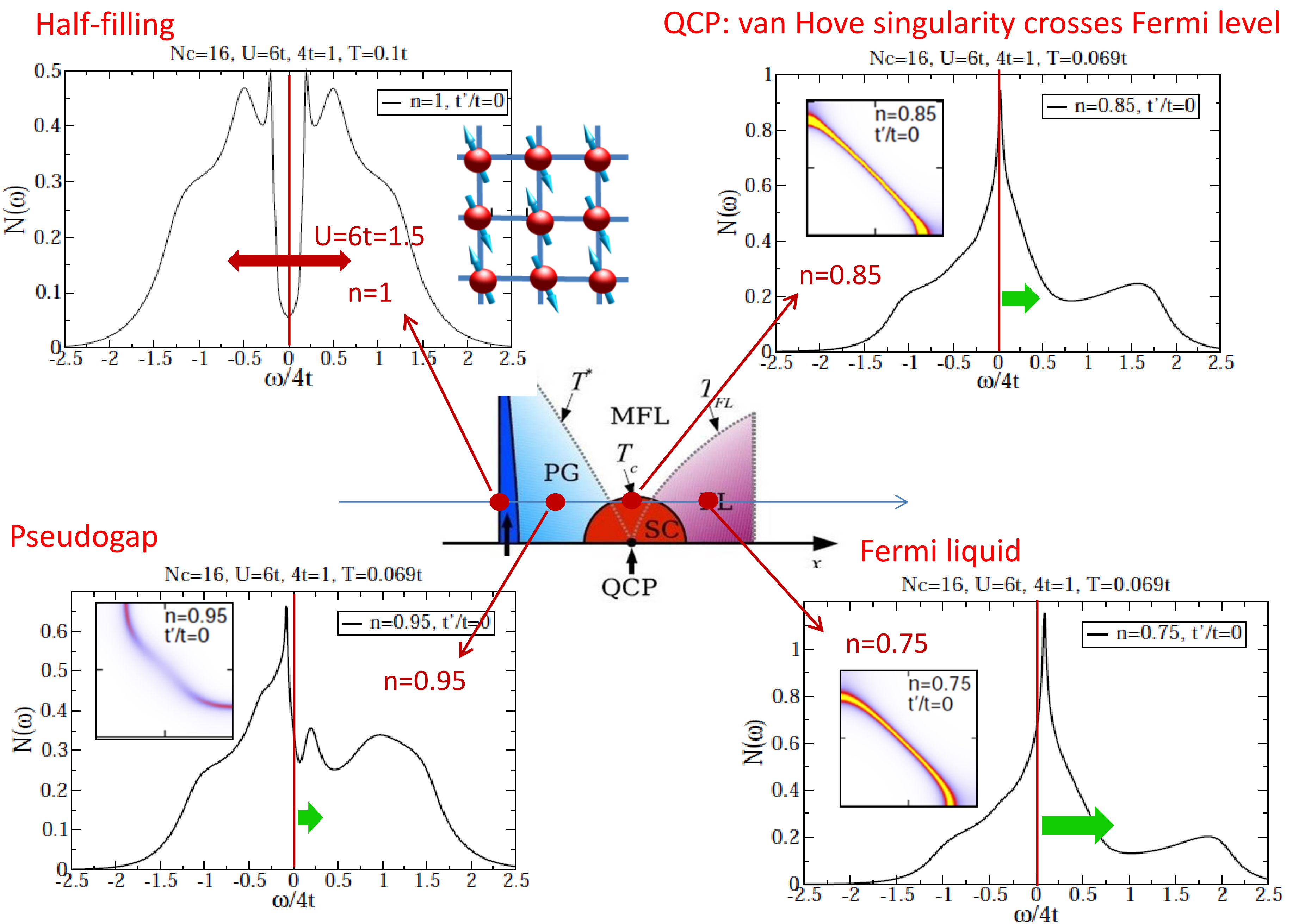
Nc=6



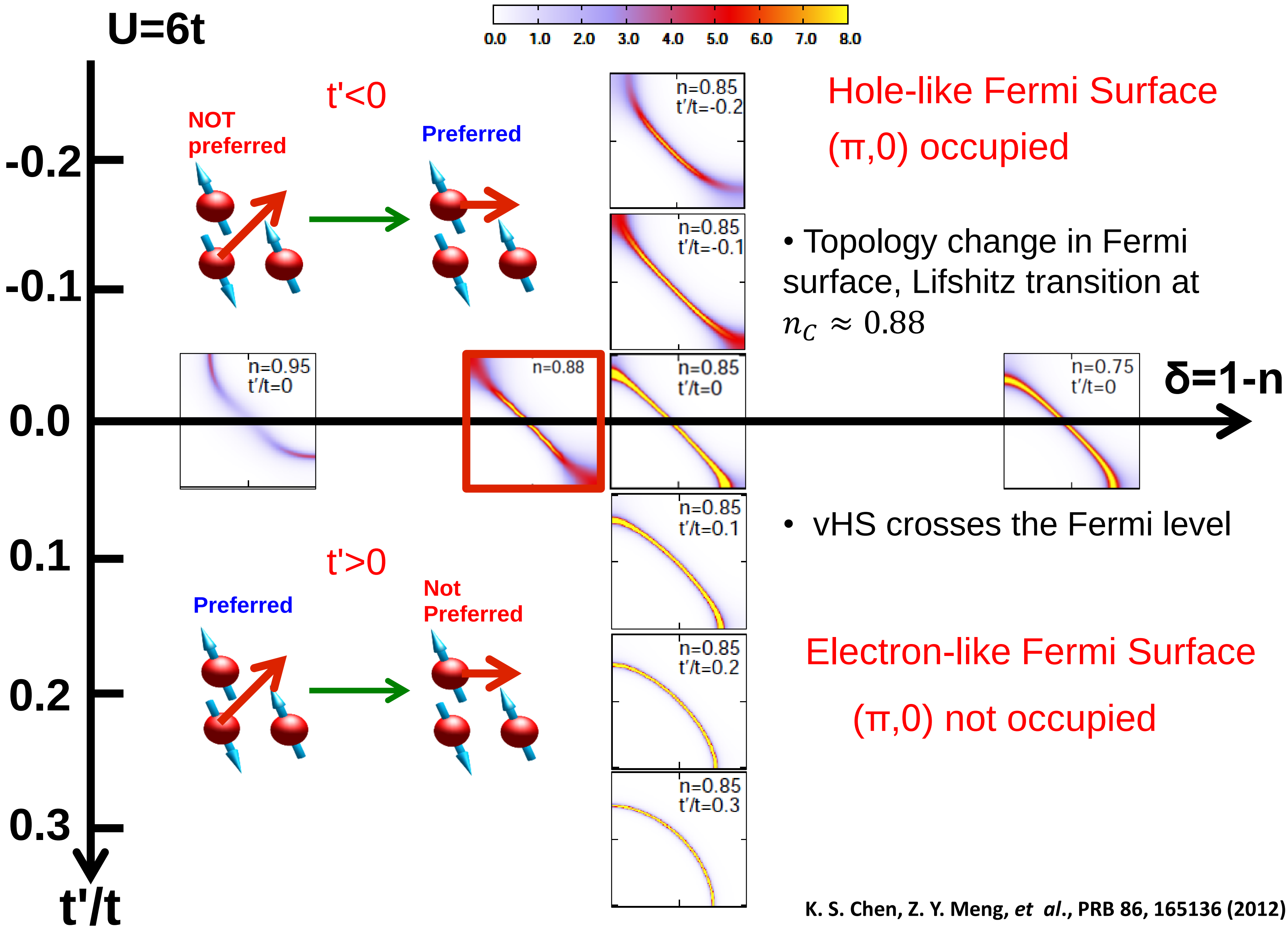
Nc=12



Square lattice Hubbard model at U=6t, t' = 0



Effect of t’: Lifshitz transition



Hole-like Fermi Surface

(π,0) occupied

- Topology change in Fermi surface, Lifshitz transition at $n_C \approx 0.88$

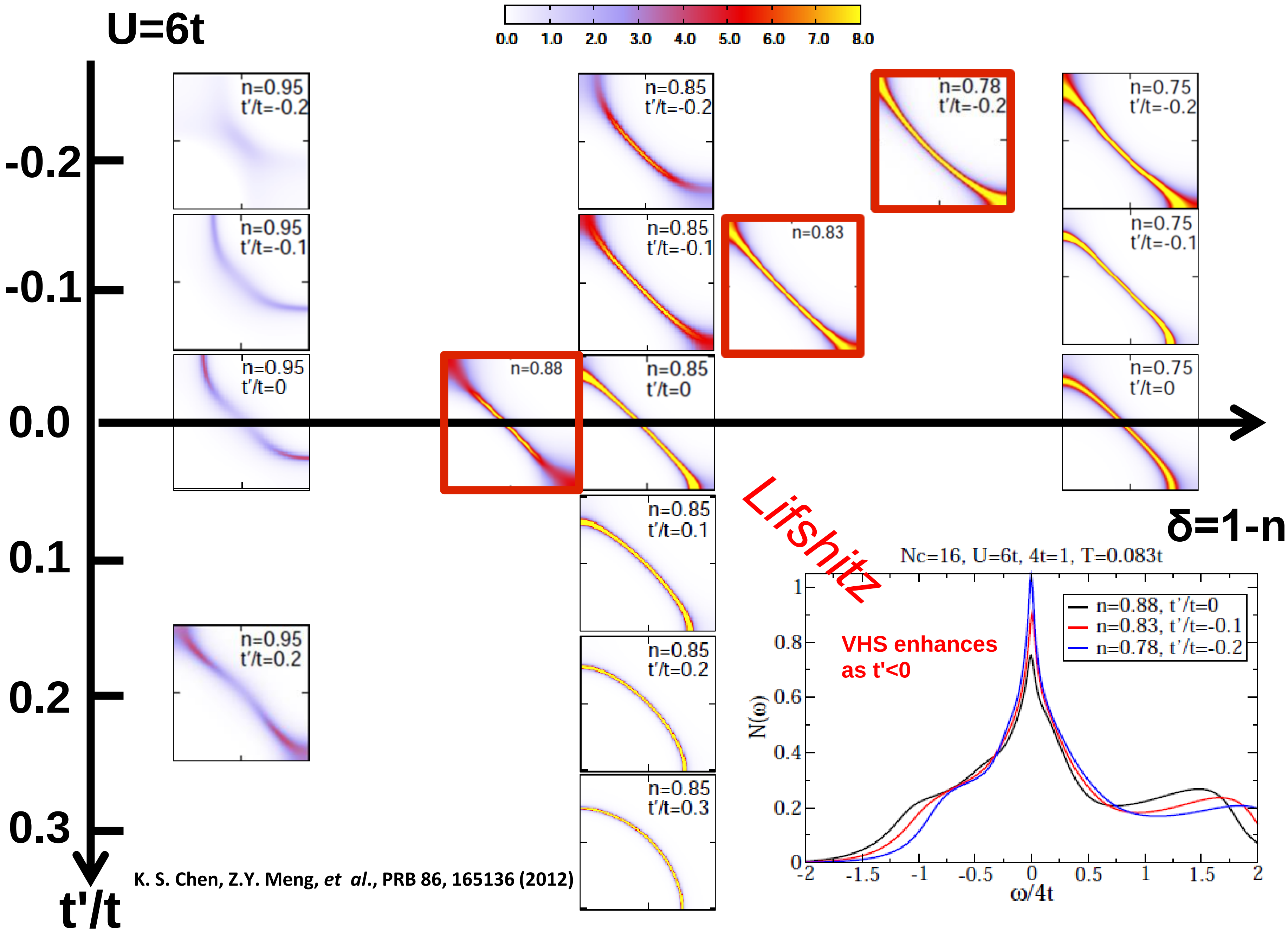
- vHS crosses the Fermi level

Electron-like Fermi Surface

(π,0) not occupied

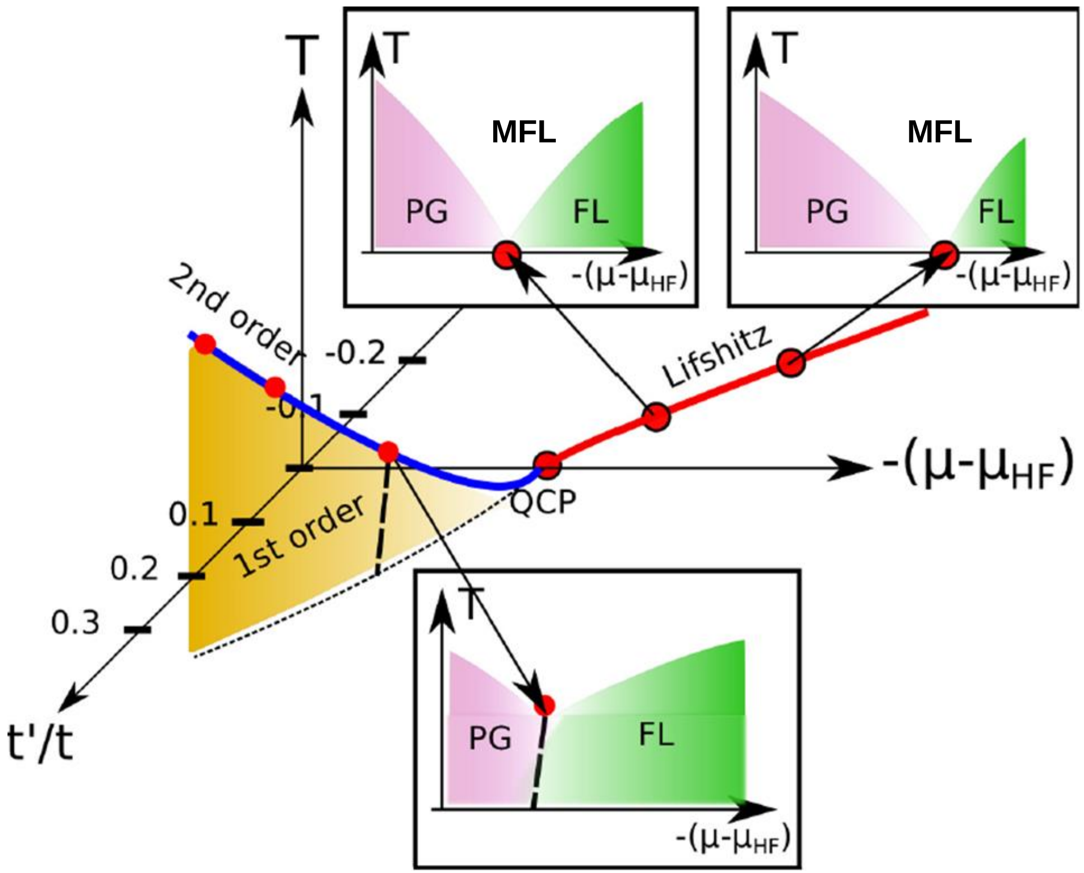
K. S. Chen, Z. Y. Meng, *et al.*, PRB 86, 165136 (2012)

