# Overcoming Fermionic Sign Problem in Lattice Quantum Monte Carlo: a Cuprate Case


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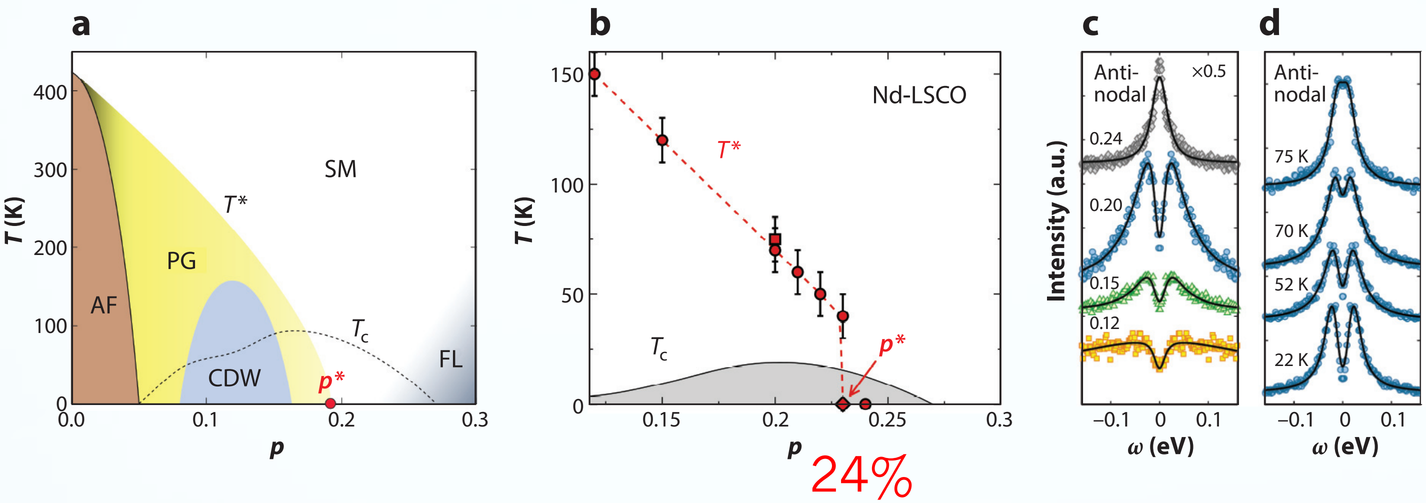
In collaboration with
S. Iskakov, E. Stepanov and M. Katsnelson

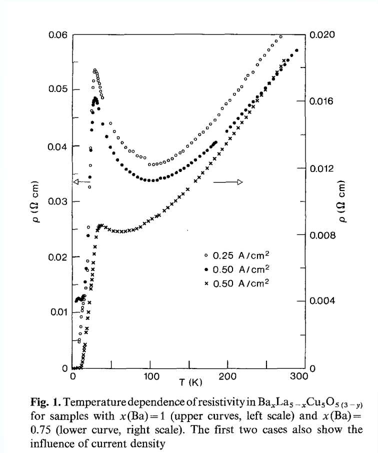
# Outline

- HTSC: Cuprate case
- Reference system: DF-QMC method
- What is “Glue” for HTSC?

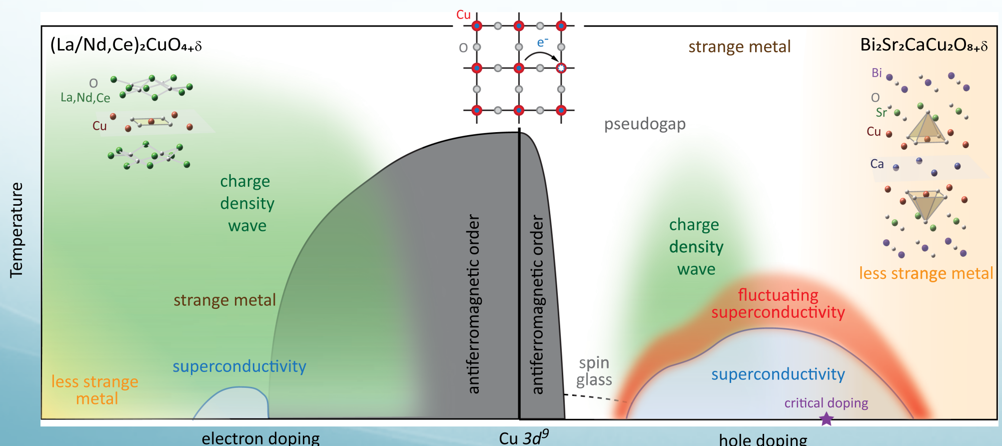
# 40 years of HTSC: What is the “glue”?




C. Proust and L.Taillefer, Annu. Rev. Condens. Matter Phys. 10, 409–429 (2019)




J. Bednorz and K. Müller
Z. Phys. B 64, 189 (1986)




J. Sobota, Yu He, and Zhi-Xun Shen, RMP 93, 025006 (2021)

# Complicated Stripes-HTSC problem

"Absence of Superconductivity in the Pure Two-Dimensional Hubbard Model"
S.R. White, S.W. Zhang et al. PRX10, 031016 (2020)

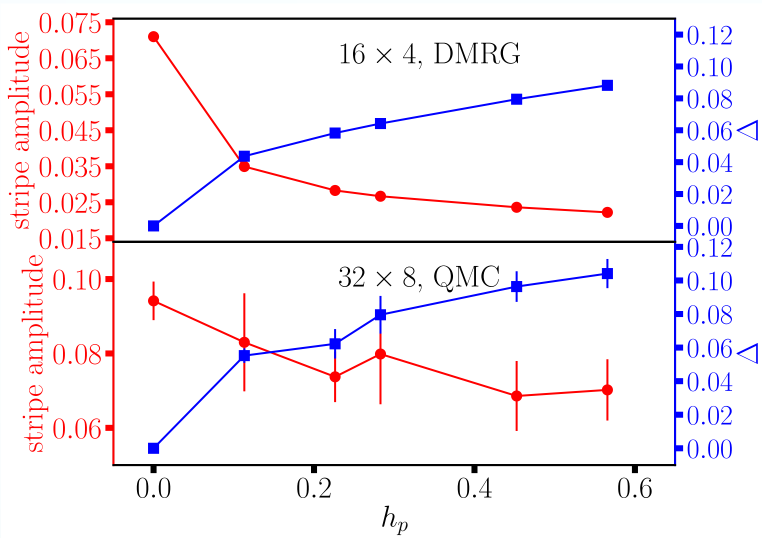
?

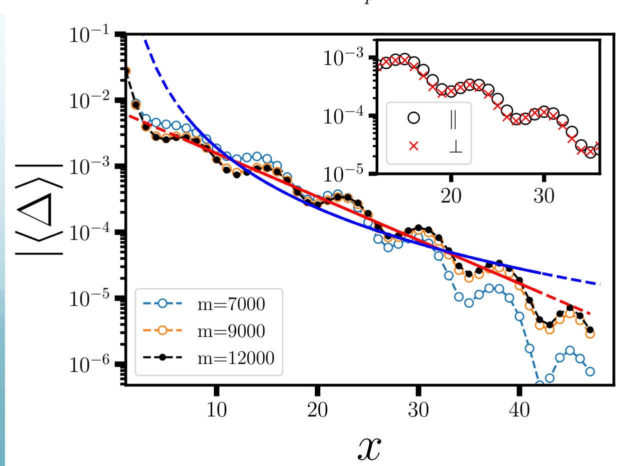
"Coexistence of superconductivity with partially filled stripes in the Hubbard model"
S.R. White, S.W. Zhang et al. Science 384, 637 (2024)

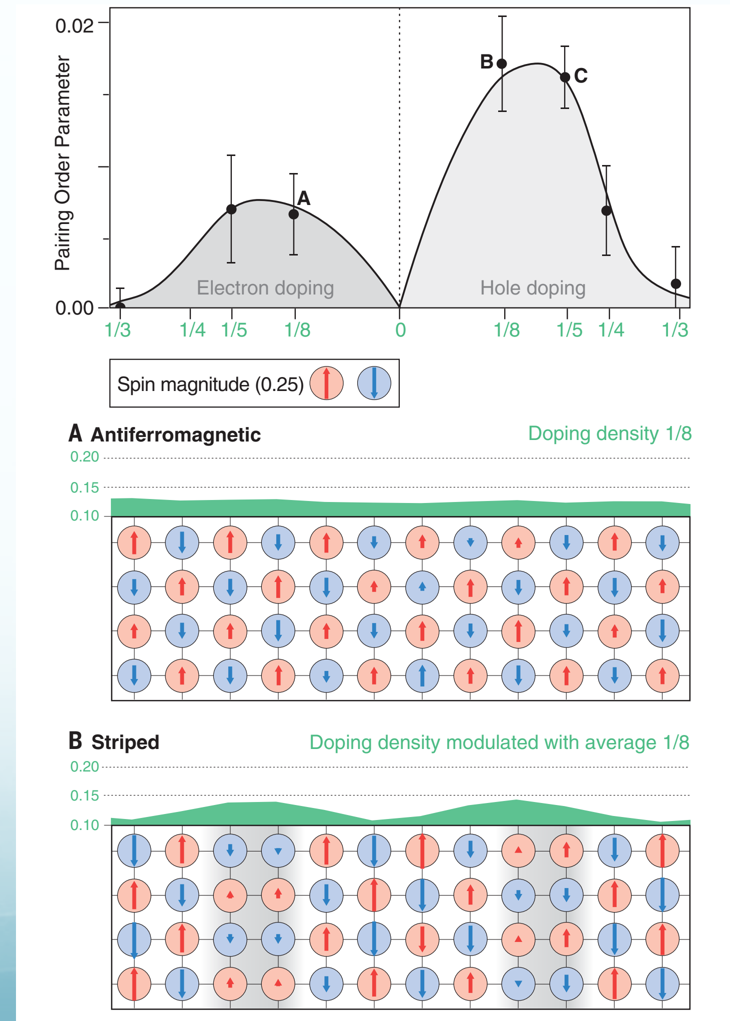
t'=0

DMRG and CP-DQMC

t'/t=-0.2

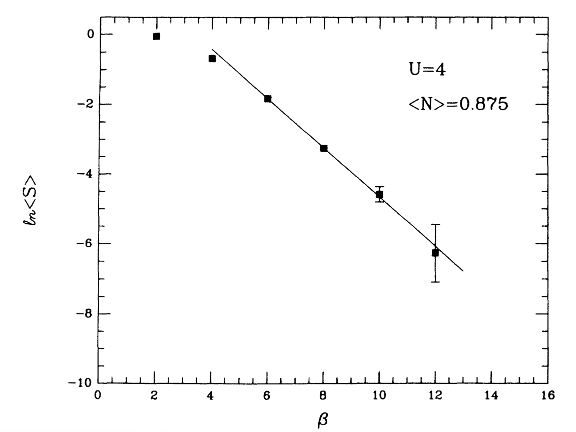


# Fermionic QMC: sign problem vs. sign blessing

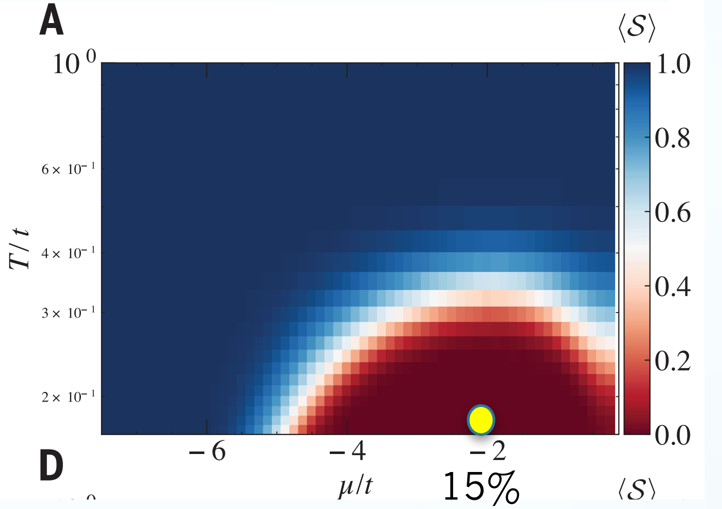
**Problem:** DQMC and CT-INT for large system about 8x8
Doped and particle-hole asymmetric case