Effect of t’: Lifshitz transition



K. S. Chen, Z.Y. Meng, *et al.*, PRB 86, 165136 (2012)

Phase diagram of square lattice Hubbard model



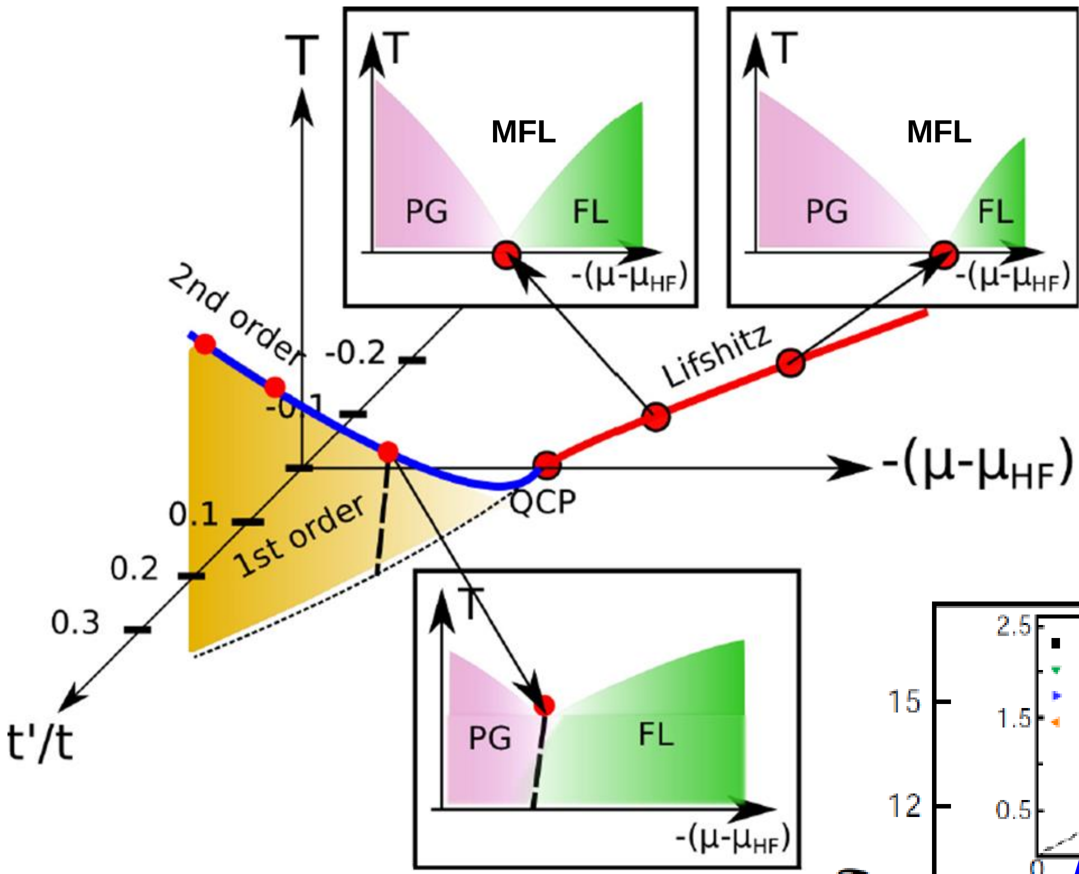
t'/t>0, previous works:

A. Macridin, *et al*., PRB **74**, 085104 (2006)
K. Mikelsons, *et al*., PRB **80**, 140505R (2009)
E. Khatami, *et al*., PRB **81**, 201101(R) (2010)

1. $\chi_c(Q = 0, T) = dn/d\mu$ diverges at 2nd order points.
2. Hysteresis of $n(\mu)$ curve is found in 1st order phase separation area.
3. QCP is the terminal point of 2nd order critical points in the limit $t'/t \to 0$ and *T=0*.

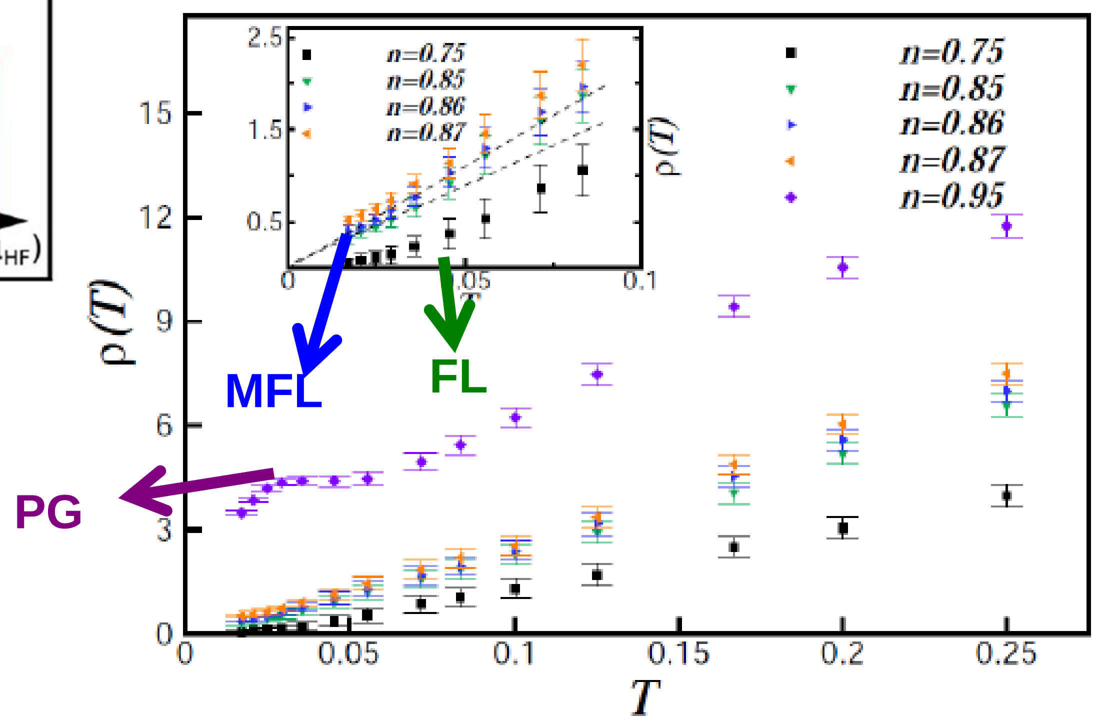
K. S. Chen, Z. Y. Meng, *et al*., PRB 86, 165136 (2012)

Phase diagram of square lattice Hubbard model



t'/t ≤ 0, Lifshitz transition:

1. Topology of Fermi surface changes (electron-/hole-like) as crossing Lifshitz line.
2. Above Lifshitz line, MFL is separats by PG and FL. Resistivity $\rho(T)$

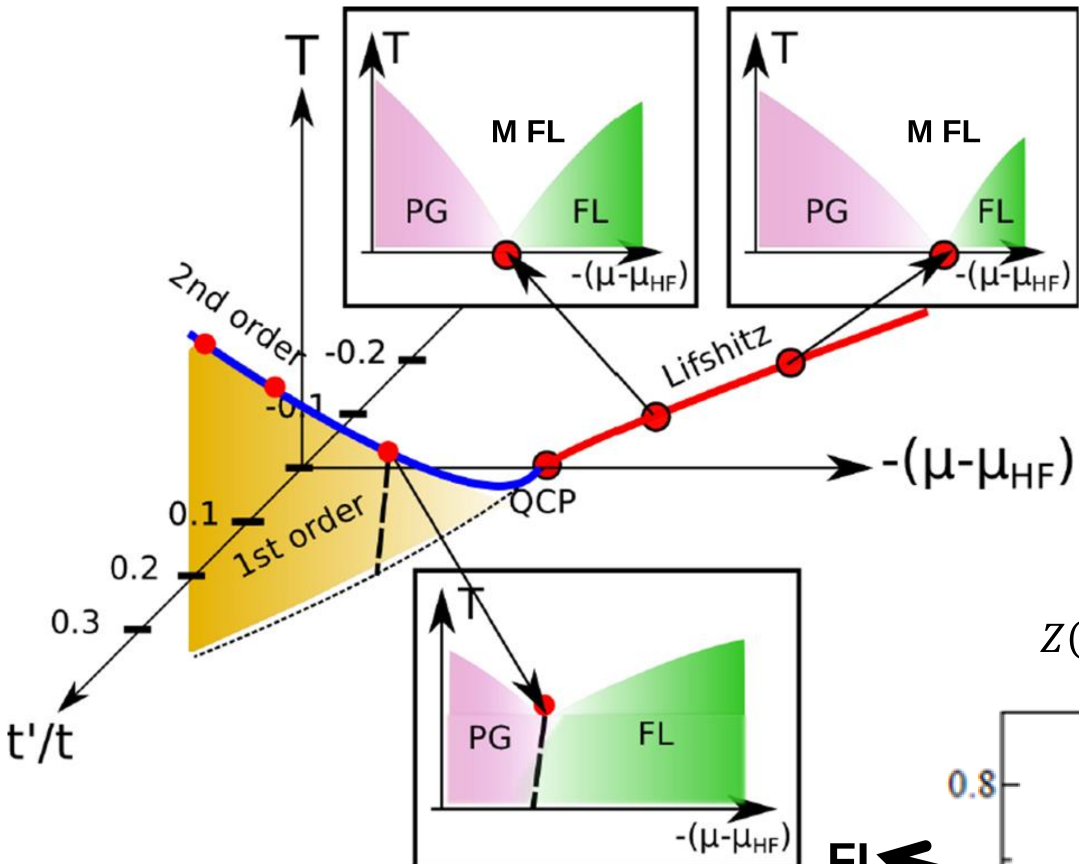


FL: $\rho(T) \propto T^2$

MFL: $\rho(T) \propto T$

K. S. Chen, Z. Y. Meng, *et al.*, PRB 86, 165136 (2012)

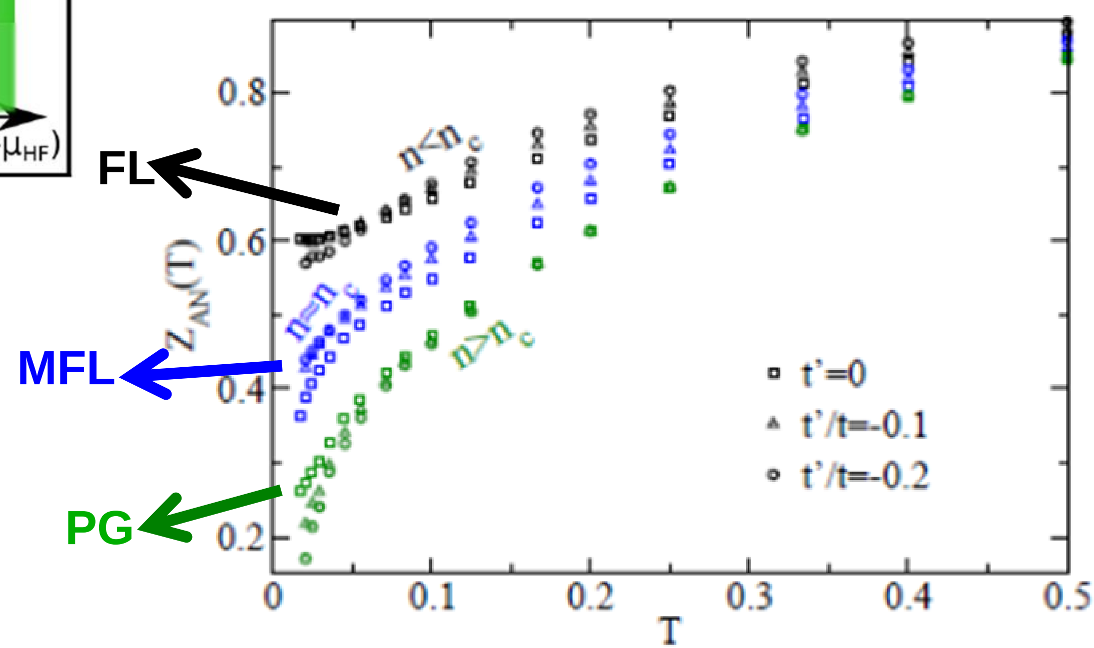
Phase diagram of square lattice Hubbard model



t'/t ≤ 0, Lifshitz transition:

1. Topology of Fermi surface changes (electron-/hole-like) as crossing Lifshitz line.
2. Above Lifshitz line, MFL is separats by PG and FL. Quasiparticle fraction $Z(T)$

$$Z(k_F,T) = (1 - \frac{\Sigma''(k_F, i\omega_0)}{\omega_0})^{-1},\ \omega_0 = \pi T$$



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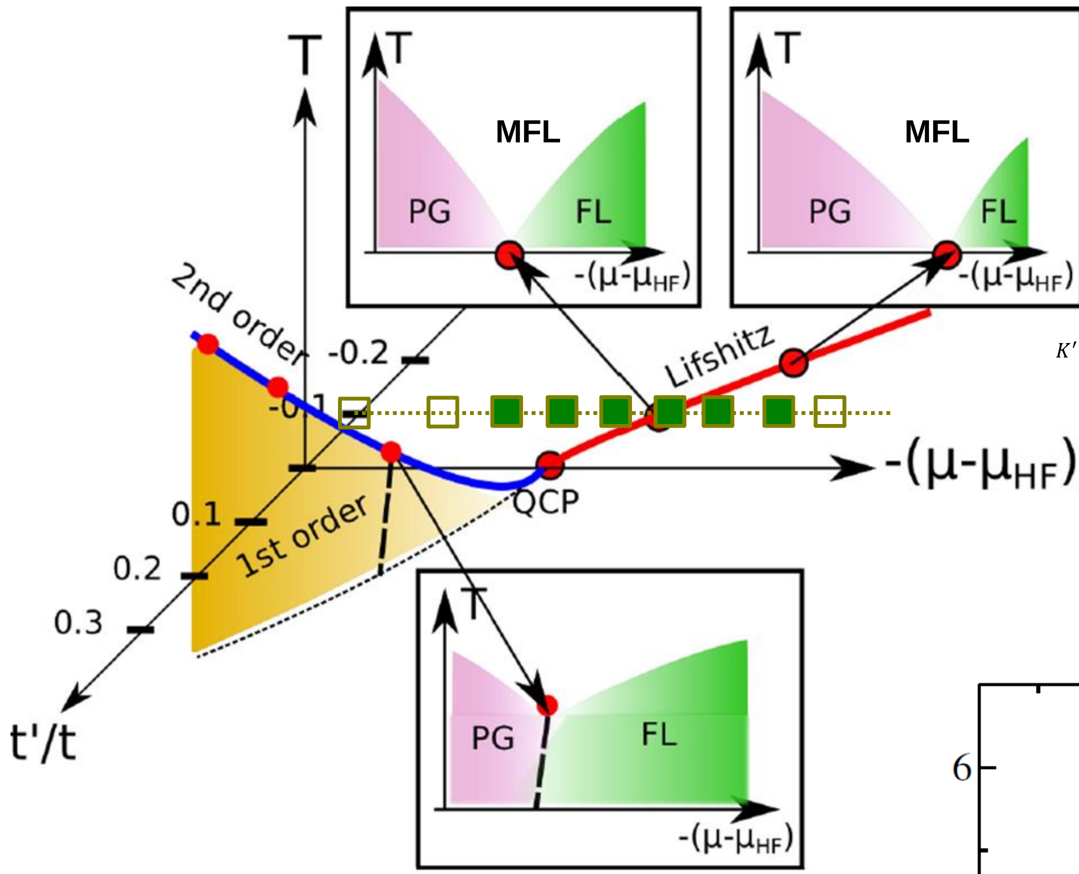
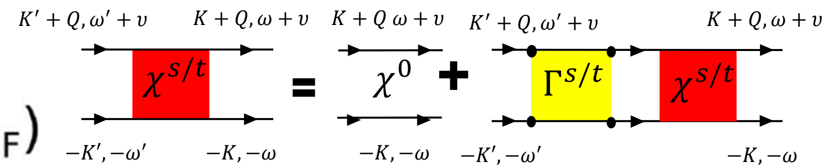
Determine the superconducting dome



t'/t ≤ 0, Lifshitz transition:

3. Superconducting dome

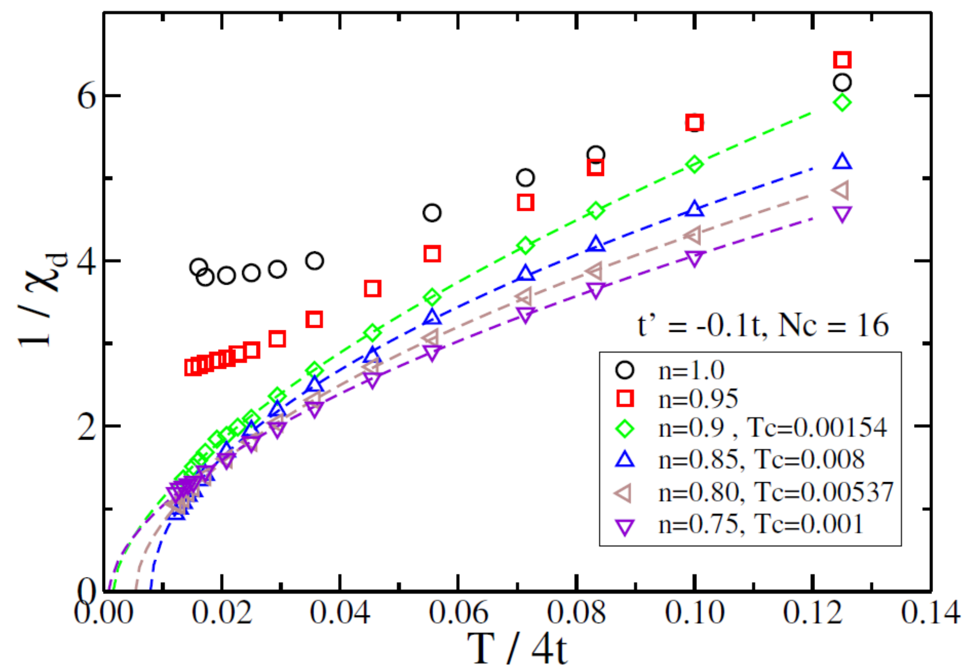
Irreducible vertex $\Gamma(P, P', Q)$



approaching to critical point

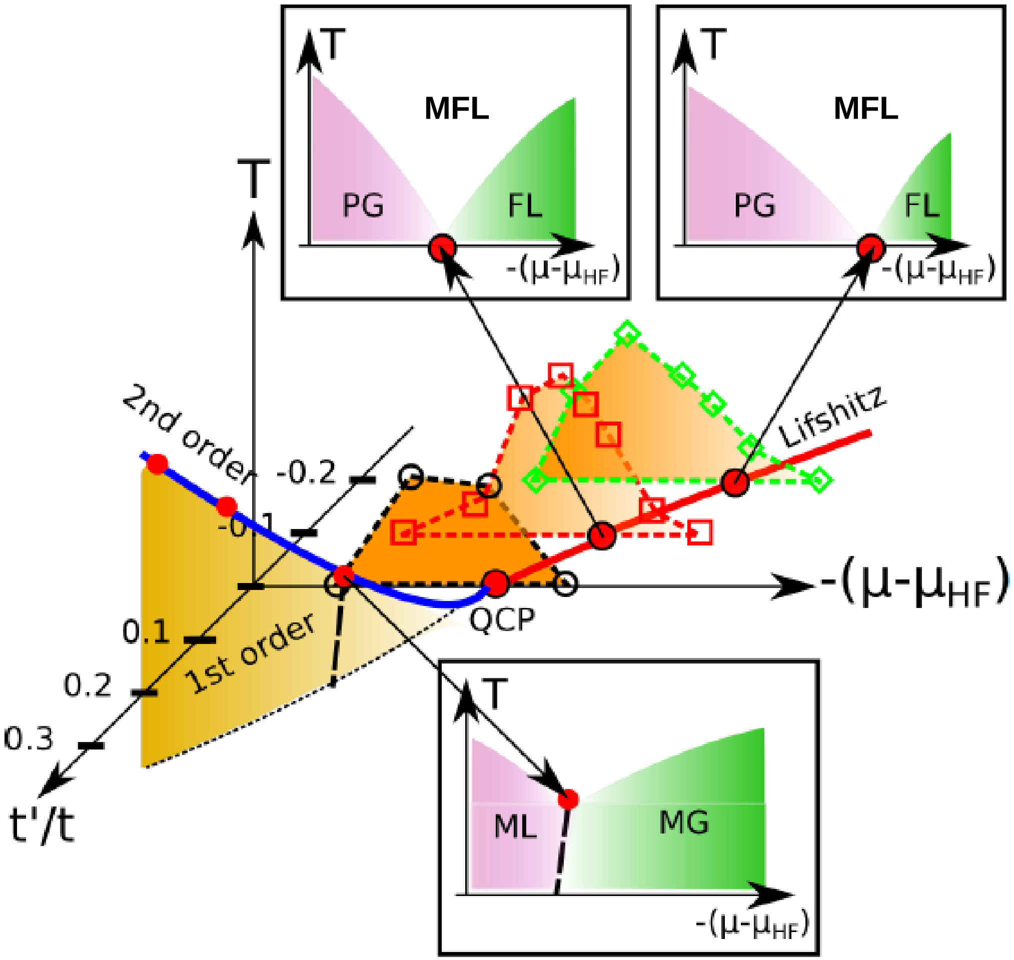
$T \to T_c,\ \chi(T) = \sum \frac{\chi_0}{1-\Gamma\chi_0}$ diverges

maximal $T_c \sim 0.03t \sim 100\ K$



Z. Y. Meng, K. S. Chen, *et al.*, in preparation

Determine the superconducting dome



maximal $T_c \sim 0.03t \sim 100\ K$

$t'/t \leq 0$, Lifshitz transition:

3. Superconducting dome

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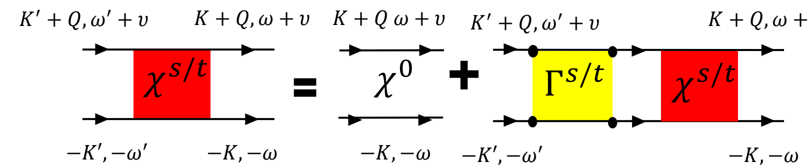

approaching to critical point

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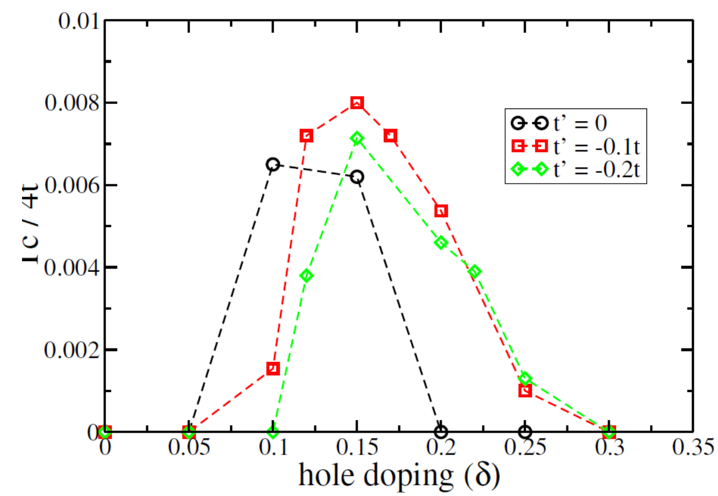
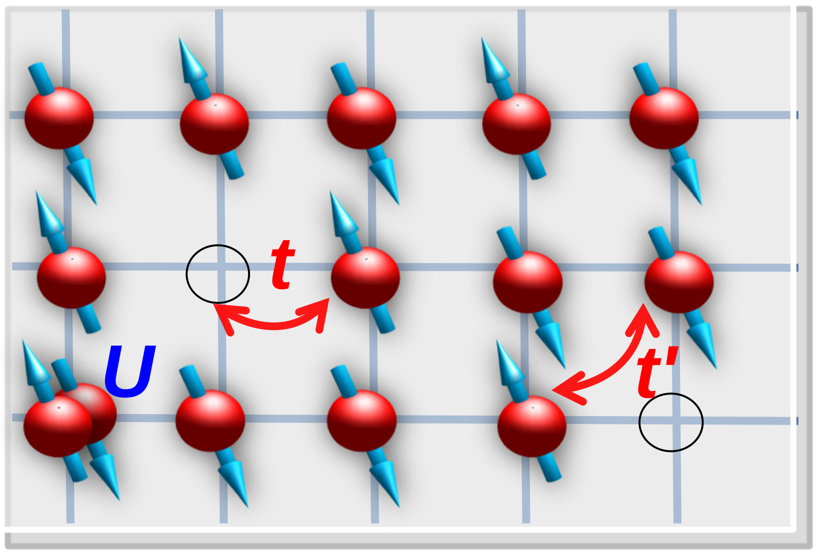


Z. Y. Meng, K. S. Chen, *et al.*, in preparation

Skewness of SC dome along the Lifshitz line requires future studies.

A tale of two strongly correlated Systems

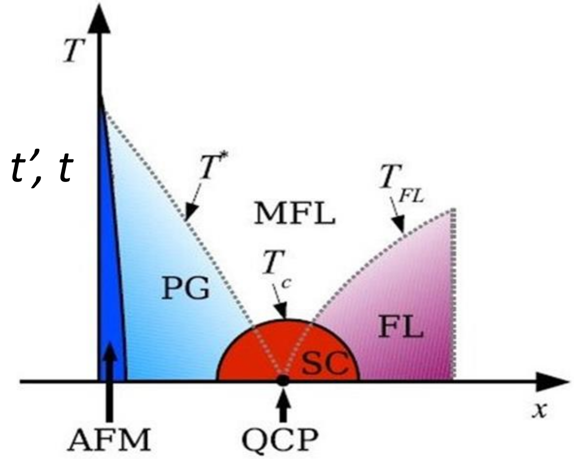


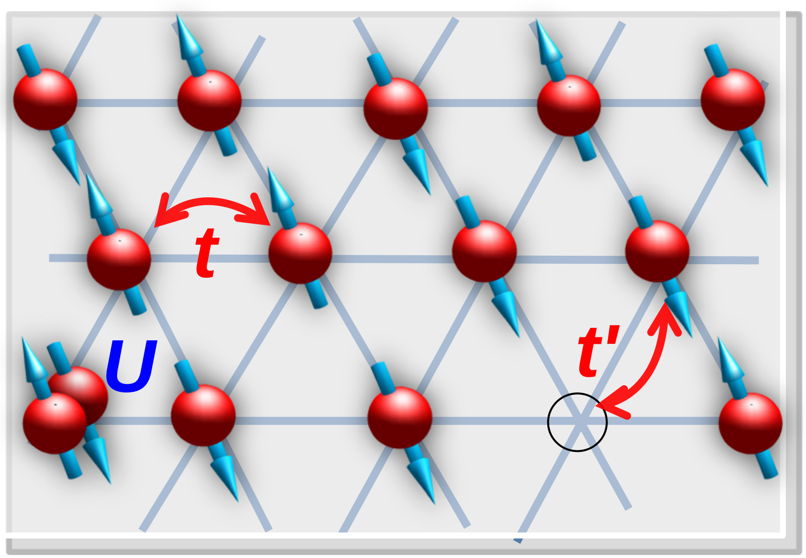
Hubbard model on square lattice

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} - t' \sum_{\langle\langle i,j \rangle\rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

parameters:

- Interaction U/t
- NN, NNN, hopping t', t
- Temperature T/t
- Hole doping



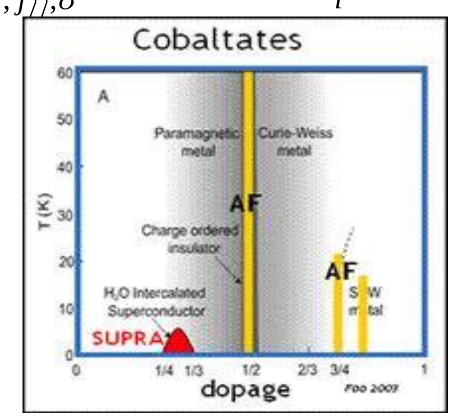


Hubbard model on triangular lattice

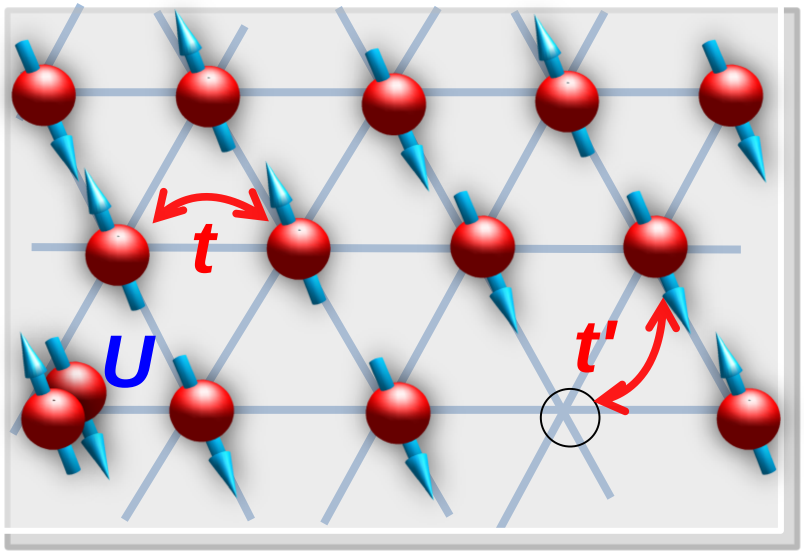
$$H = -t \sum_{\langle i,j \rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} - t' \sum_{\langle\langle i,j \rangle\rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

Phase diagram:

- Mott transition
- d+id chiral superconductivity



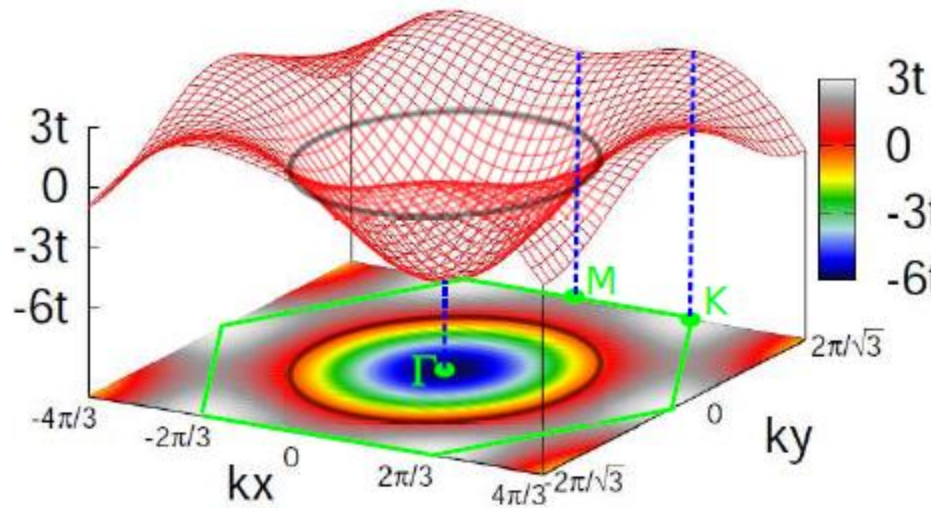
Hubbard Model on triangular Lattice

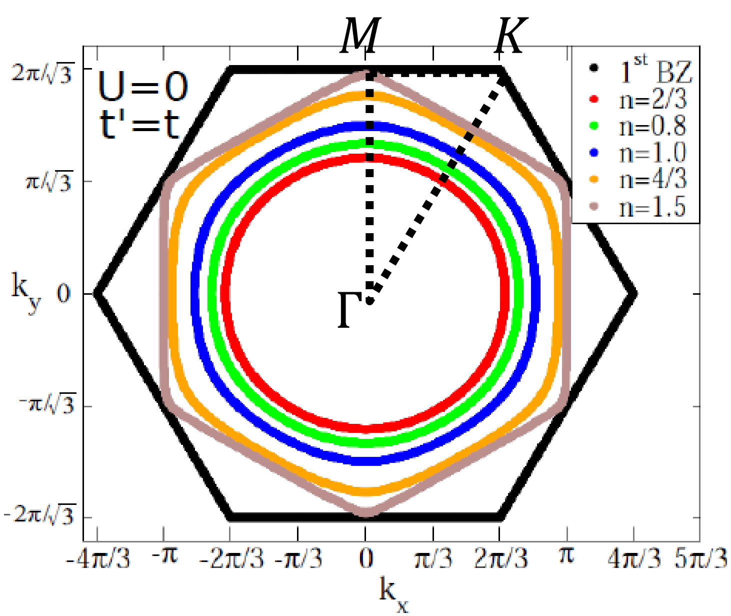


$$H = \sum_{\boldsymbol{k},\sigma} \epsilon^0_{\boldsymbol{k}}\, c^\dagger_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