$$< S > \sim e^{-\beta U N}$$

U/t=6 t'/t=-0.2

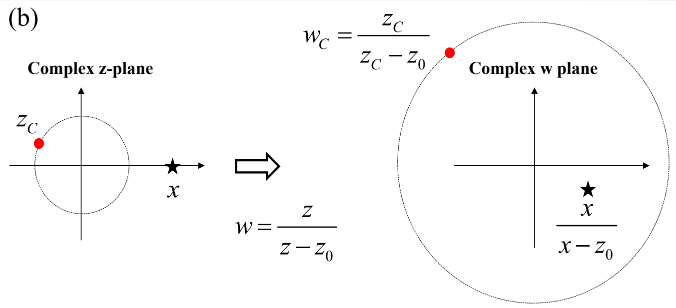
Sign is physical and related with QCP




E. Loh, Phys. Rev. B 41, 9301 (1990)

R. Mondaini, S. Tarat, R. Scalettar, Science 375, 418 (2022)

**Blessing:** DiagMC and Cdet (Riccardo Rossi)
Cancellation of high-order Feynman diagram
10-12 order is converge with "shifted-action" and conformal mapping

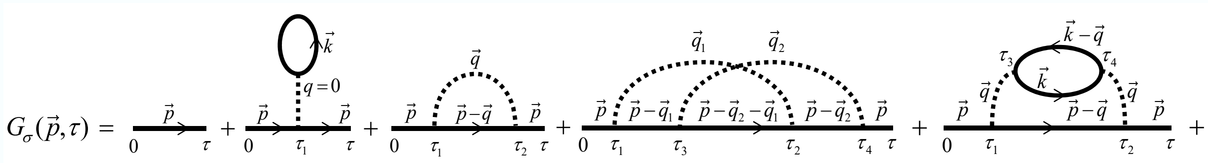



N. Prokof'ev "DiagMC" Jülich school 2019

# Weak and Strong coupling: QMC

$$H = c_1^\dagger t_{12} c_2 + \frac{1}{4} c_1^\dagger c_2^\dagger U_{1234} c_3 c_4$$

Weak: U<<t , "normal" perturbation diagram




Diagrammatic MC (Worm)

N. Prokof'ev, B. Svistunov, I. Tupitsyn,
JETP Lett. 64, 911 (1996), Sov. Phys. JETP 87, 310 (1998)
N. Prokof'ev, B. Svistunov, Phys. Rev. Lett. 81, 2514 (1998)

CT-QMC: CT-INT ("det $G_0$")

A. Rubtsov, and A. L., JETP Lett. 80, 61 (2004)
A. Rubtsov, V. Savkin, and A. L., Phys. Rev. B 72, 035122 )2005)

CDet: $$C(V) = \det(V) - \sum_{S \subsetneq V} C(S) \det(V \backslash S)$$

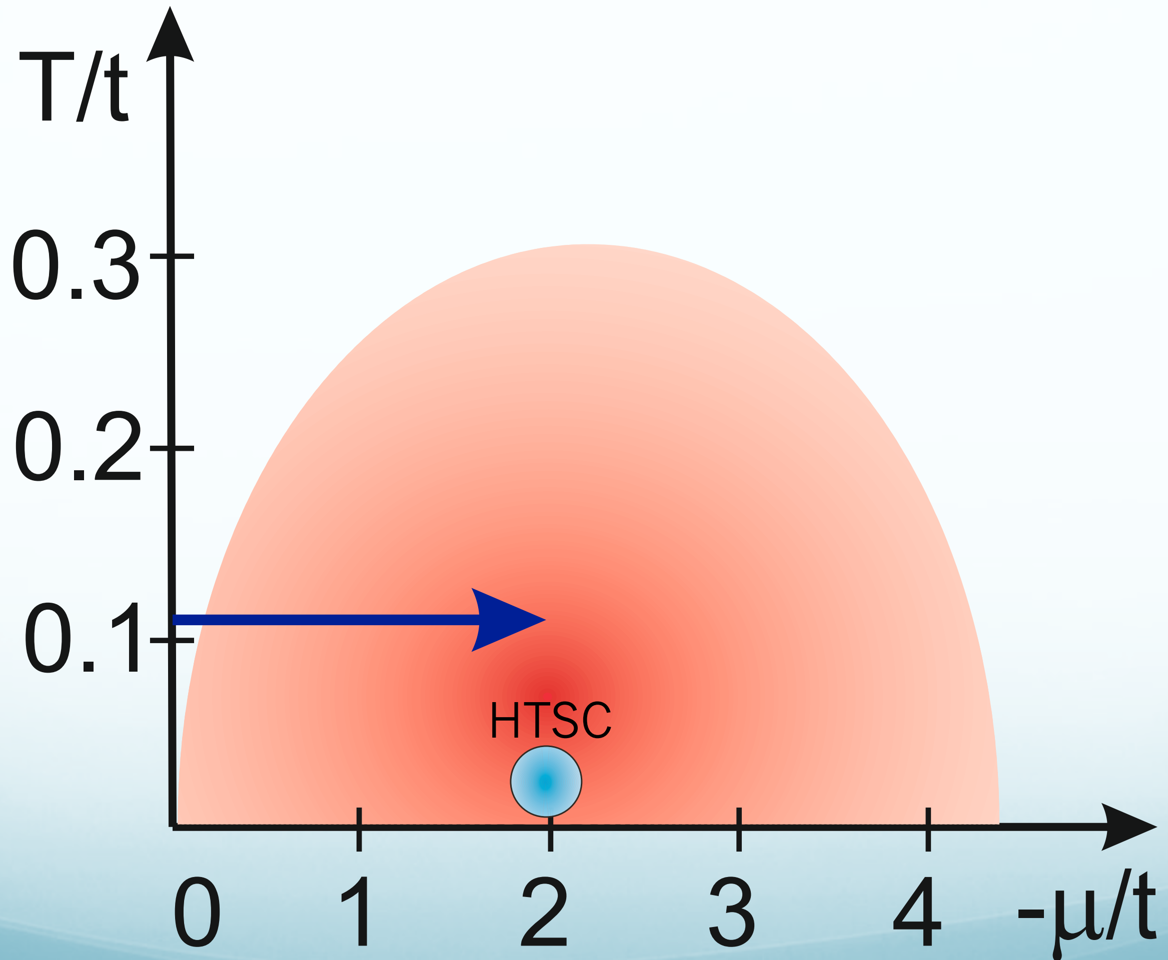
R. Rossi, Phys. Rev. Lett. 119, 045701 (2017)

Strong: U>>t complicated perturbation diagram

CT-QMC: CT-HYB ("det $\Delta$")

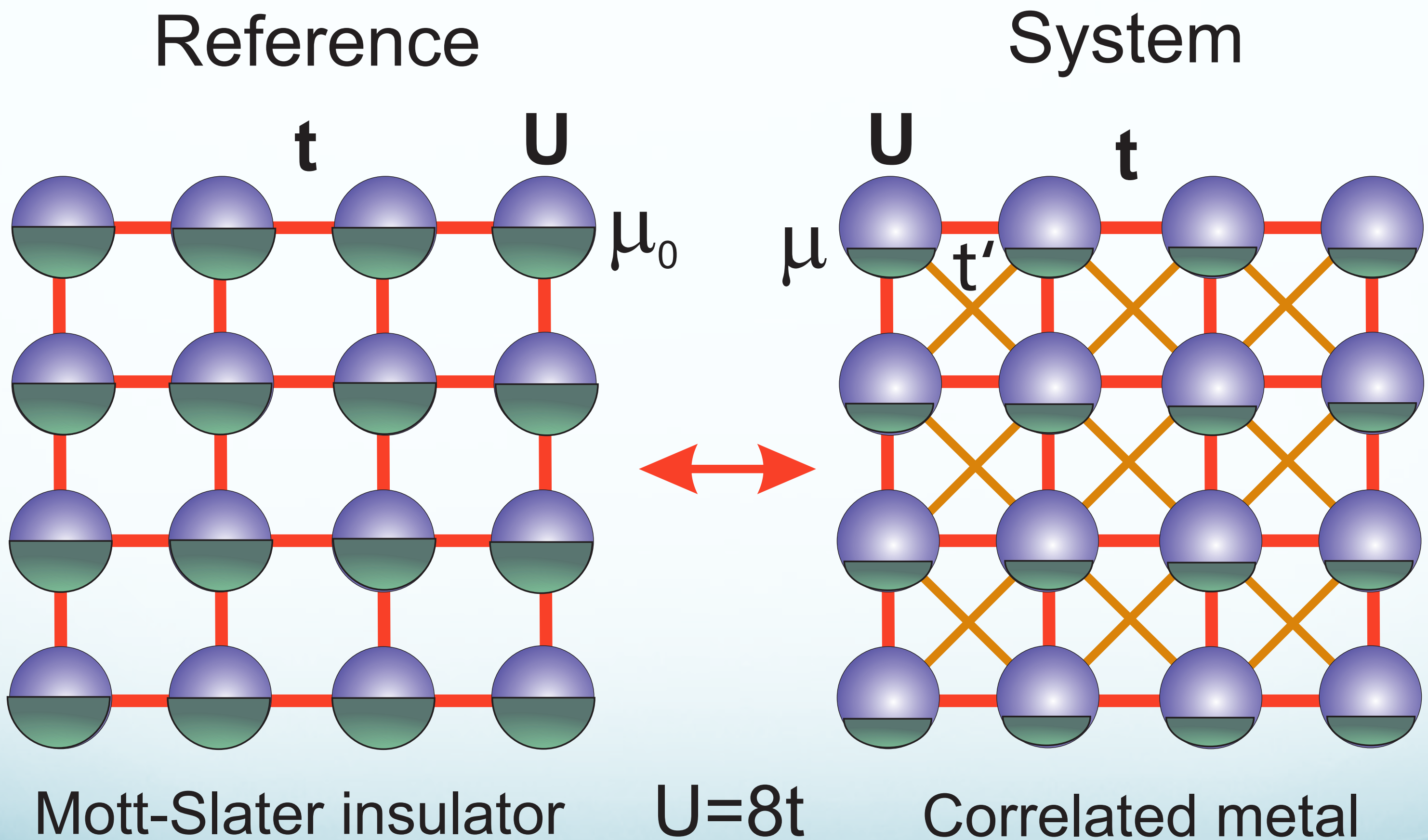
P. Werner, A. Comanac, L. de' Medici, M. Troyer, A. Millis
Phys. Rev. Lett. 97, 076405 (2006).

# Can we "shift $\mu$"?



# Super-perturbation: DF-QMC

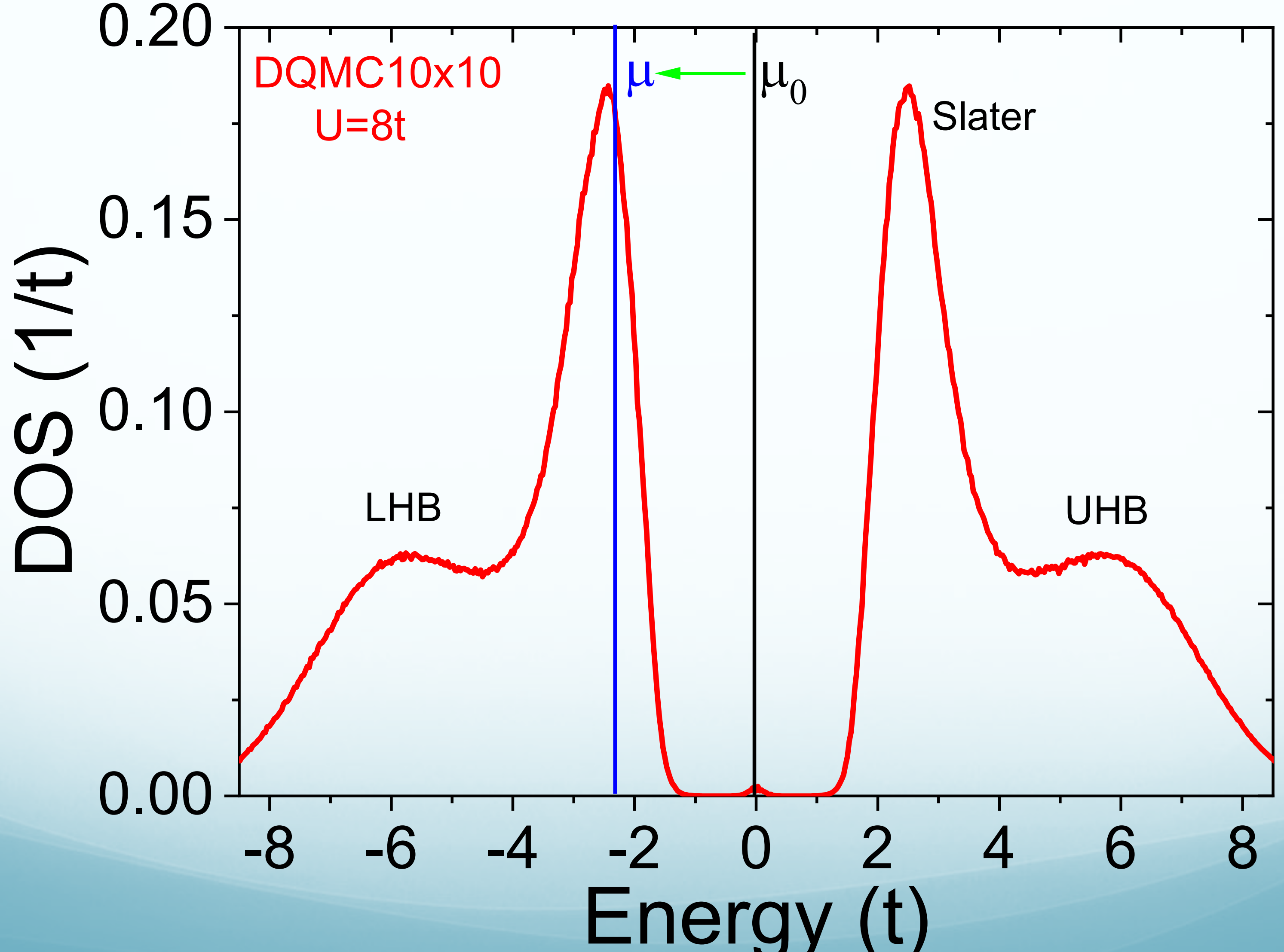
- Controllable perturbative solution of doped Hubbard model for HTSC
- Developed DF expansion around DQMC for N=1, t'=0



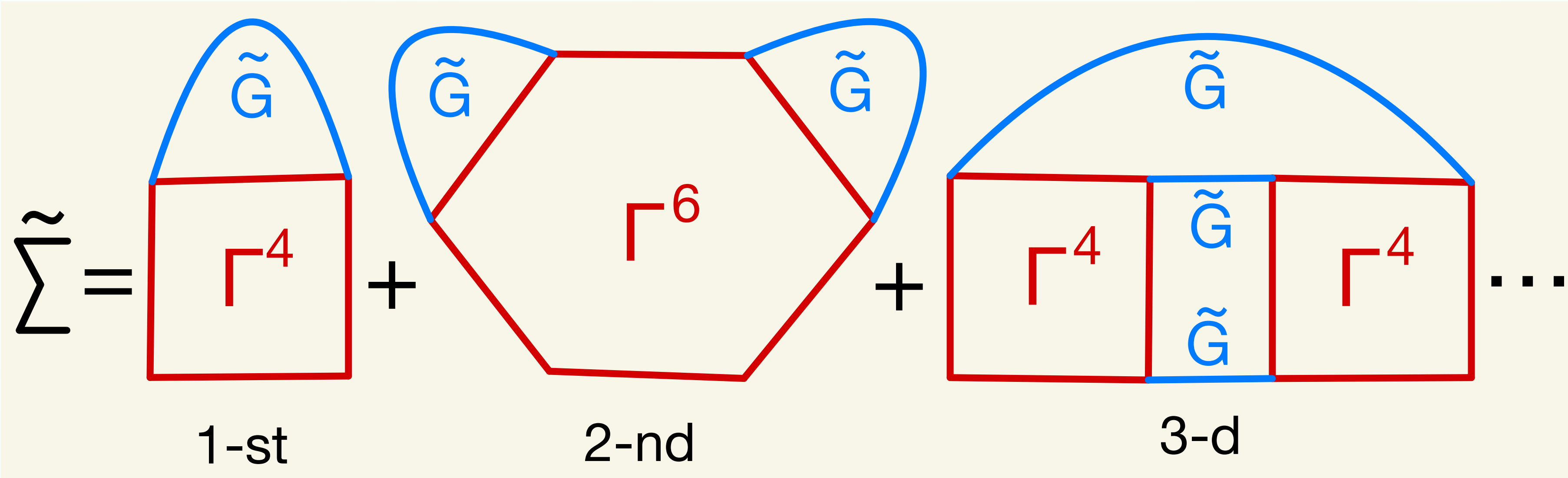

DQMC – no sign problem

DF QMC super-perturbation

# DOS for Reference System



# DF-exact diagrammatics




S. Brener, E. Stepanov, A. Rubtsov, M. Katsnelson, A.L., Ann. Phys. 422, 168310 (2020)

Similar "strong-coupling" cumulant expansion:

S.K. Sarker, JPC 21, L667 (1988)
S. Pairault et al, EPJ B16, 85 (1990)
W. Metzner, PRB 43, 8549 (1991)

# DF-QMC scheme: Real Space

Hamiltonian and Action

$$\hat{H}_\alpha = \sum_{i,j,\sigma} t^\alpha_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_i U(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})$$

$$t^\alpha_{ij} = \begin{cases} t & \text{if } i \text{ and } j \text{ are nearest neighbours,} \\ \alpha t' & \text{if } i \text{ and } j \text{ are next nearest neighbours,} \\ \alpha\mu & \text{if } i = j, \\ 0 & \text{otherwise,} \end{cases}$$

$$S_\alpha[c^*, c] = -\sum_{1,2} c^*_1 \, (\mathcal{G}_\alpha)^{-1}_{12} \, c_2 + \frac{1}{4} \sum_{1234} U_{1234} c^*_1 c^*_2 c_4 c_3$$

Perturbation: $\tilde{t} = \mathcal{G}_0^{-1} - \mathcal{G}_1^{-1}$

Dual Action:

$$\tilde{S}[d^*, d] = -\sum_{12\,\nu\sigma} d^*_{1\nu\sigma} \, (\tilde{G}^0_\nu)^{-1}_{12} \, d_{2\nu\sigma} + \frac{1}{4} \sum_{1234} \gamma_{1234} d^*_1 d^*_2 d_3 d_4 \; + \ldots$$

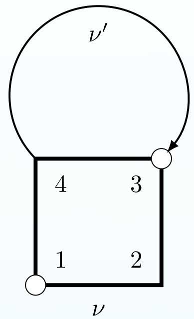
Dual GF: $\tilde{G}^0_{12} = \left[\, \tilde{t}^{-1} - \hat{g} \,\right]^{-1}_{12}$

g exact GF of $H_0$

Vertex:

$$\gamma_{1234} = \langle c_1 c^*_2 c_4 c^*_3 \rangle - \langle c_1 c^*_2 \rangle \langle c_4 c^*_3 \rangle + \langle c_1 c^*_3 \rangle \langle c_4 c^*_2 \rangle$$

1-st order diagram




DF-QMC: $$\tilde{\Sigma}^{(1)}_{12} = -\sum_{s-QMC} \sum_{3,4} \gamma^d_{1234}(s) \tilde{G}^0_{34}$$