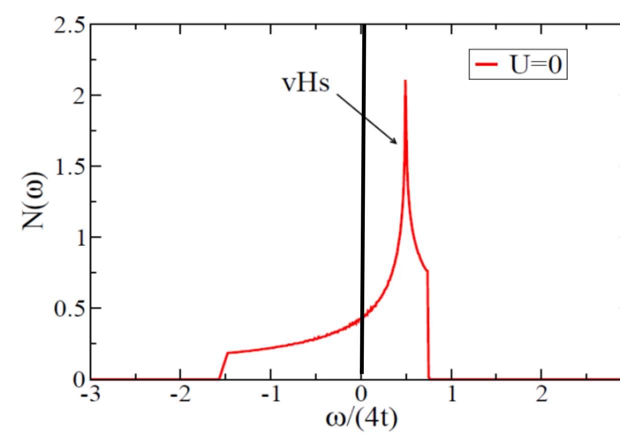
$$\epsilon^0_{\boldsymbol{k}} = -2t\cos k_x - 4t'\cos\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2}$$

Isotropic limit: $t = t'$ Band width: W = 9t

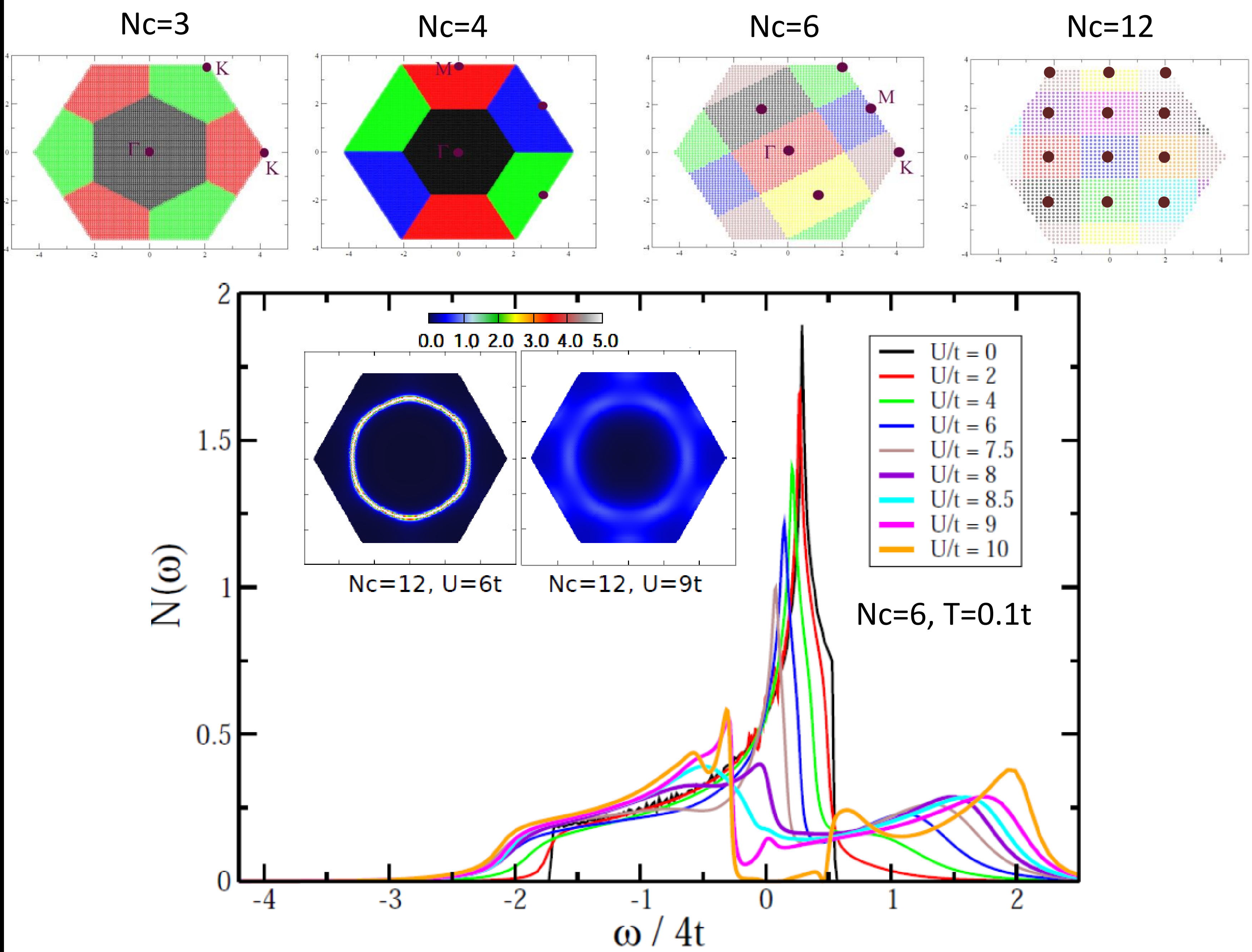




Stable Fermi surface at half filling

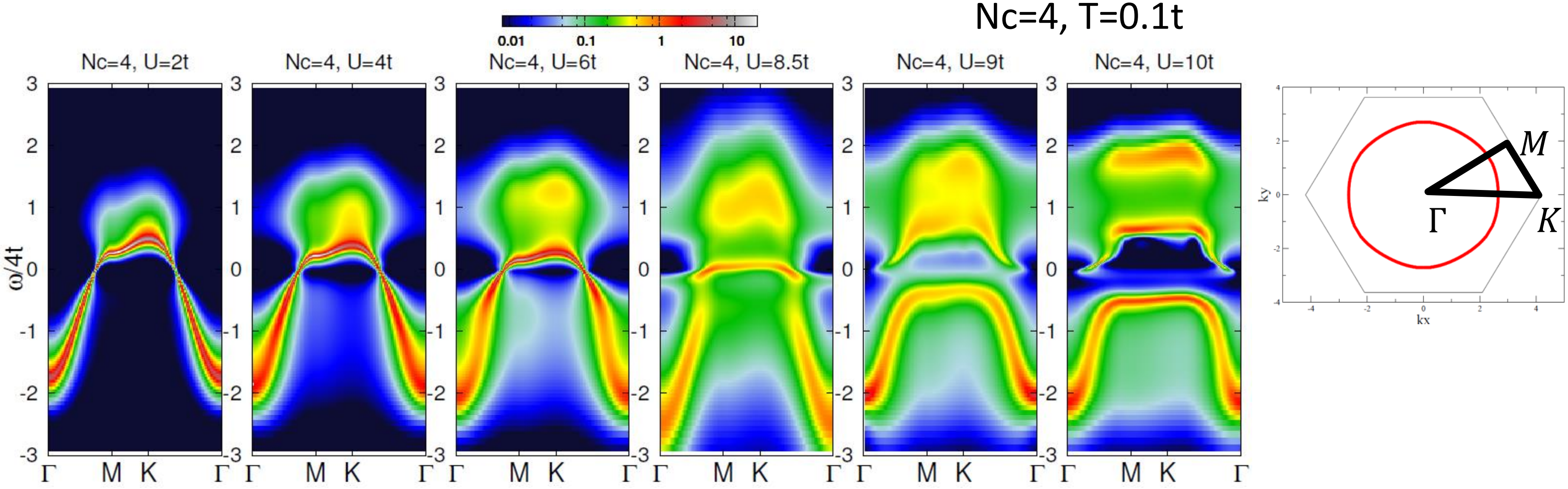


Mott Transition

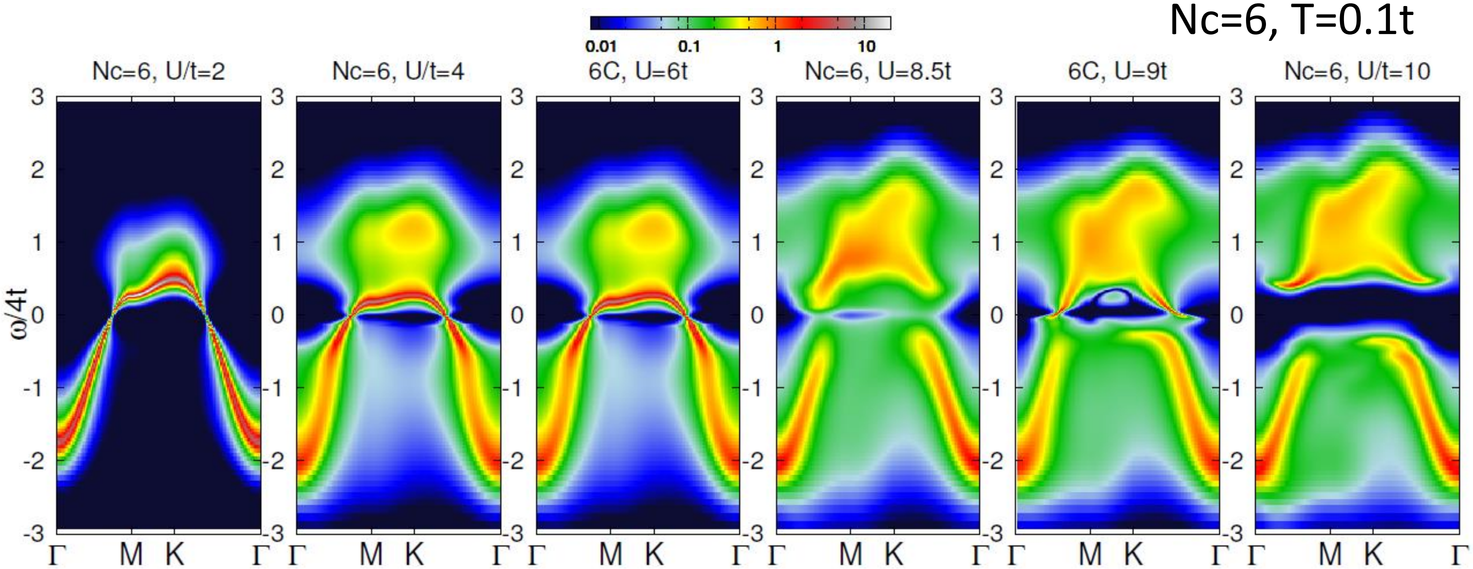


Mott Transition: $A(\boldsymbol{k},\omega)$

Nc=4, T=0.1t



Nc=6, T=0.1t

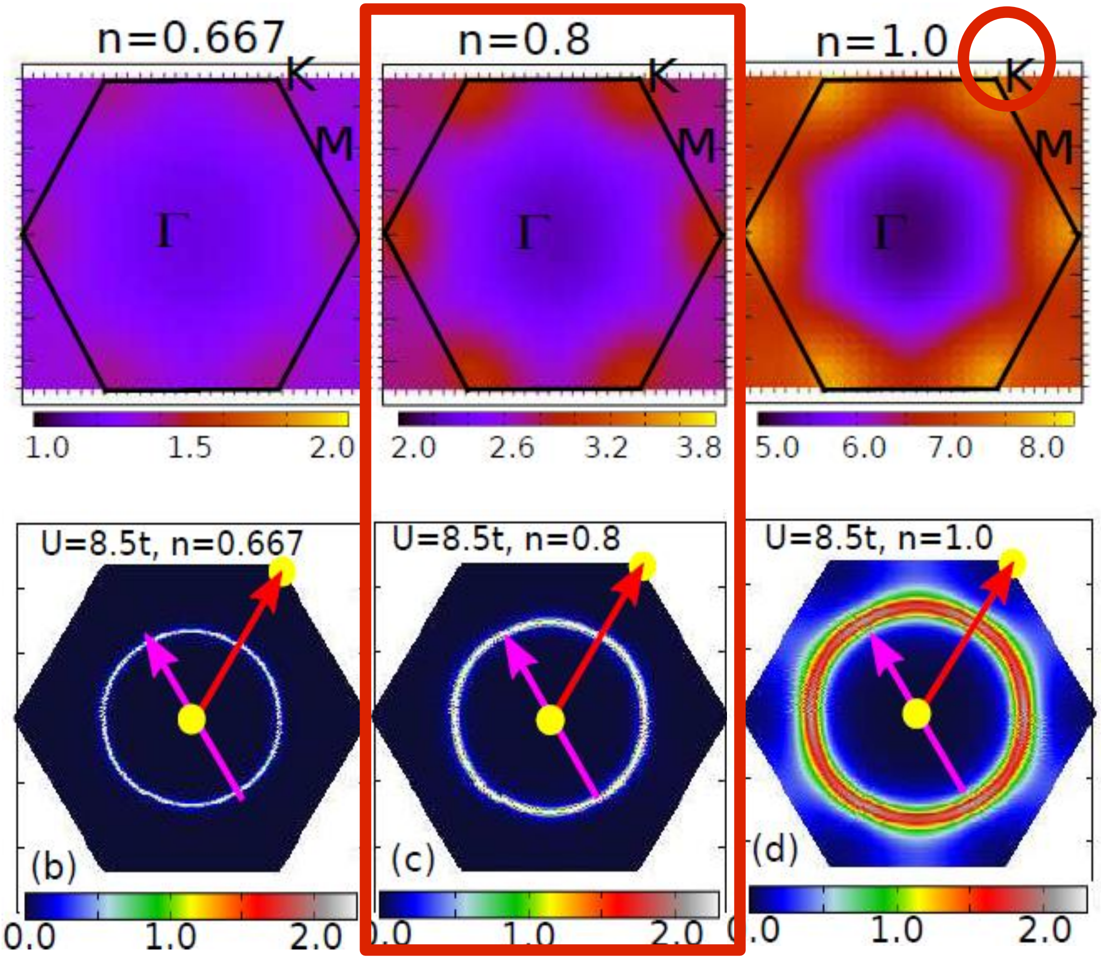


Superconductivity: FS nesting

U=8.5t
T=0.1t

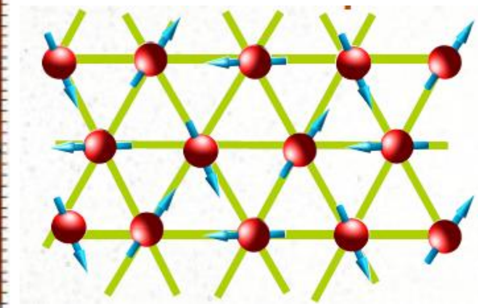
$\chi_s(K)$

Superconducting!