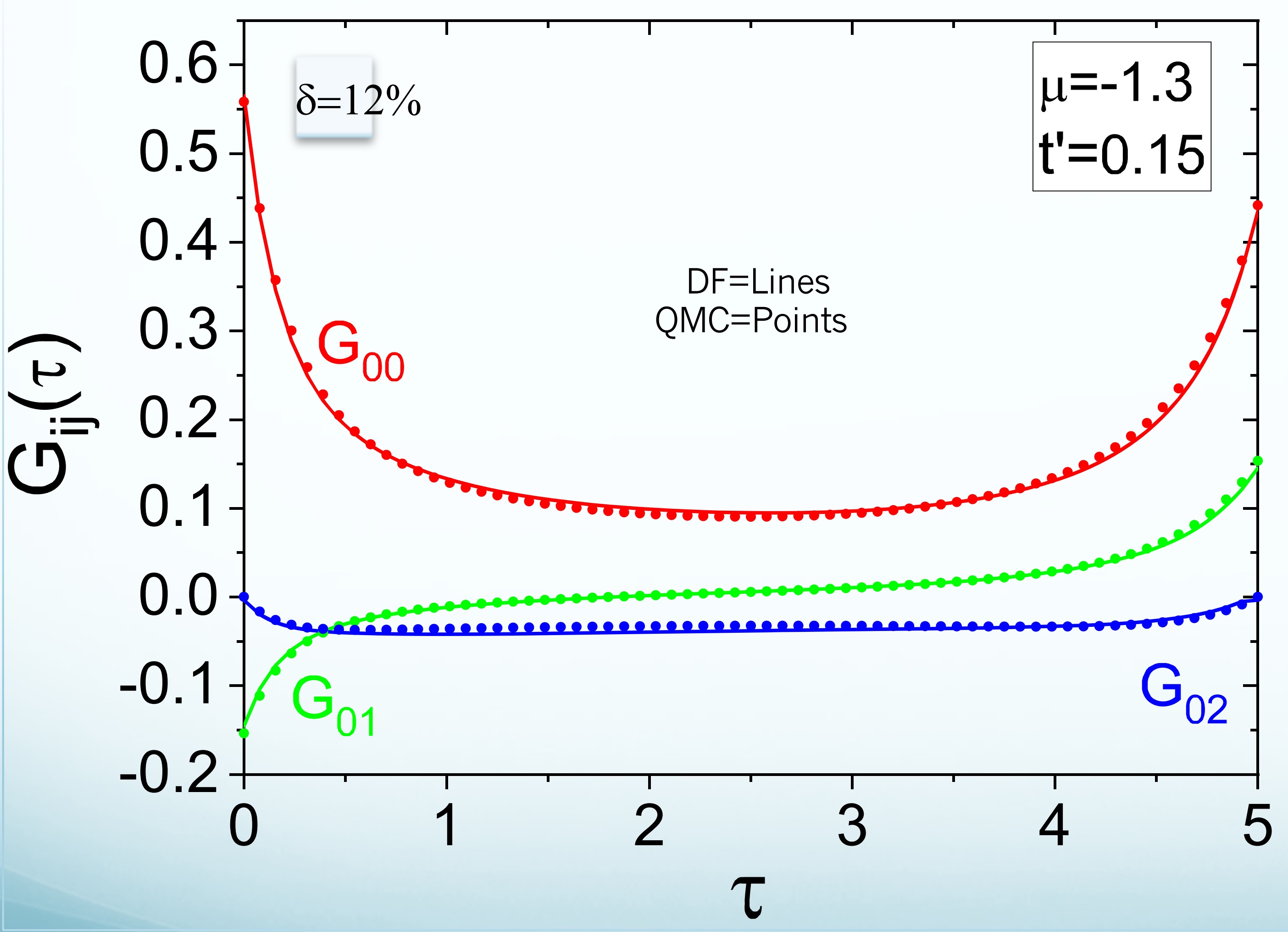
Final GF:

$$G_{12} = \left[ \left( g + \tilde{\Sigma} \right)^{-1} - \tilde{t} \right]^{-1}_{12}$$

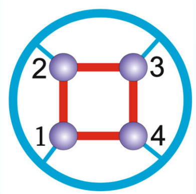
Inside QMC - Wick: $$\gamma_{1234}(s) \equiv \langle c_1 c^*_2 c_3 c^*_4 \rangle_s = \langle c_1 c^*_2 \rangle_s \langle c_3 c^*_4 \rangle_s - \langle c_1 c^*_4 \rangle_s \langle c_3 c^*_2 \rangle_s$$

Disconnected part - subtraction $\tilde{g}^s_{12} = g^s_{12} - g_{12}$

# Super-DF-QMC 2x2 compare with exact QMC




DF-perturbation
Hirsch-Fay DQMC




U=5.56

β=5

L=64

# DF-QMC scheme: K - Space

Action in Fourier-space

$k \equiv (\mathbf{k}, \nu_n)$ and $\nu_n = (2n+1)\pi/\beta$

$$\tilde{S}[d^*, d] = -\sum_{\mathbf{k}\,\nu\sigma} d^*_{\mathbf{k}\nu\sigma}\, \tilde{G}^{-1}_{0\mathbf{k}\nu}\, d_{\mathbf{k}\nu\sigma} + \frac{1}{4}\sum_{1234} \gamma_{1234} d^*_1 d^*_2 d_3 d_4$$

Bare dual GF: $\tilde{G}^0_k = \left(\tilde{t}_k^{-1} - \hat{g}_k\right)^{-1}$

First order diagram

$$\tilde{\Sigma}^{(1)}_k = \frac{-1}{(\beta N)^2 Z_{QMC}} \sum_{s-QMC} \sum_{k'} \left[\tilde{g}^{\uparrow\uparrow}_{kk} \tilde{g}^{\uparrow\uparrow}_{k'k'} - \tilde{g}^{\uparrow\uparrow}_{kk'} \tilde{g}^{\uparrow\uparrow}_{k'k} + \tilde{g}^{\uparrow\uparrow}_{kk} \tilde{g}^{\downarrow\downarrow}_{k'k'}\right]_s \tilde{G}^0_{k'}$$

Subtraction of disconnected part: $\tilde{g}^s_{kk'} = g^s_{kk'} - g_k \delta_{kk'}$

Lattice Green's function $G_k = \left[\left(g_k + \tilde{\Sigma}_k\right)^{-1} - \tilde{t}_k\right]^{-1}$

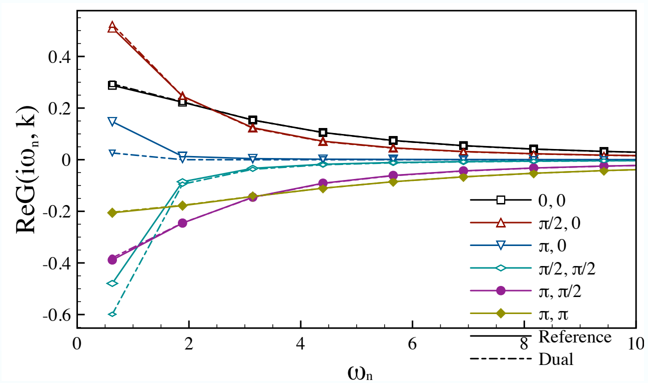
N.B.: $\tilde{\Sigma}_k = 0$ corresponds to CPT approximation

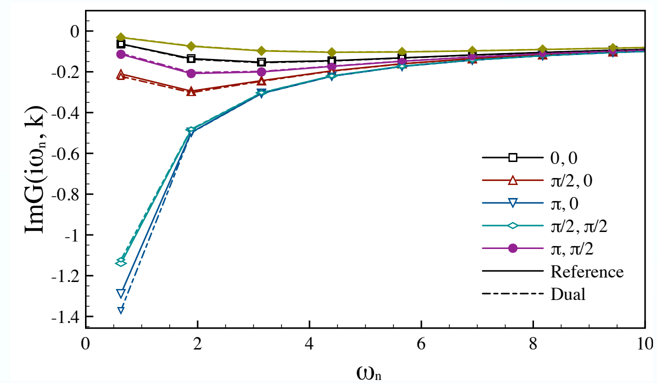
# K-space test 4x4 system DQMC & CT-INT

$\mu/t$=-0.5
t'/t=-0.1

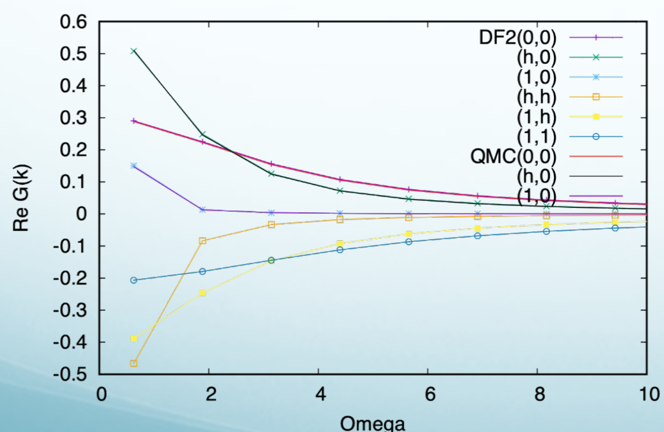
U/t=2
T/t=0.2

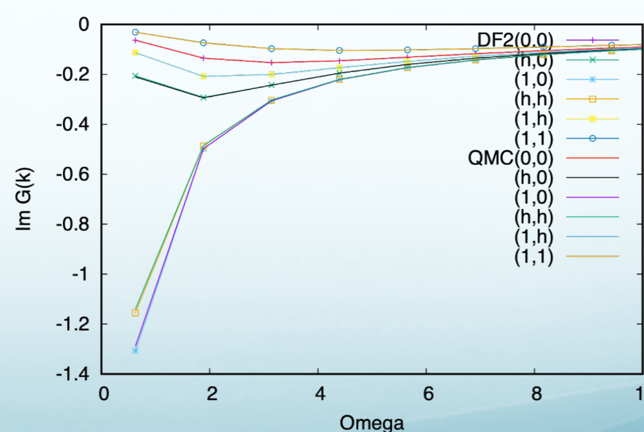
DF-1 order



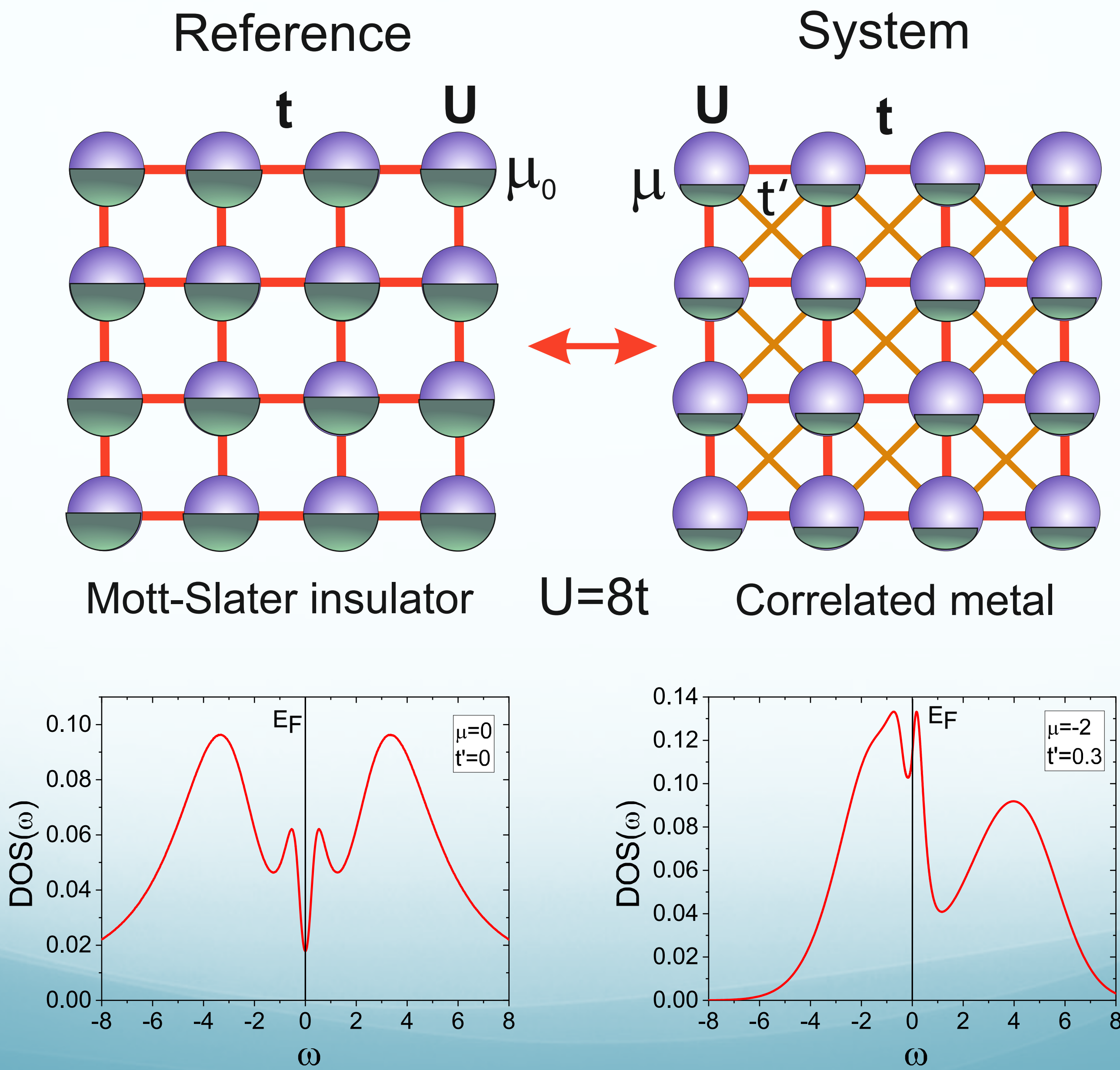




DF-2 order

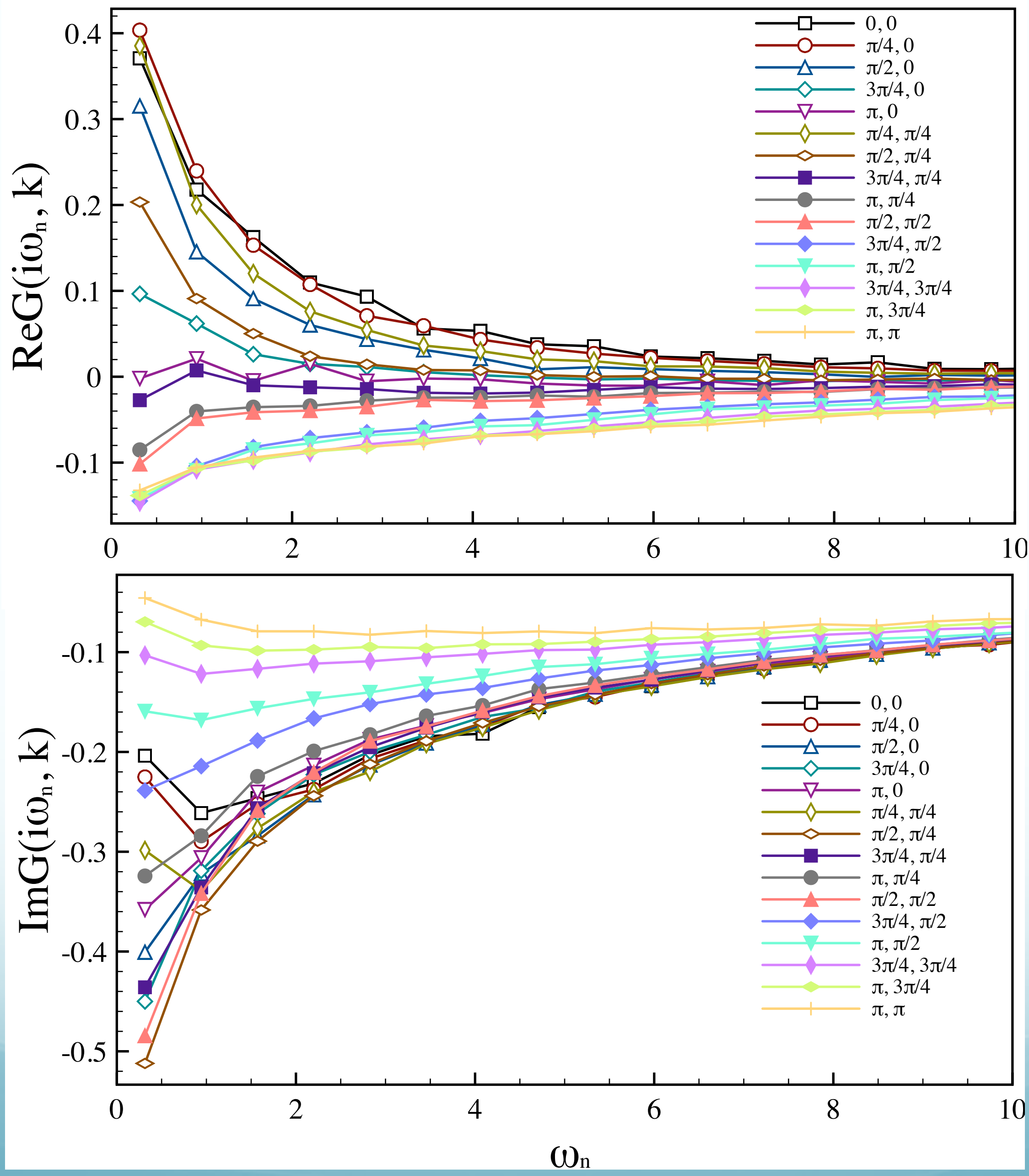


# DF-QMC 8x8 CT-INT



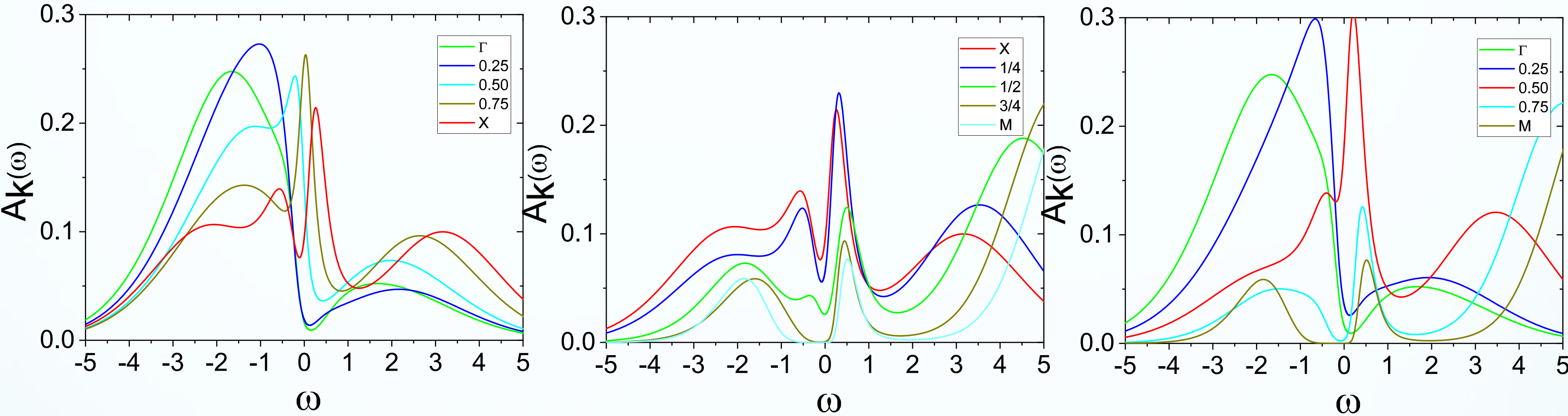
# Matsubara Green's Function

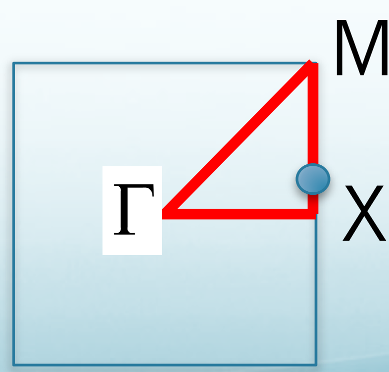



β=10
U=8
t'/t=-0.3
μ=-2
x=16%

CT-INT
Sergey
Iskakov

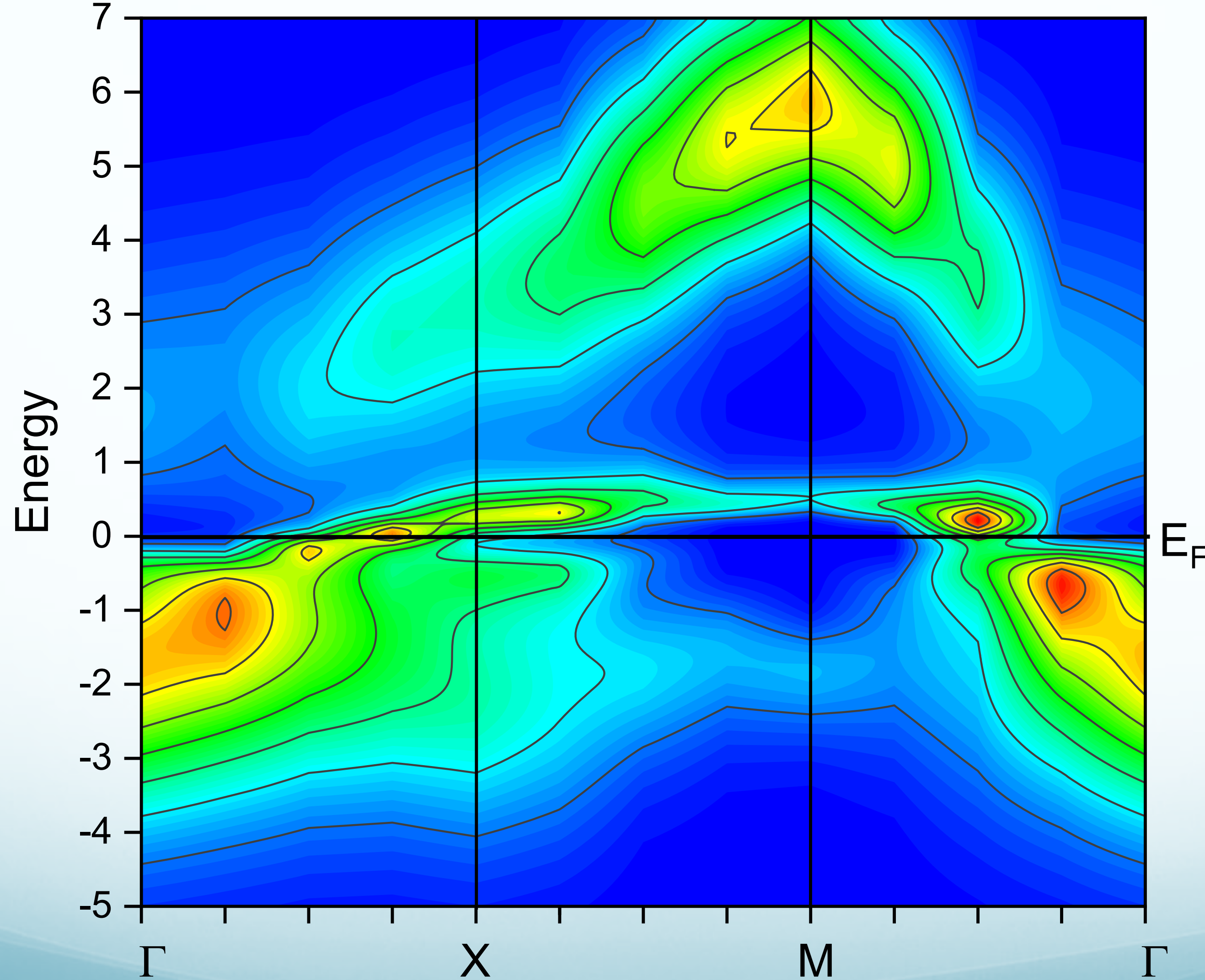
# Spectral Function




Strong PG
"shift" c.f.
F. Šimkovic, R. Rossi,
A. Georges, M. Ferrero,
arXiv:2209.09237