Fermi Surface

Heisenberg limit
AF 120°-order



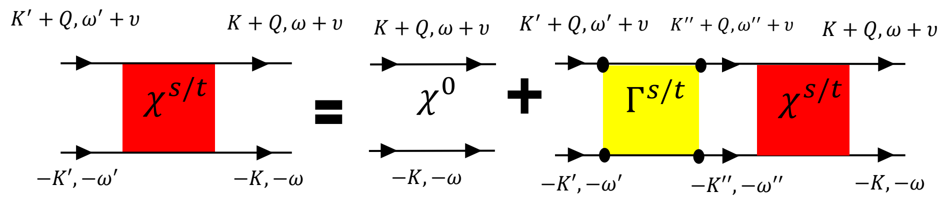
AF wavevector

$$\mathbf{Q_{AF}} = K - \Gamma$$

K. S. Chen, Z .Y. Meng, *et al.*, PRB 88, 041103(R) (2013)

Superconductivity: d+id singlet pairing

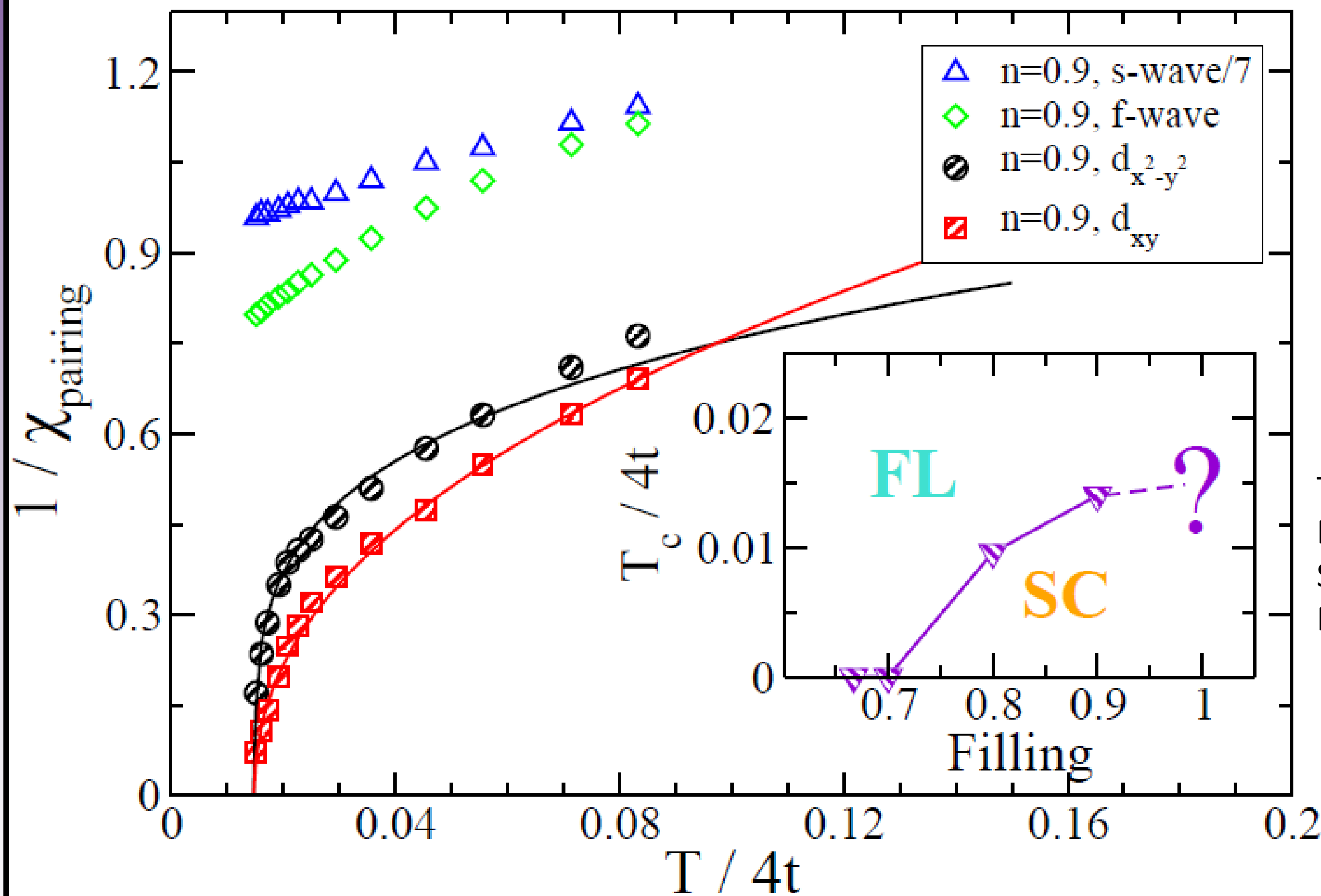
particle-particle: pairing vertex $\Gamma^{s/t}$



$T \rightarrow T_c,\ \chi(T) = \sum \frac{\chi_0}{1-\Gamma\chi_0}$ diverges

Projected onto:

- s-wave singlet
- dx2-y2 and dxy singlet
- f-wave triplet



dx2-y2 and dxy degenerate, chrial d+id pairing ground state.

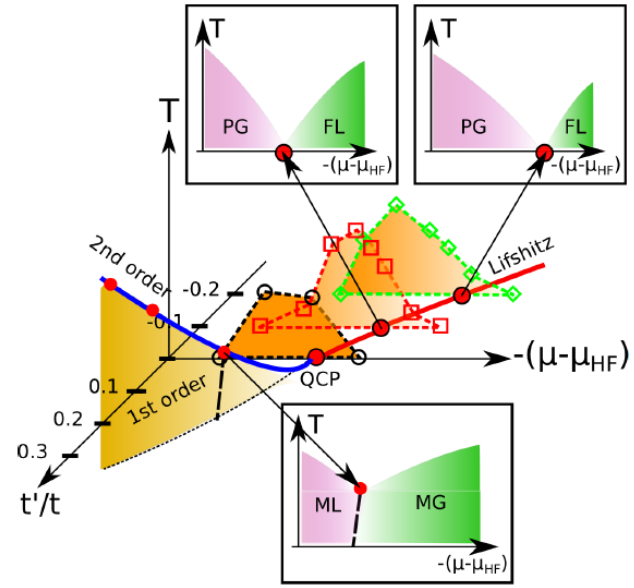
T. Senthil *et al.*, PRB (1999)
Powell and McKenzie, PRL (2007)
S. Zhou and Z. Wang, PRL (2008)
M. Kiesel *et al.*, arXiv:1301.5662

K. S. Chen, Z .Y. Meng, *et al.*, PRB 88, 041103(R) (2013)

Open Questions

Hubbard model on the square lattice:

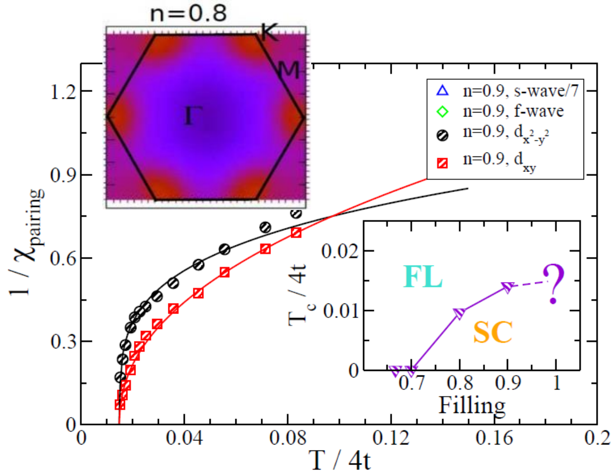
- ❑ Lifshitz transition,Pseudogap, marginal Fermi liquid, Fermi liquid....
- ❑ *d*-wave superconductivity, evolution of superconducting dome
- ❑ Asymmetry of t' > 0 and t'<0 ?
- ❑ Skewness of superconducting dome ?



K. S. Chen, Z. Y. Meng, *et.al.*, PRB 86, 165136 (2012)
Z. Y. Meng, K. S. Chen, *et al.*, in preparation

Hubbard model on the triangular lattice:

- ❑ FS nesting + AF fluctuations = d+id pairing
- ❑ Topological chiral superconductor?
- ❑ Electron-doped side?
- ❑ Nature of the Mott transition?
- ❑ Nature of the insulating phase?

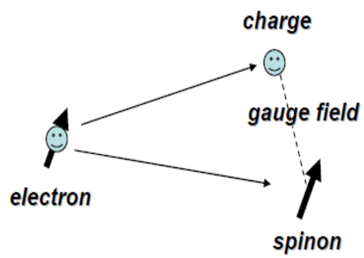


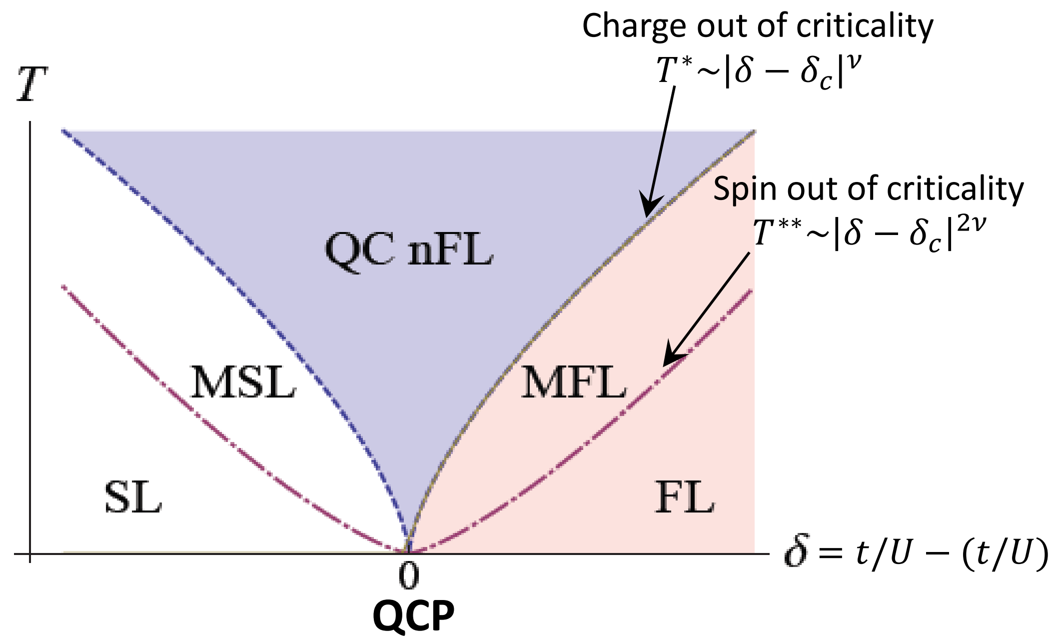
K. S. Chen, Z .Y. Meng, *et al.*, PRB 88, 041103(R) (2013)

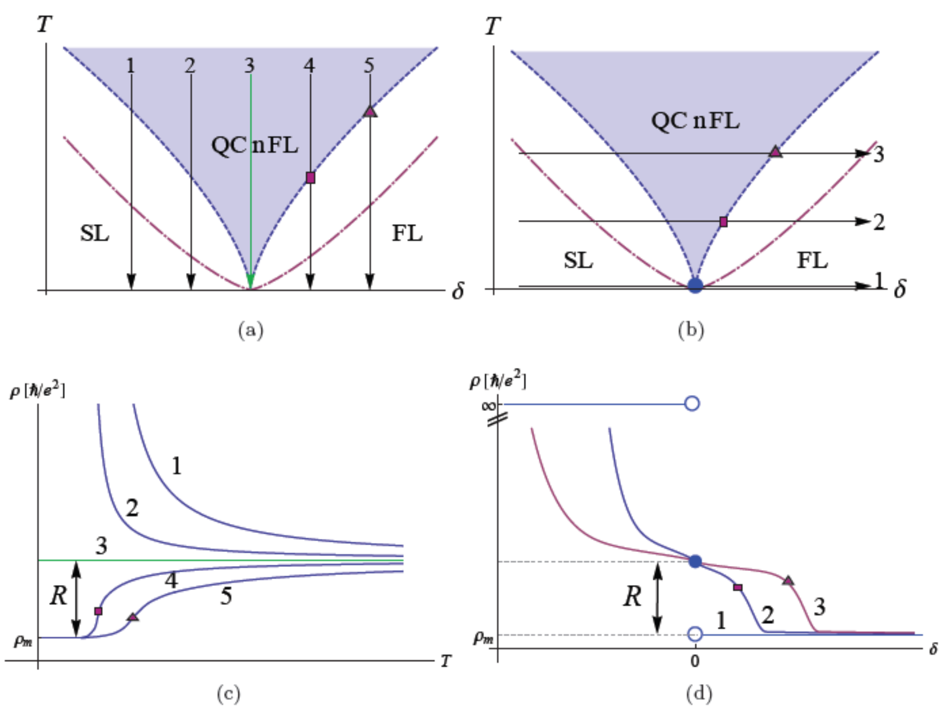
Quantum critical Mott Transition Scenario

- T. Senthil, PRB 78, 035103 (2008)
- T. Senthil, PRB 78, 045109 (2009)
- W. Witczak-Krempa, *et al.*, arXiv:1206.3309

Slave rotor: $c_{i,\sigma} = \psi_{i,\sigma} b_i$







Rotor resistivity dominates close to QCP

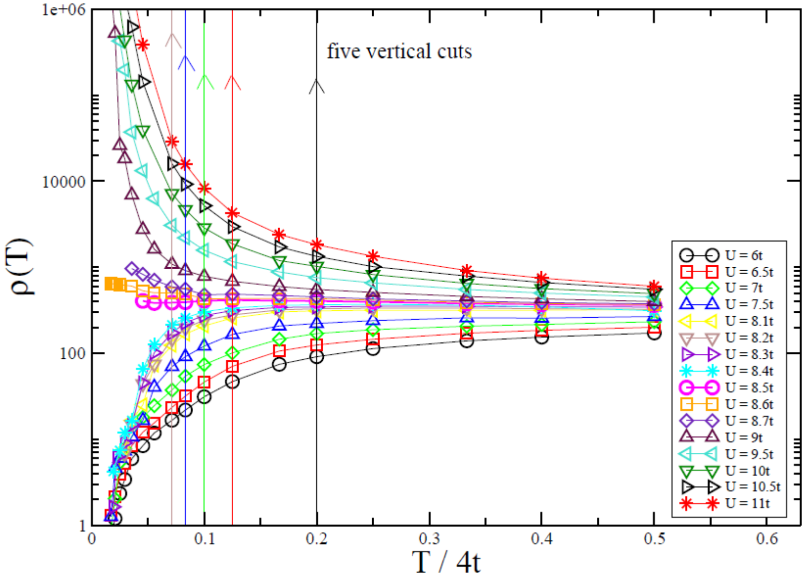
$$\rho - \rho_m = \frac{\hbar}{e^2} G\left(\frac{\delta^{z\nu}}{T}\right)$$

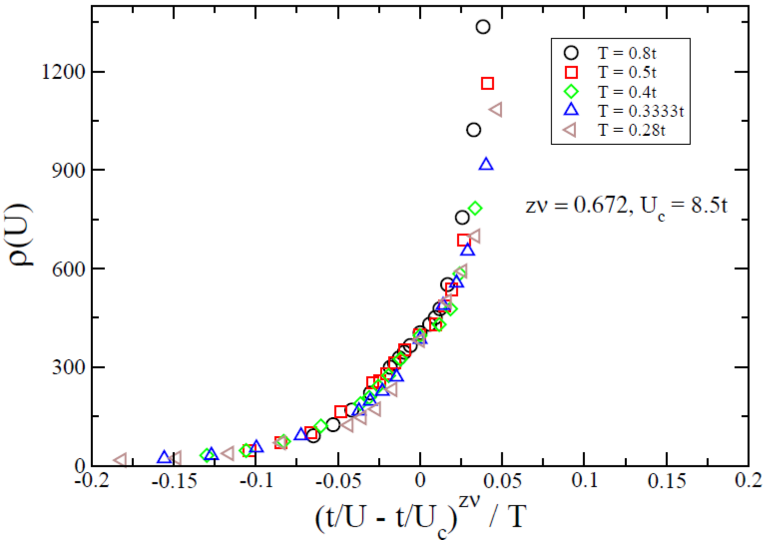
3D XY: $z = 1, \nu = 0.672$

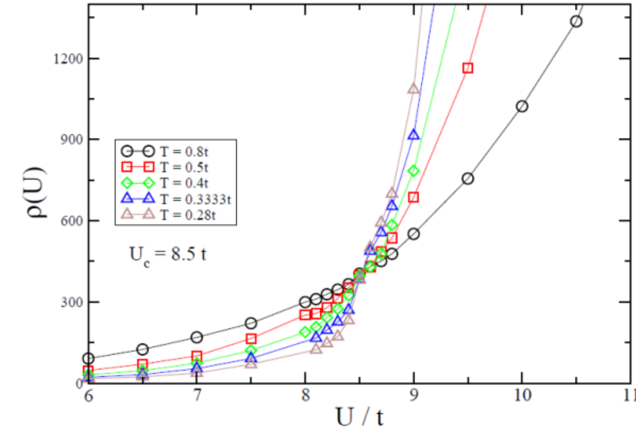
Resistivity measurements: Nc = 6

Kubo + relaxation time approximation:

$$\rho_{\alpha,\beta} \propto 1/\int d\omega\,(-\frac{\partial f(\omega)}{\partial \omega})\frac{1}{N}\sum_{\boldsymbol{k},\sigma} v_\alpha(\boldsymbol{k})v_\beta(\boldsymbol{k})A^2(\boldsymbol{k},\omega)$$