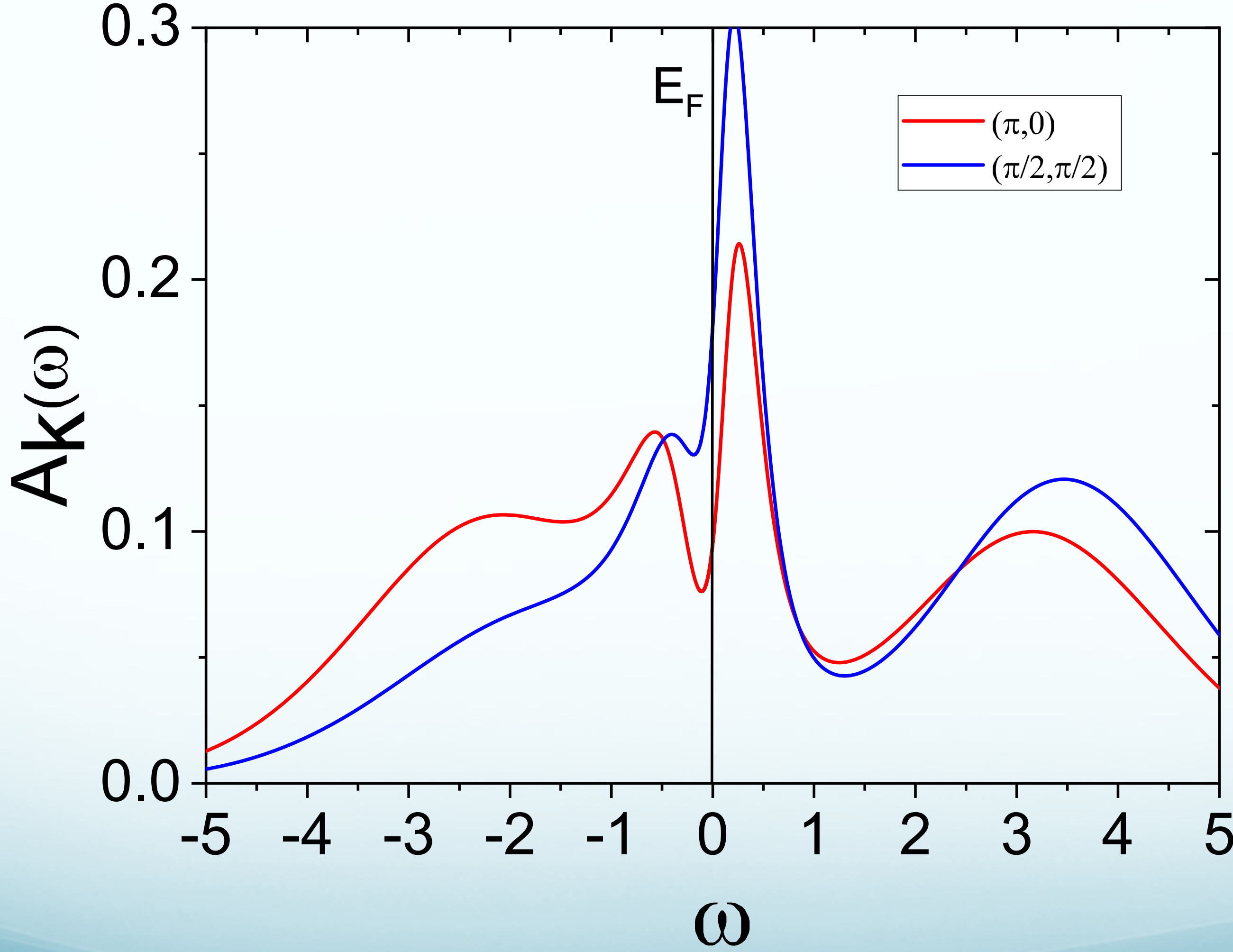
# DF-QMC for 8x8: Spectral Function




T=t/10
t'/t=-0.3
U=8
β=10
μ=-2
x=167%

S. Iskakov, et al, npj Computational Materials 10, 36 (2024)

# Nodal-Antinodal dichotomy



# Superconductivity: D-wave instability

Perturbation action with external symmetry breaking fields $\Delta_k = h_{dw}(\cos k_x - \cos k_y)$

$$\Delta S = \sum_{\mathbf{k},\nu,\sigma} c^*_{\mathbf{k},\nu,\sigma} \tilde{t}_{\mathbf{k},\nu} c_{\mathbf{k},\nu,\sigma} + \sum_{\mathbf{k},\nu} \Delta_{\mathbf{k}} \left( c^*_{\mathbf{k},\nu,\uparrow} c^*_{-\mathbf{k},-\nu,\downarrow} - c_{-\mathbf{k},-\nu,\uparrow} c_{\mathbf{k},\nu,\downarrow} \right)$$

Bare Dual Green's Function – Spinor From

$$\tilde{\mathcal{G}}_\nu = \left[ \begin{pmatrix} \tilde{t}_{\mathbf{k},\nu} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}} & -\tilde{t}_{-\mathbf{k},-\nu} \end{pmatrix}^{-1} - \begin{pmatrix} g^{\uparrow}_{\mathbf{k},\nu} & 0 \\ 0 & -g^{\downarrow}_{-\mathbf{k},-\nu} \end{pmatrix} \right]^{-1}$$

Dual Self-energy – Spinor From

$$\tilde{\Sigma}^{\uparrow\uparrow}_k = \frac{-1}{Z} \sum_{QMC} \sum_{k'} \left[ \left( \tilde{g}^{\uparrow}_{kk} \tilde{g}^{\uparrow}_{k'k'} - \tilde{g}^{\uparrow}_{kk'} \tilde{g}^{\uparrow}_{k'k} \right) \tilde{G}^{\uparrow\uparrow}_{k'} + \tilde{g}^{\uparrow}_{kk} \tilde{g}^{\downarrow}_{k'k'} \tilde{G}^{\downarrow\downarrow}_{k'} \right]$$

$$\tilde{\Sigma}^{\uparrow\downarrow}_k = \frac{1}{Z} \sum_{QMC} \sum_{k'} \tilde{g}^{\uparrow}_{kk'} \tilde{g}^{\downarrow}_{k'k} \tilde{G}^{\uparrow\downarrow}_{k'}$$

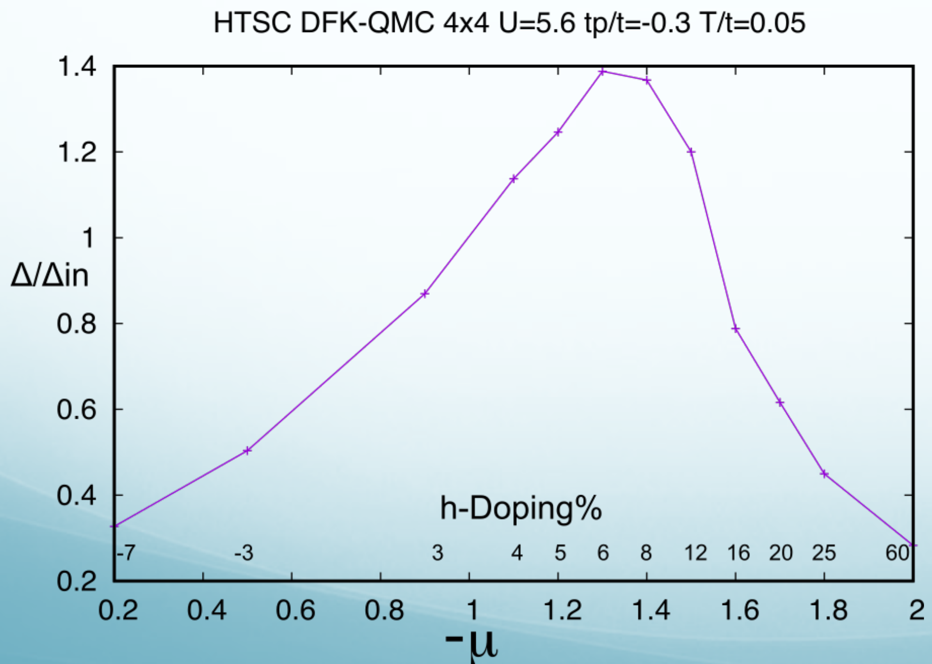
$$\tilde{\Sigma}^{\downarrow\downarrow}_k = \frac{-1}{Z} \sum_{QMC} \sum_{k'} \left[ \left( \tilde{g}^{\downarrow}_{kk} \tilde{g}^{\downarrow}_{k'k'} - \tilde{g}^{\downarrow}_{kk'} \tilde{g}^{\downarrow}_{k'k} \right) \tilde{G}^{\downarrow\downarrow}_{k'} + \tilde{g}^{\downarrow}_{kk} \tilde{g}^{\uparrow}_{k'k'} \tilde{G}^{\uparrow\uparrow}_{k'} \right]$$

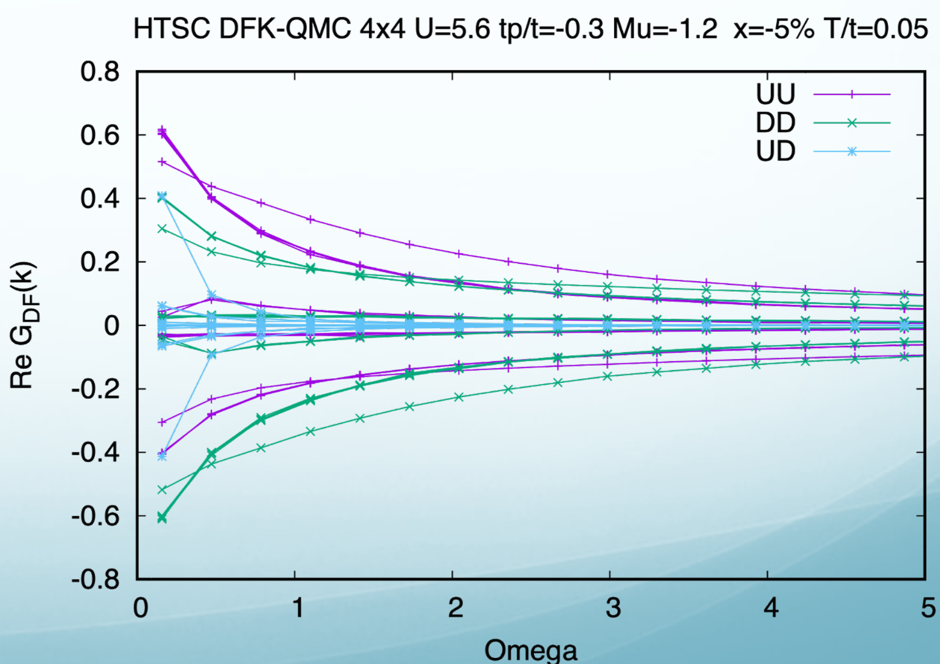
$$\tilde{\Sigma}^{\downarrow\uparrow}_k = \frac{1}{Z} \sum_{QMC} \sum_{k'} \tilde{g}^{\downarrow}_{kk'} \tilde{g}^{\uparrow}_{k'k} \tilde{G}^{\downarrow\uparrow}_{k'}$$

# Superconductivity: D-wave instability

Lattice Green's Function: Spinor Form:

$$G_k = \left[ \begin{pmatrix} g_k + \tilde{\Sigma}_k^{\uparrow\uparrow} & \tilde{\Sigma}_k^{\uparrow\downarrow} \\ \tilde{\Sigma}_k^{\downarrow\uparrow} & -g_k^* + \tilde{\Sigma}_k^{\downarrow\downarrow} \end{pmatrix}^{-1} - \begin{pmatrix} \tilde{t}_k & 0 \\ 0 & -\tilde{t}_k^* \end{pmatrix} \right]^{-1}$$

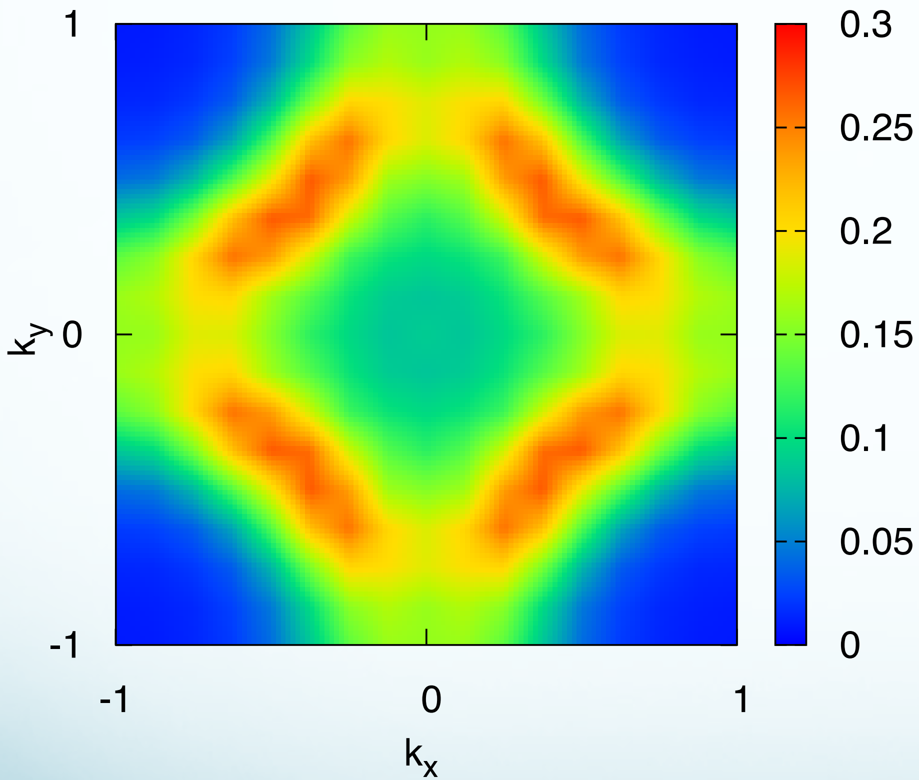


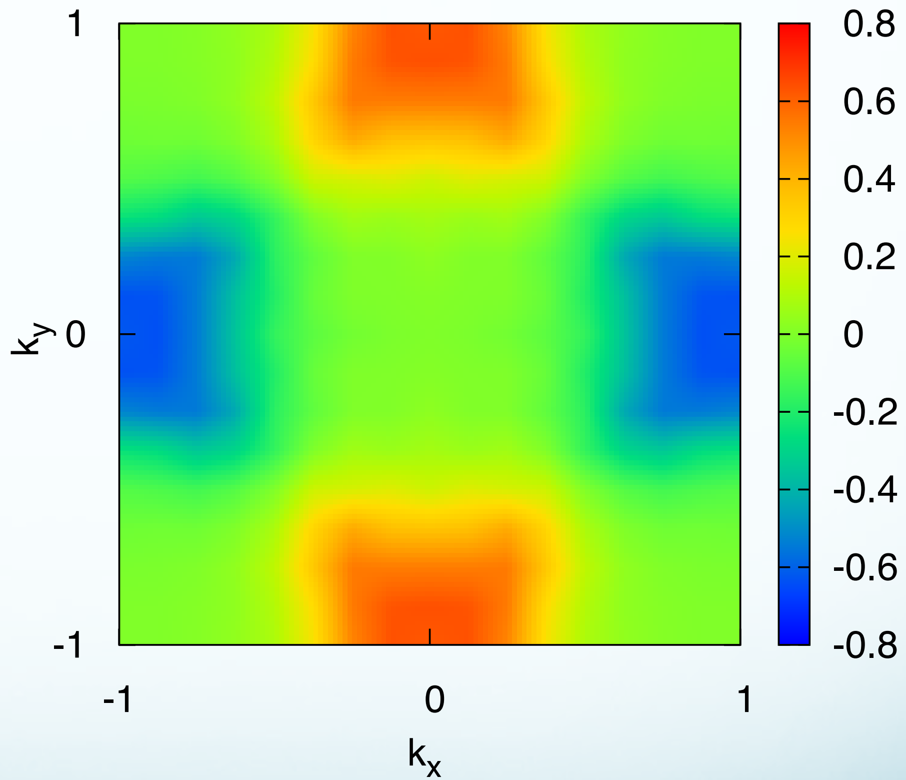



# Fermi Surface and d-waves: Superconductivity of the "bad" electrons

Normal: $A(k)=-1/\pi\, G(k,\omega_0)$

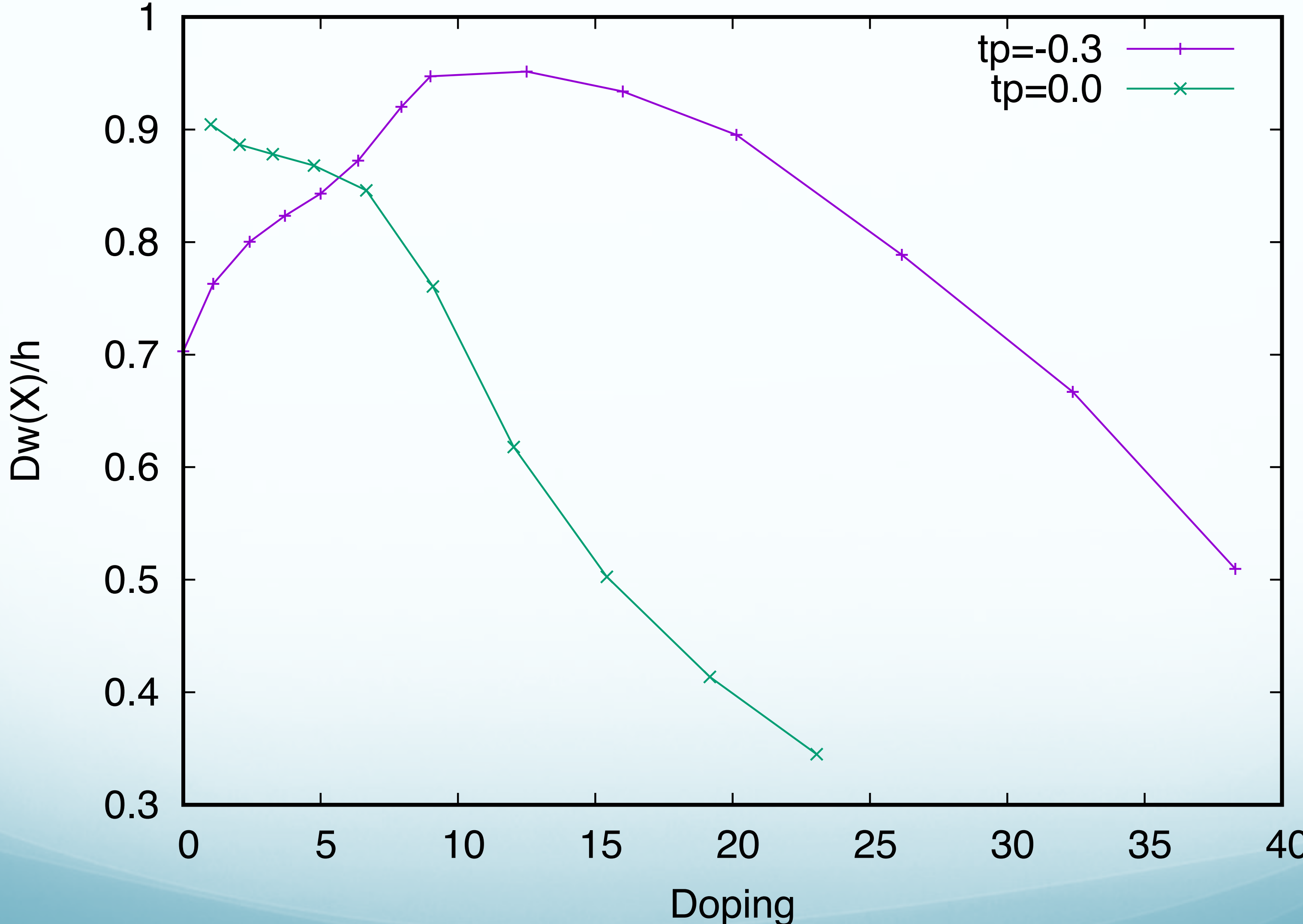
Anomalous: $F\,(k,\omega_0)$



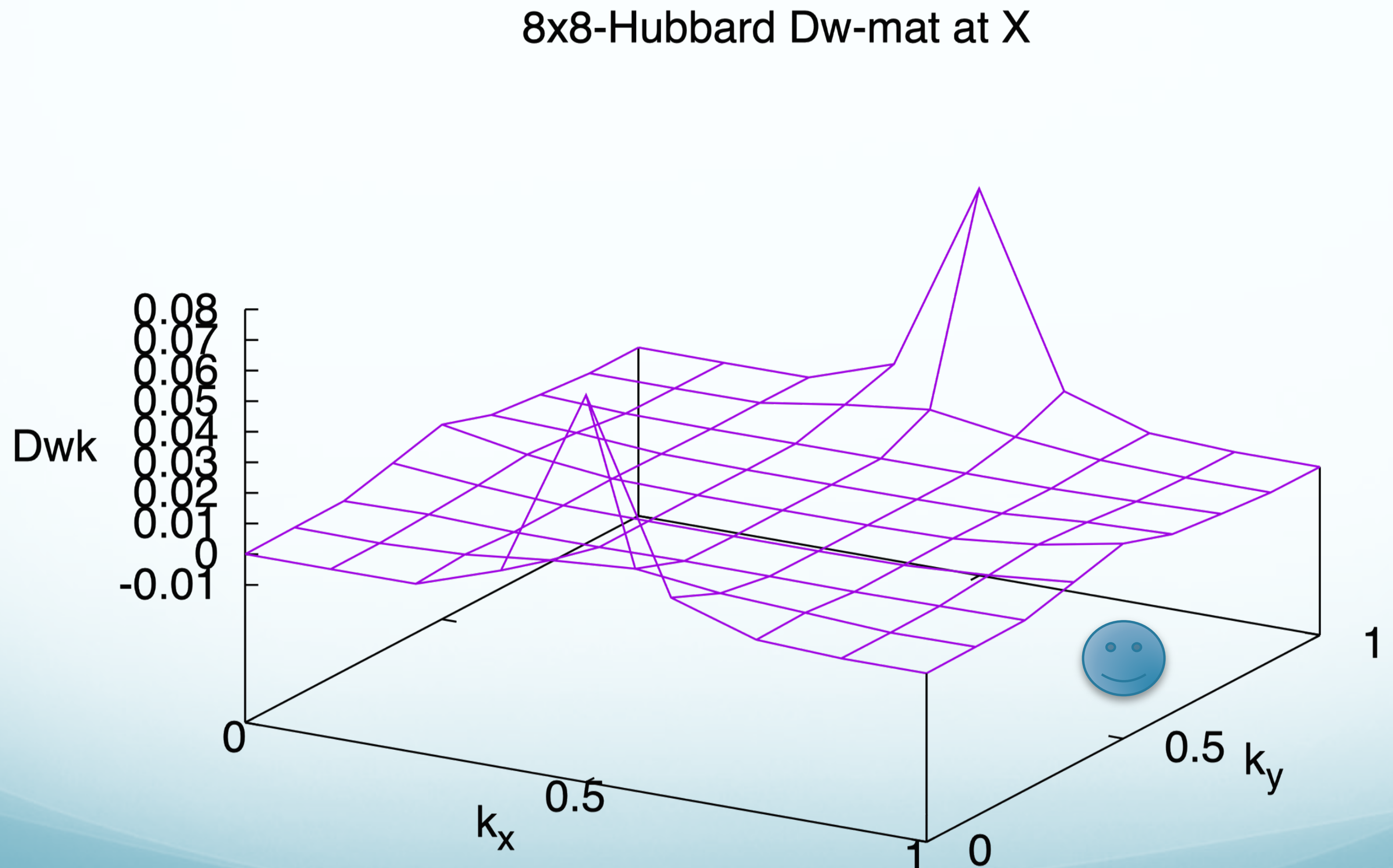




16x16 lattice U=5.6 t'/t=-0.3 T=0.2t

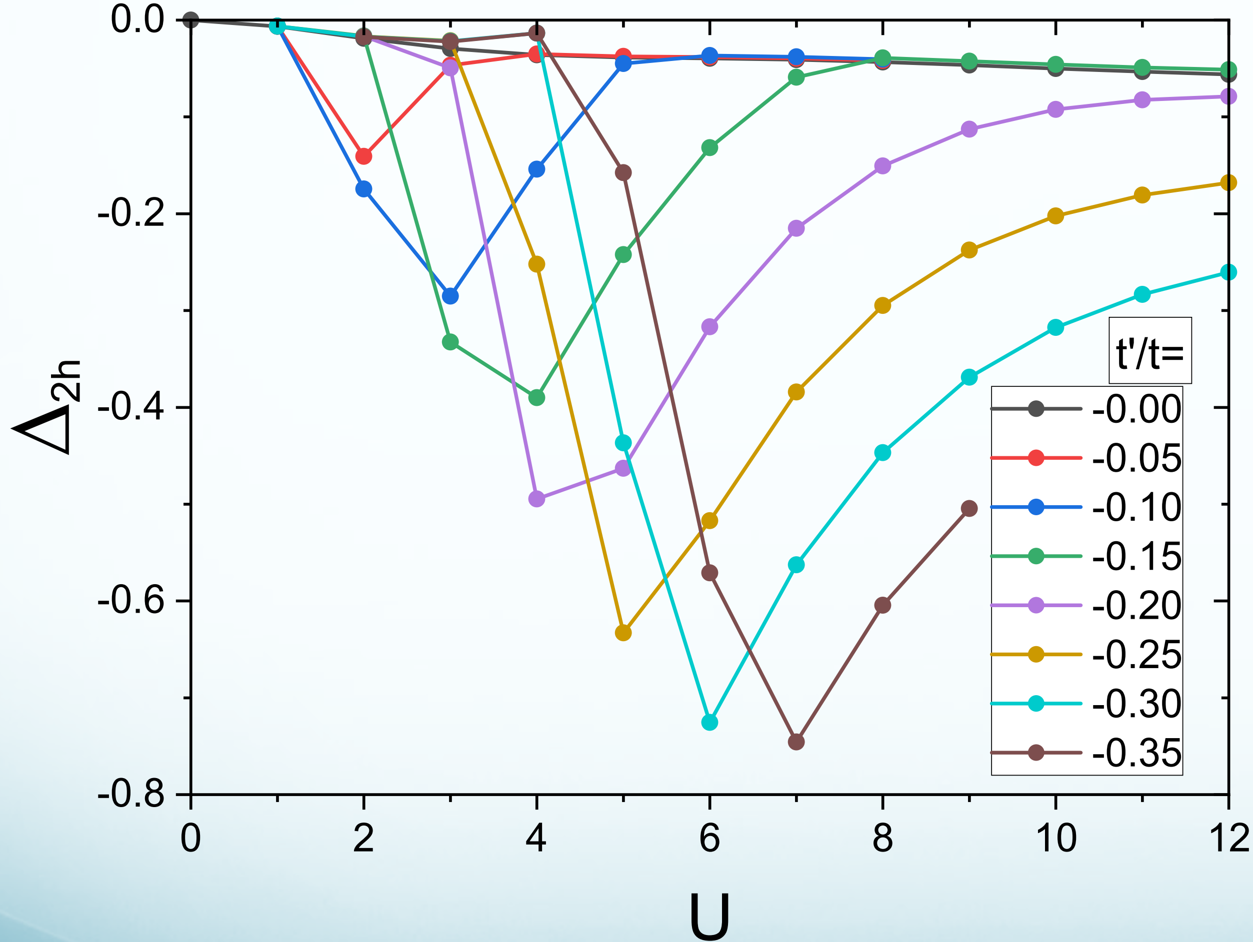
# Effect of t'



# Effect of eVH



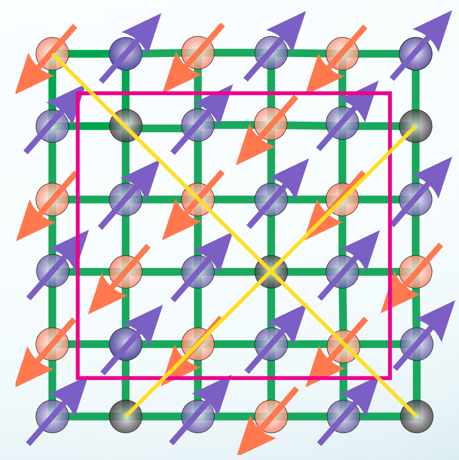
# ED 4x4 cluster: Local Pairs




$$\Delta_{2h} = \tilde{E}_{2h} - 2\tilde{E}_{1h}$$

$$\tilde{E}_{Nh} = E_{Nh} - E_0$$

$\Delta_{2h}$=0.7t=3000 K

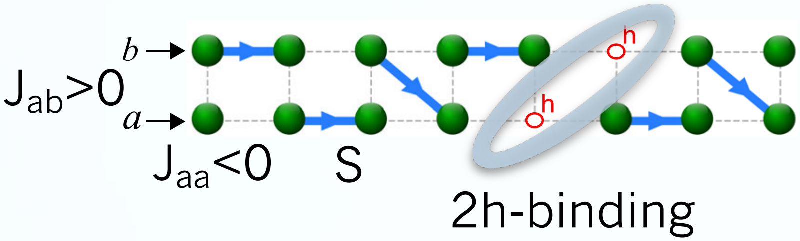


M. Danilov, E.G.C.P. van Loon, S. Brener, S. Iskakov, M. Katsnelson, and A.L.
npj Quantum Materials **7,** 50 (2022)