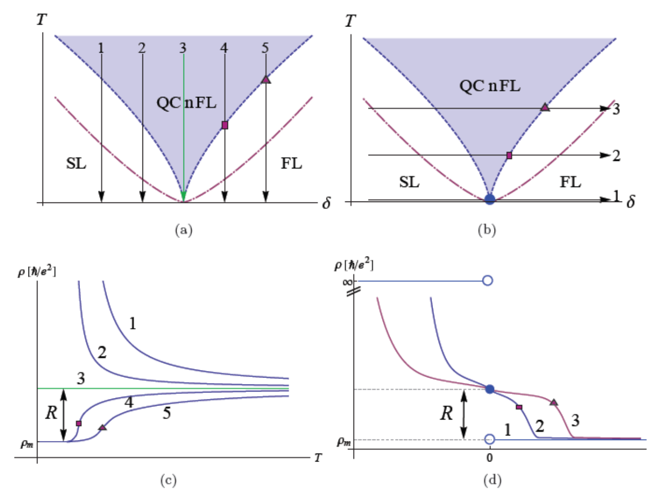




Rotor resistivity dominates close to QCP

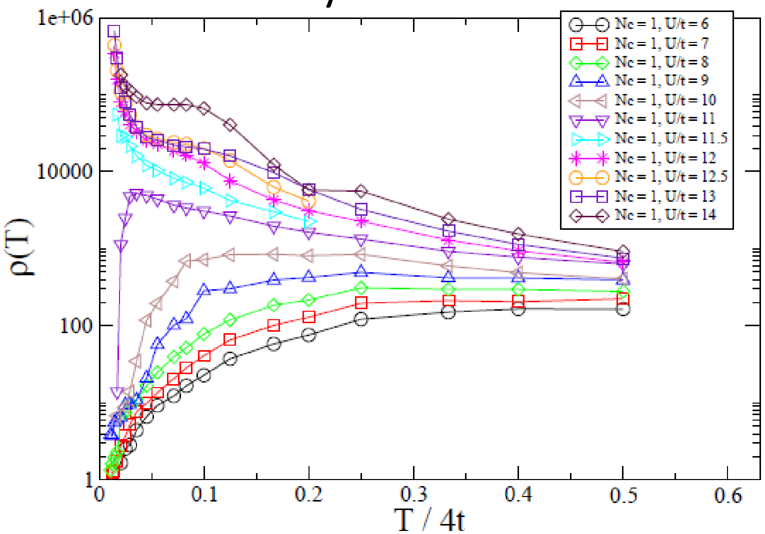
$$\rho - \rho_m = \frac{\hbar}{e^2} G\left(\frac{\delta^{z\nu}}{T}\right) \qquad \delta = t/U - (t/U)_c$$

3D XY: $z = 1, \nu = 0.672$

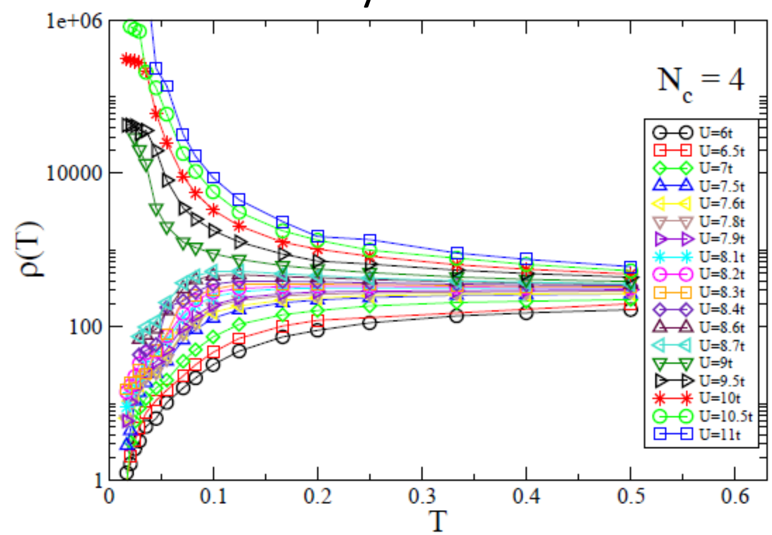


backup slide: resistivity

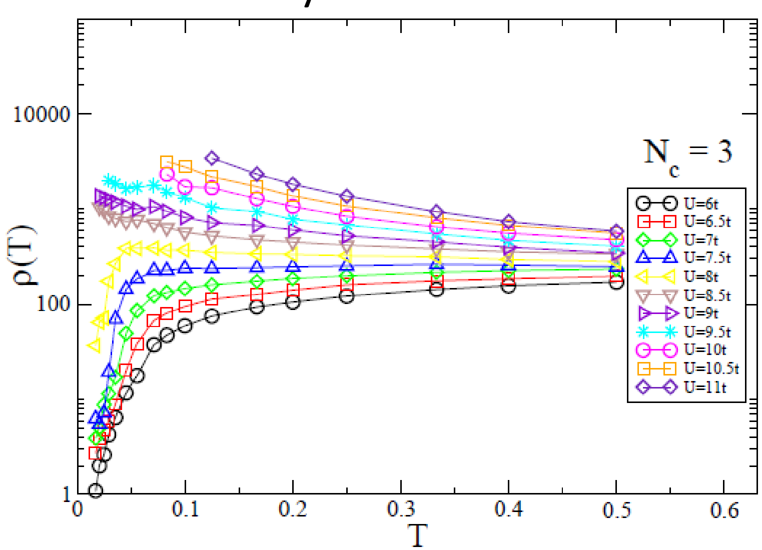
Resistivity data:Nc =1



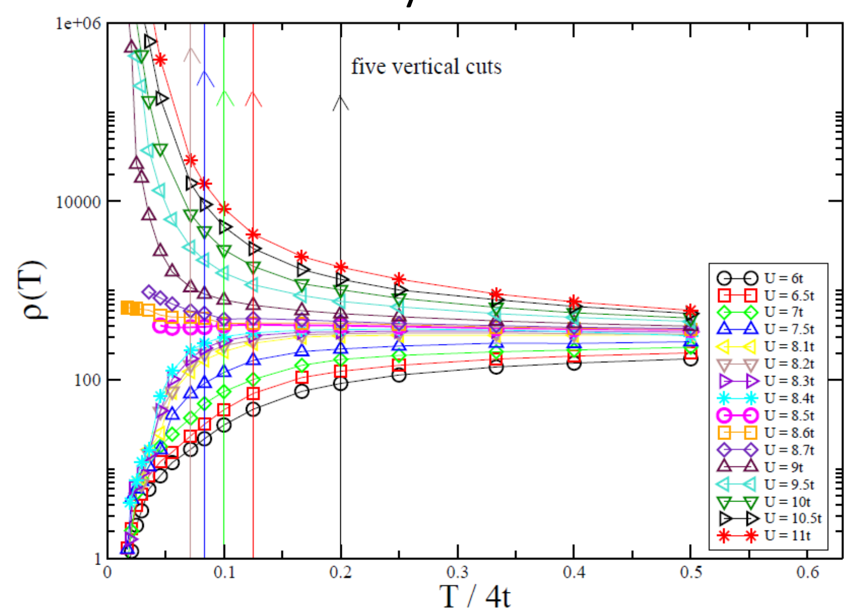
Resistivity data:Nc =4



Resistivity data:Nc =3

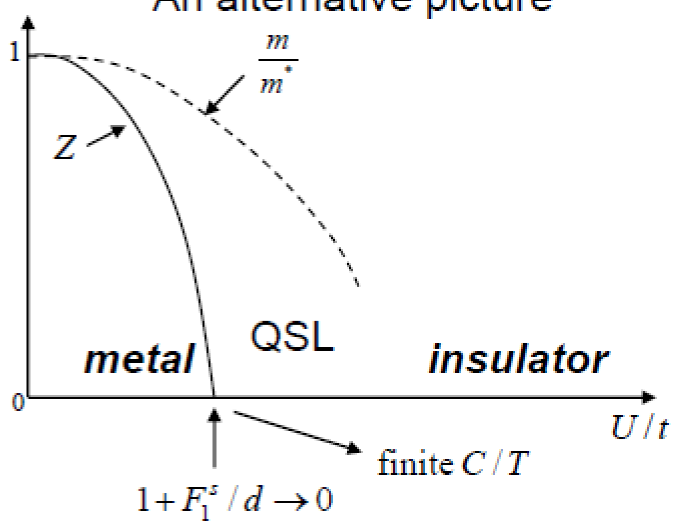


Resistivity data:Nc =6



backup slide: effective mass

Idea from Yi Zhou & Tai Kai Ng



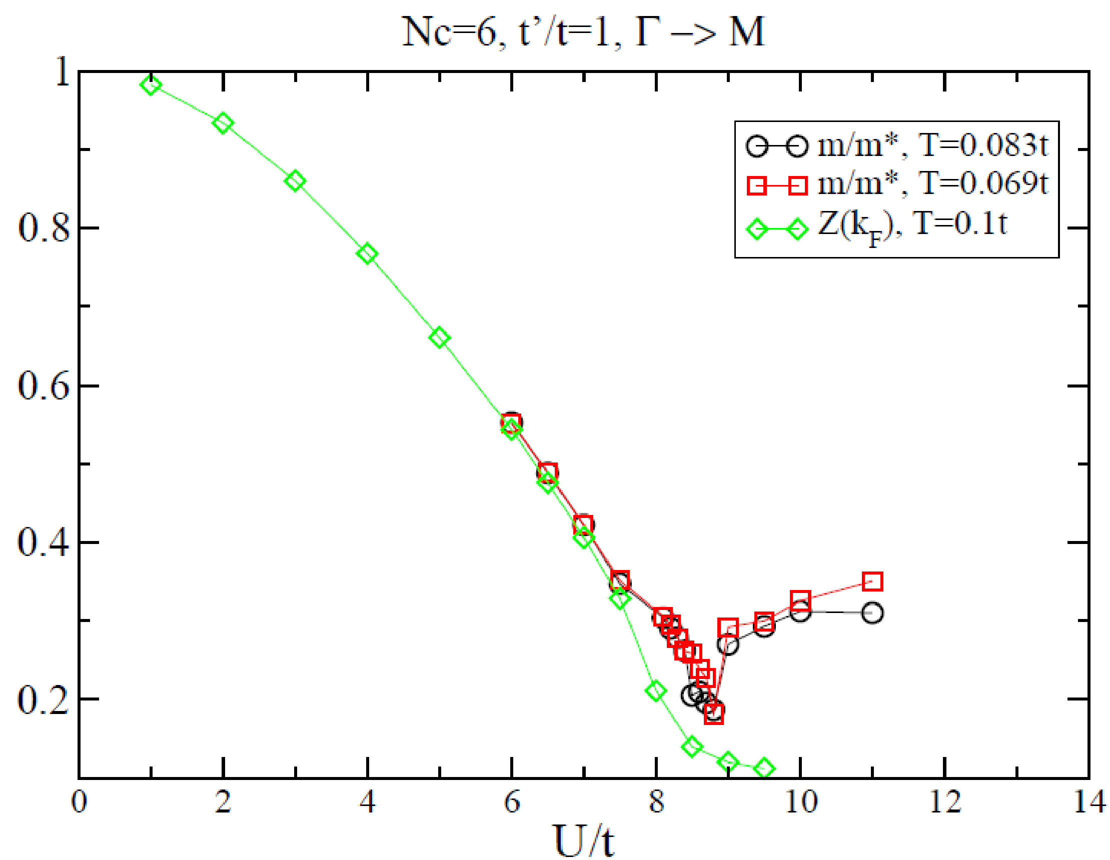
The quasiparticle Fermi surface is not destroyed but is converted to a spinon Fermi surface.

Quasiparticle weight vanishes

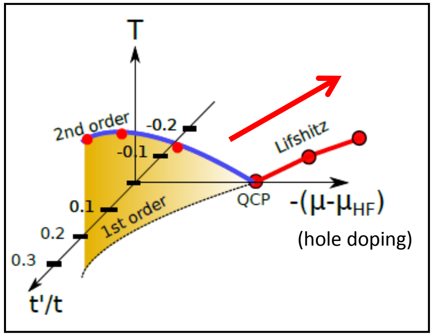
$$Z_k = [1 - \frac{\partial}{\partial \xi}\Sigma(k,\xi)\,|_{\xi=\xi_k}]^{-1}$$

Effective mass stays finite

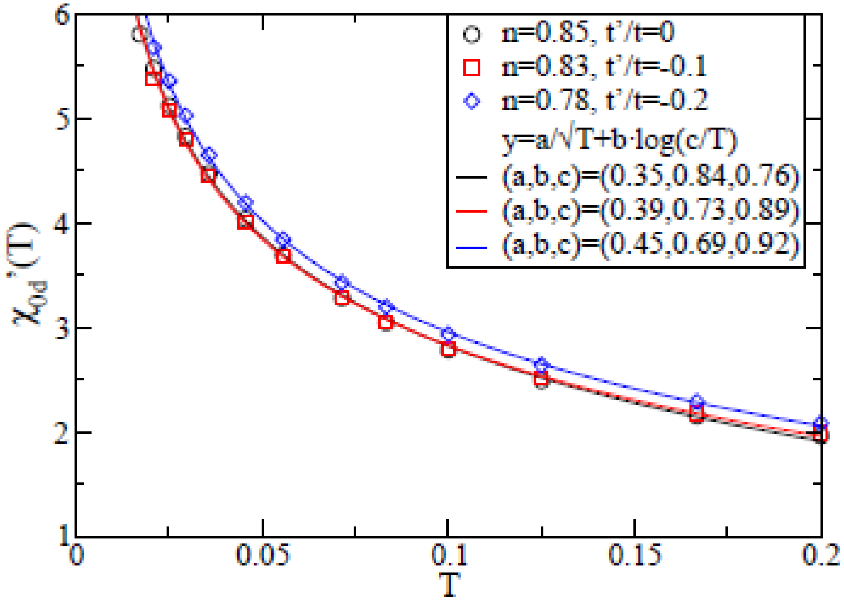
$$\frac{m}{m^*} = \lim_{\xi_k^0 \to 0} \frac{\partial \varepsilon_k}{\partial \varepsilon_k^0} = \lim_{\xi_k^0 \to 0} \frac{1 + (\partial/\partial \varepsilon_k^0)\Sigma(k,\xi)}{1 - (\partial/\partial \xi)\Sigma(k,\xi)}$$



backup: scaling behavior at t'<0



Algebraic divergence become stronger as $t' \rightarrow$ negative values



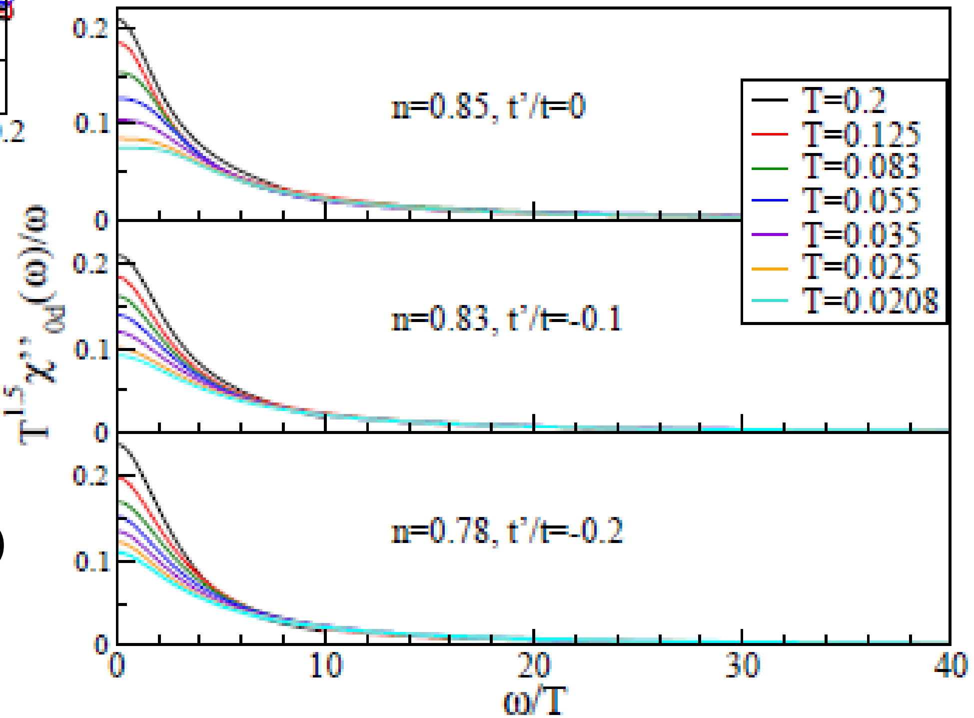
$$\frac{T^{1.5}\chi''_{0d}(\omega)}{\omega} = H(\omega/T)$$

$$\chi_{0d}'(T) = \int d\omega \chi_{0d}''(\omega)/\omega$$

$$\int d\omega T^{-1.5} H\left(\frac{\omega}{T}\right) = \frac{B}{\sqrt{T}}, B = \int dx H(x)$$

$$\chi_{0d}'(T) = slowpart + B/\sqrt{T}$$

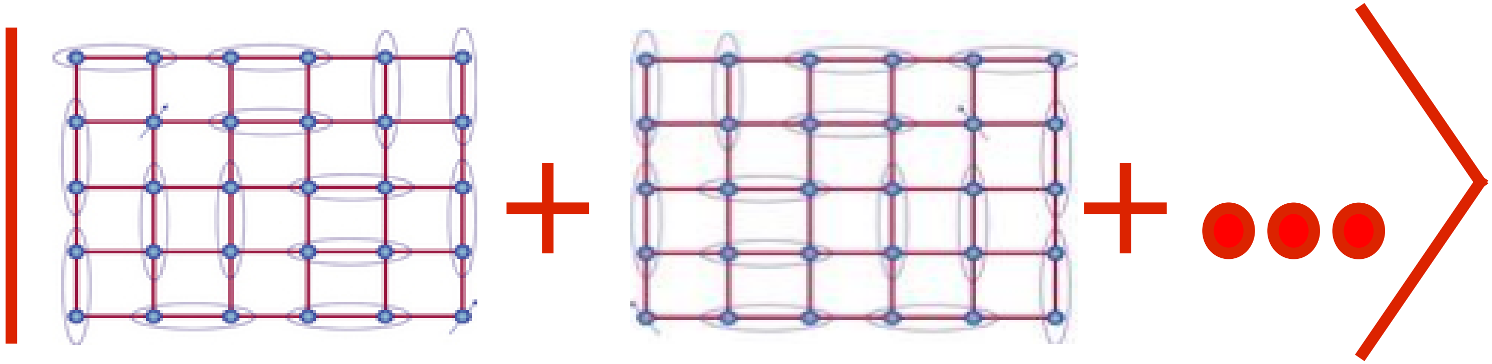
Scale-invariant proximity to QCP



backup: Pseudogap = RVB ?

Quasi-particle weight vanishes at (pi,0) for the Pseudogap region

|RVB>=



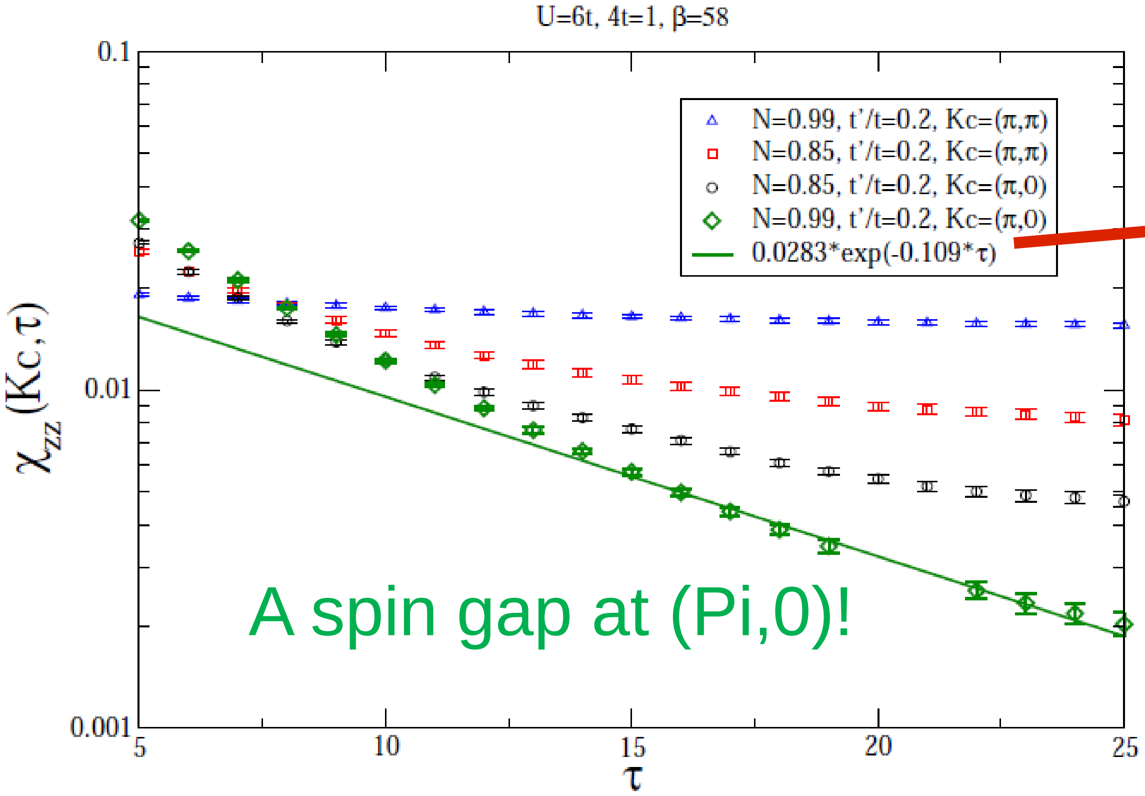
The singlet is formed mainly along the x or y directions and is short-ranged.

backup: pseudogap = RVB ?

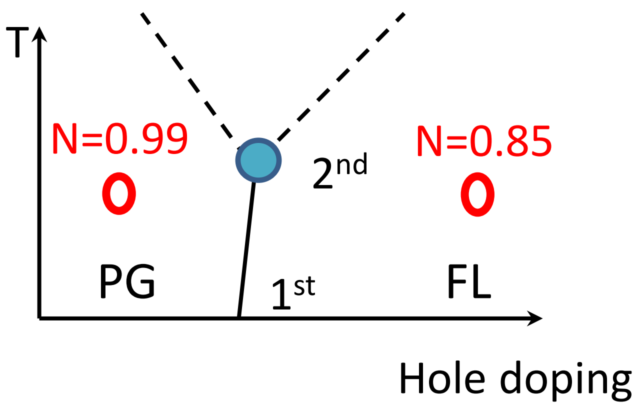
Dynamic spin-spin correlation function

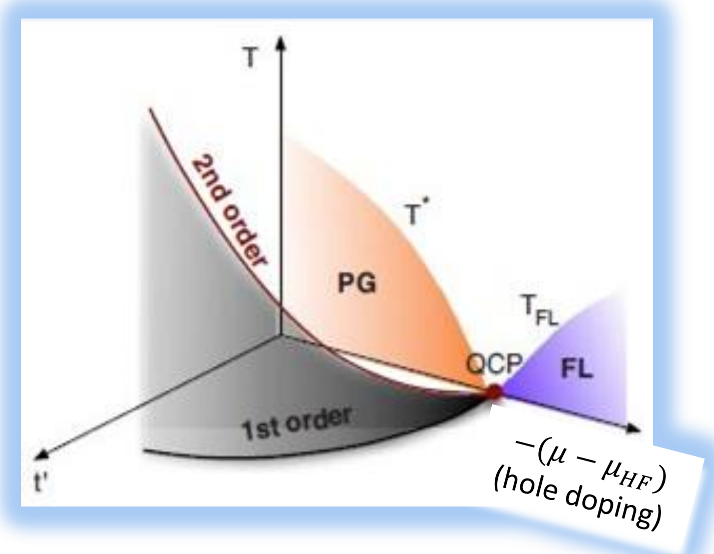
$$\chi_{zz}(K_C,\tau) = \frac{1}{N_C}\sum_{R_i,R_j} e^{-iK_C(R_i-R_j)}\left\langle S^z_{R_i}(\tau)S^z_{R_j}(0)\right\rangle$$

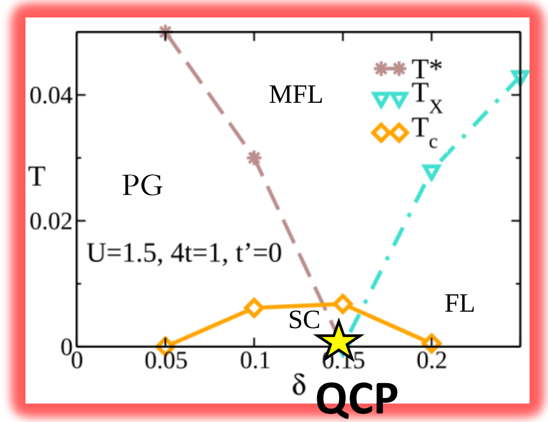
$$\tau\to\infty\,,\ \chi_{zz}(K_C,\tau)\to\exp(-\Delta_S(K_C)\tau)$$

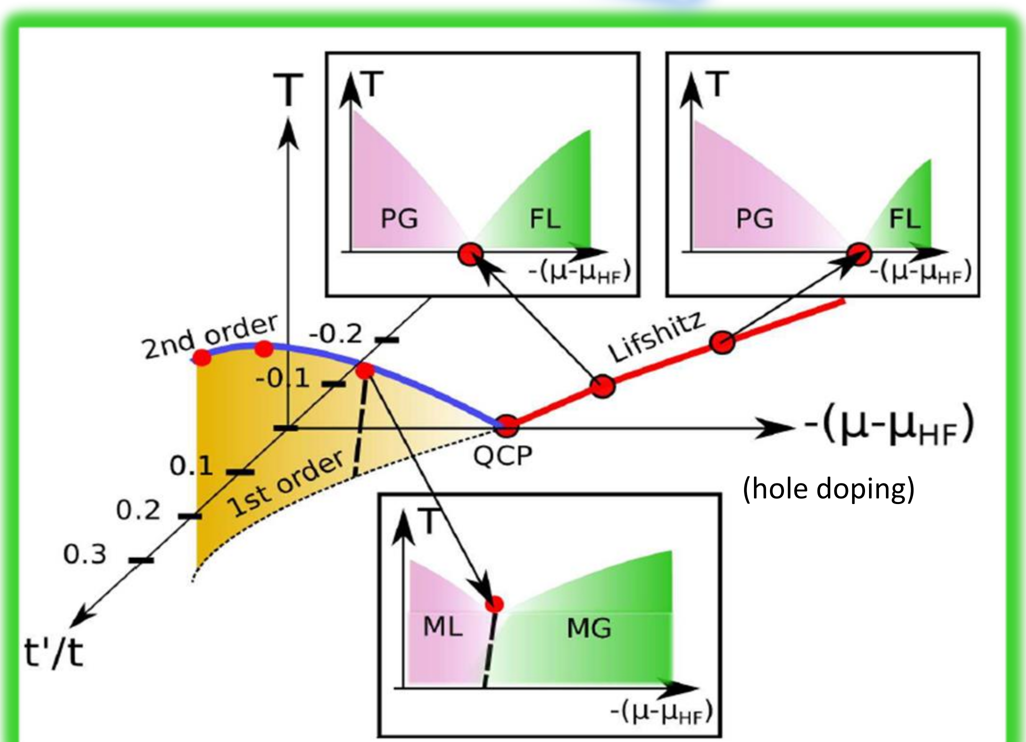


J=4t^2/U=1/6=0.167









Superconductivity and QCP in the 2D Hubbard Model

- QCP : Due to a T=0 second order terminus of a line of first-order phase separation transitions.
- QCP accompanied by vHs
- SC enhanced near QCP by chi not V.
- Dependence on t'/t

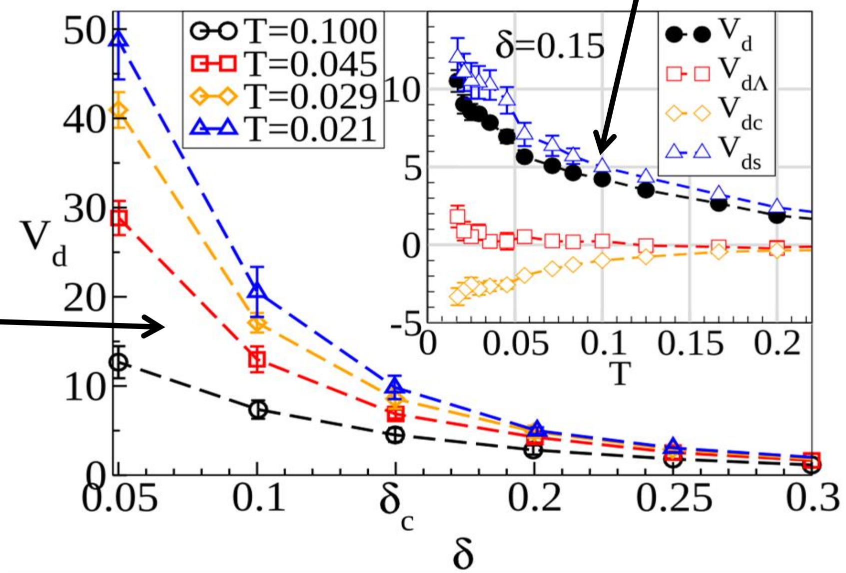
backup: pairing and Tc

- $T \to T_c,\ \chi(T) = \sum \frac{\chi_0}{1-\Gamma\chi_0} \to \infty$

  pairing matrix $\Gamma\chi_0\varphi = \lambda\varphi,\ \lambda \to 1$

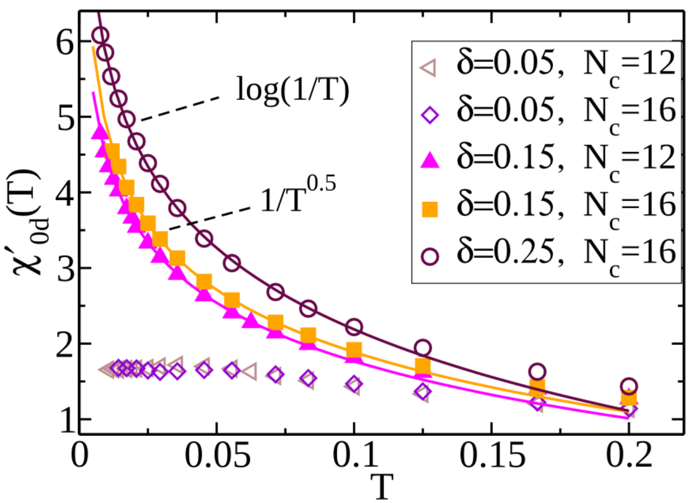
  $V_d = \langle g_d|\Gamma|g_d\rangle \quad \chi_{0d} = \langle g_d|\chi_0|g_d\rangle$

- spin channel is dominant

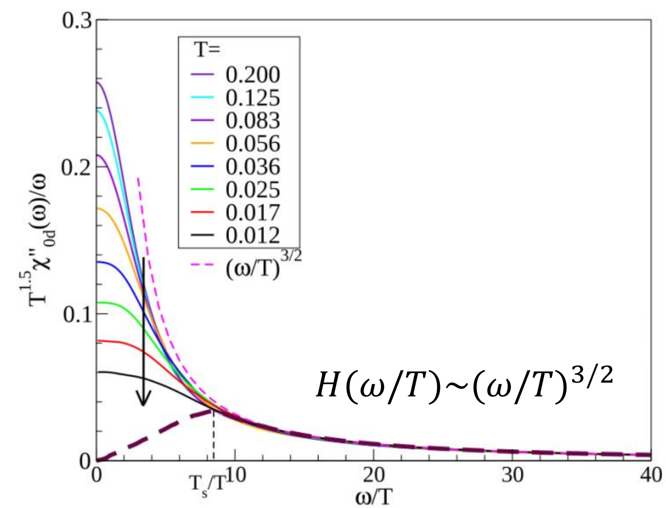


- V_d decays monotonically with doping

- χ'_{0d} has a power-law divergence at QCP



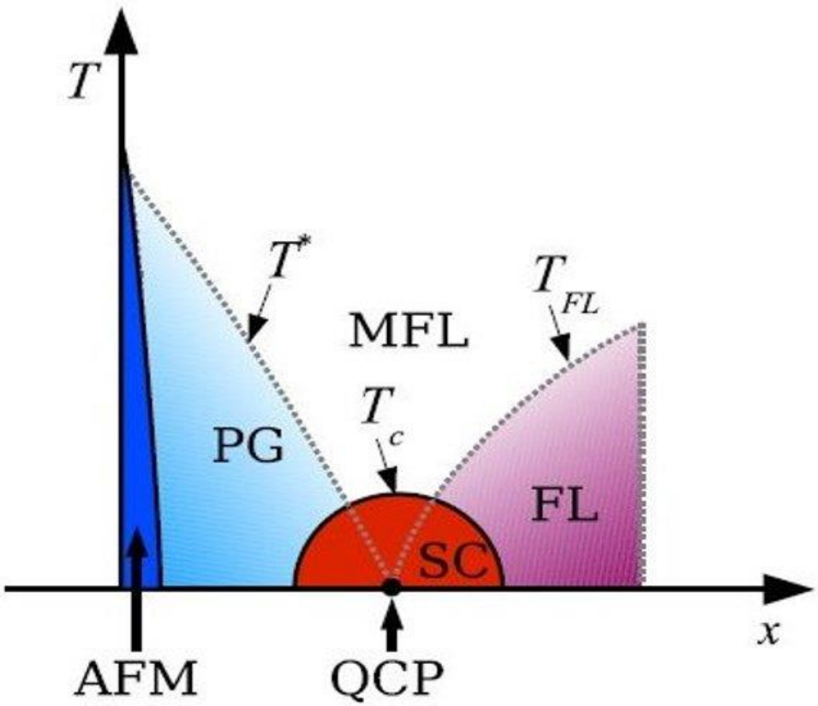
- $T^{1.5}\chi''_{0d}(\omega)/\omega$ scales as $(\omega/T)^{1.5}$ at QCP



- $T_c \sim (BV_d)^2$ unbounded! $B = \int dx H(x)$ different from BCS $T_c \sim e^{-1/N(0)V}$

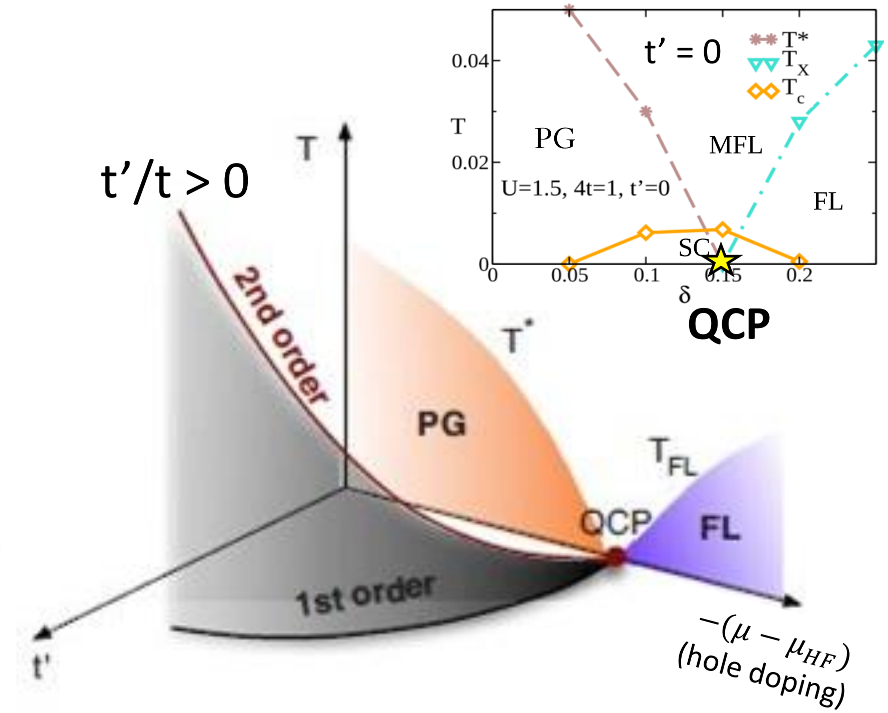
J.-H. She and J. Zaanen, PRB 80, 184518 (2009)
S.-X. Yang, et.al. PRL 106, 047004 (2011)

backup: QCP in the 2D Hubbard Model



Theory and Experiment:
QCP lying beneath the SC dome.

C. M. Varma, PRL 83, 3538 (1999)
Y. Ando et al., PRL 93, 267001 (2004)
D. M. Broun, Nat. Phys. 4, 170 (2008)
R. A. Cooper et al., Science 323, 603 (2009)
R. Daou et. al. Nat. Phys. 5, 31 (2009)
F. F. Balakirev et. al. PRL 102, 017044 (2009)
S. Sachdev, Phys. Status Solidi B 247, 537 (2010)
S. E. Sebastian et al., PNAS, 107, 6175(2010)



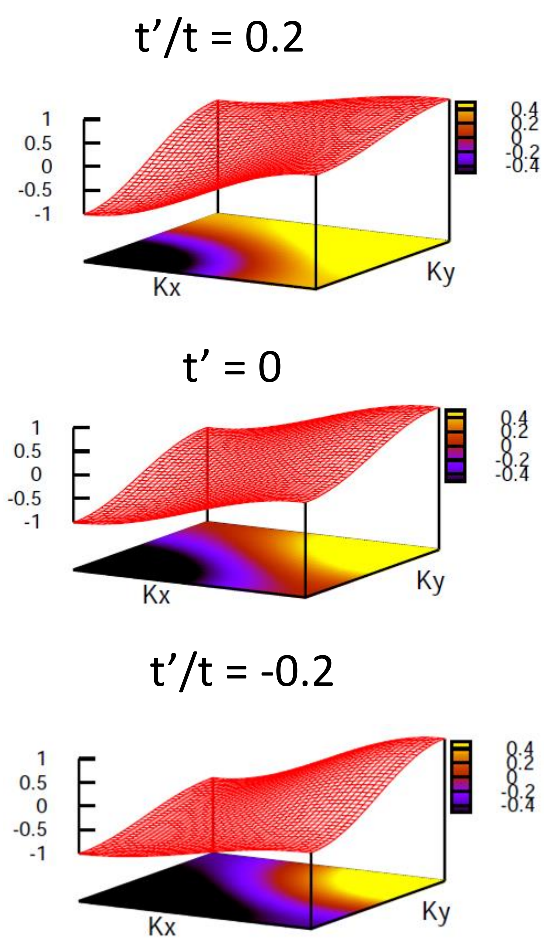
Numerical: **QCP is the point where the 1st order phase separation area and 2nd order transition lines coincide at t'=0 & T=0.**

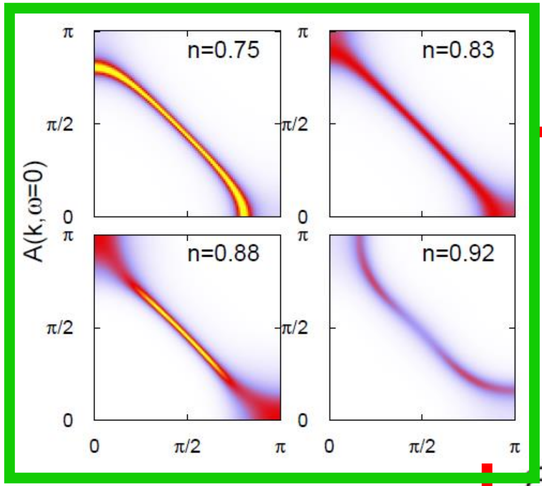
A. Macridin et al., PRB 74, 085104 (2006)
K. Mikelsons et. al. PRB 80, 140505R (2009)
E. Khatami, et. al. PRB 81, 201101(R) (2010)
N.S.Vidhyadhiraja et al., PRL 102, 206407, (2009)
S.-X. Yang et.al. PRL 106, 047004 (2011)
K.-S. Chen et.al. PRB 84, 245107 (2011)

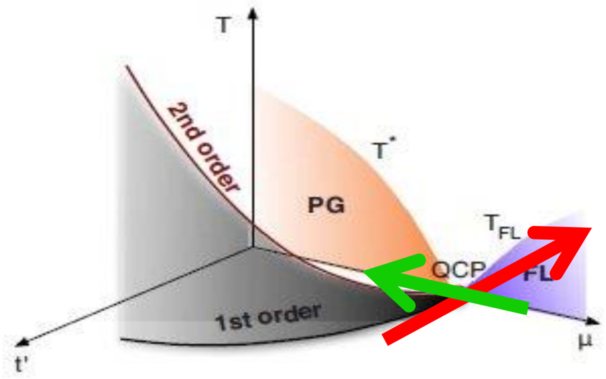
backup: (t', n) : control Parameter of Lifshitz Transition

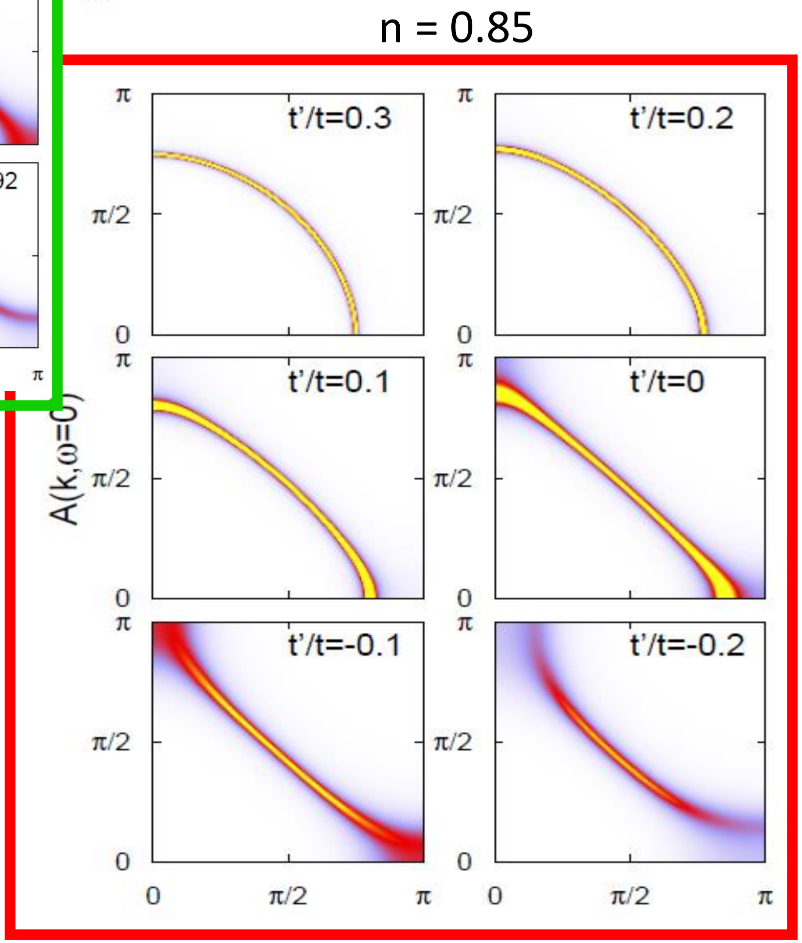
Effect of t' on bare dispersion

$$\epsilon^0_{\boldsymbol{k}} = -2t\left(\cos k_x + \cos k_y\right) - 4t'\left(\cos k_x \cos k_y - 1\right)$$







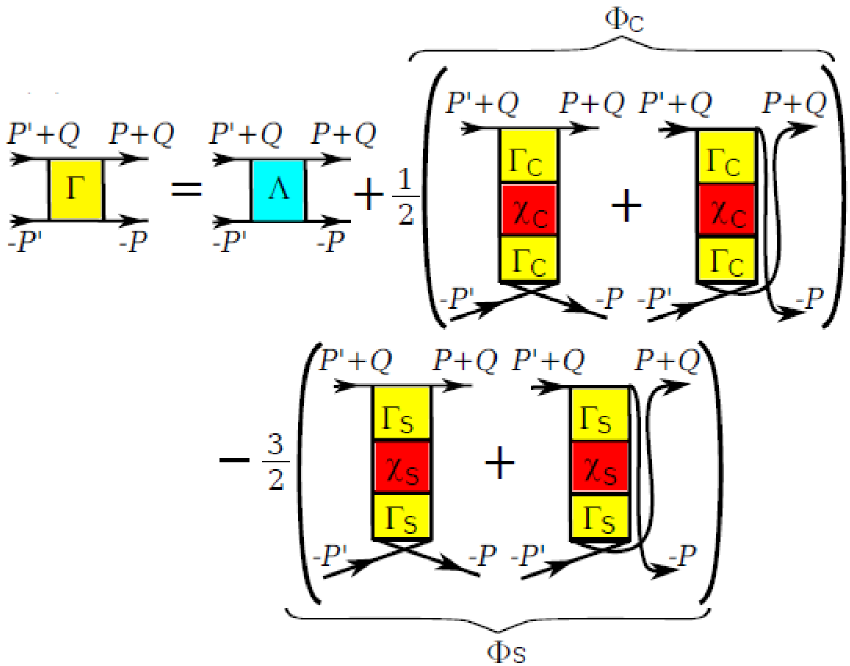


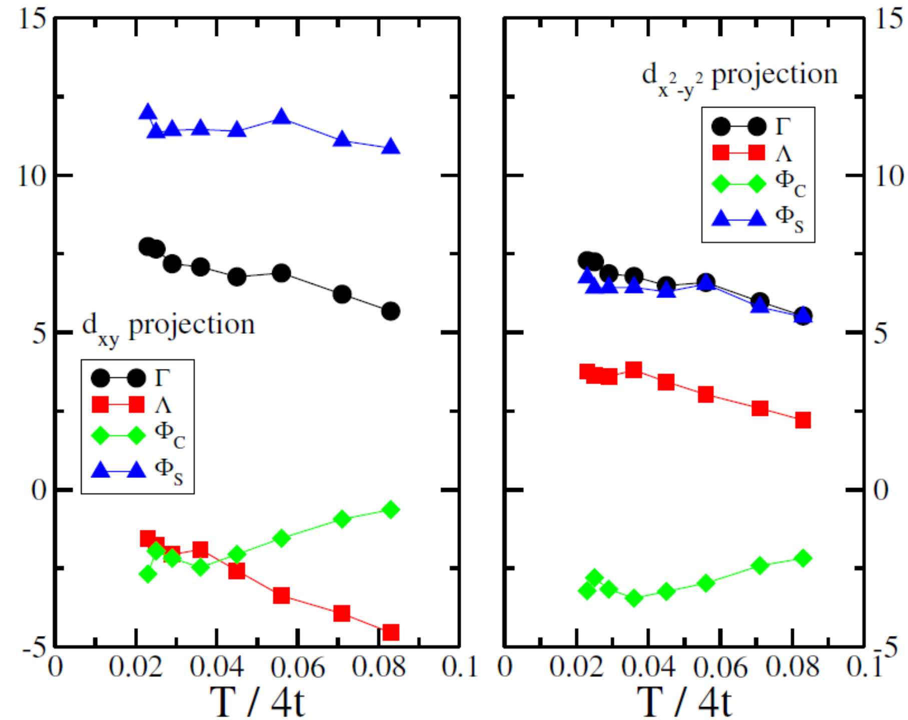
K.-S. Chen, Z. Y. Meng et.al., PRB 86, 165136 (2012)

Superconductivity: vertex decomposition

Vertex decomposition, parquet formalism:

$$\Gamma(P,P',Q) = \Lambda(P,P',Q) + \Phi_C(P,P',Q) + \Phi_S(P,P',Q), \quad P = (K, i\omega)$$





- Spin part Φ_S dominates the pairing vertex Γ;
- Momentum transfer $Q = \mathbf{Q}_{\mathbf{AF}}$ contributes most to Φ_S , AF fluctuation mediated pairing

K. S. Chen, Z .Y. Meng, et al, PRB 88, 041103(R) (2013)