# Strong Coupling HTSC: RVB

Interlayer Tunneling $T_c = \frac{T_J}{64}\left(1 + \frac{2t - \varepsilon_F}{4t' + 2t}\right)^4$

P.W. Anderson, Science 258, 1154 (1995)
261, 337 (1993)

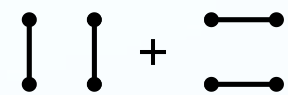


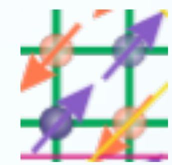

Elbio Dagotto NPJ-QM 5, 27 (2020)

2 Hole in Plaquette = D-Wave!

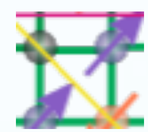
E. Altman, A. Auerbach, PRB 65, 104508 (2002)

$$|\Omega\rangle = \frac{\mathcal{P}}{\sqrt{Z_\Omega}}\left(c^\dagger_{(\pi,0)\uparrow}c^\dagger_{(\pi,0)\downarrow} - c^\dagger_{(0,\pi)\uparrow}c^\dagger_{(0,\pi)\downarrow}\right)c^\dagger_{(0,0)\uparrow}c^\dagger_{(0,0)\downarrow}|0\rangle \approx$$



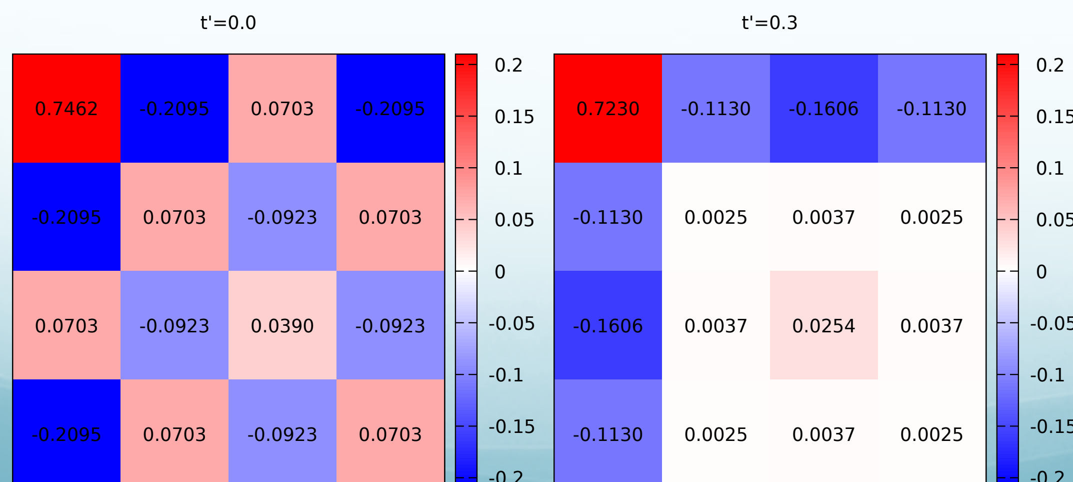


$$b^\dagger_\alpha|\Omega\rangle = \frac{1}{\sqrt{Z_b}}\mathcal{P}c^\dagger_{(0,0)\uparrow}c^\dagger_{(0,0)\downarrow}|0\rangle = \frac{1}{\sqrt{Z'_b}}\left(\sum_{ij} d_{ij}c_{i\uparrow}c_{j\downarrow} + \ldots\right)|\Omega\rangle$$



$d_{ij}$ is +1 (-1) on vertical (horizontal) bonds

AFM




ED 4x4 strong effect of t' on spin-spin correlations

FM-stripes

2holes: Sector $(7\uparrow, 7\downarrow)$

# Conclusions

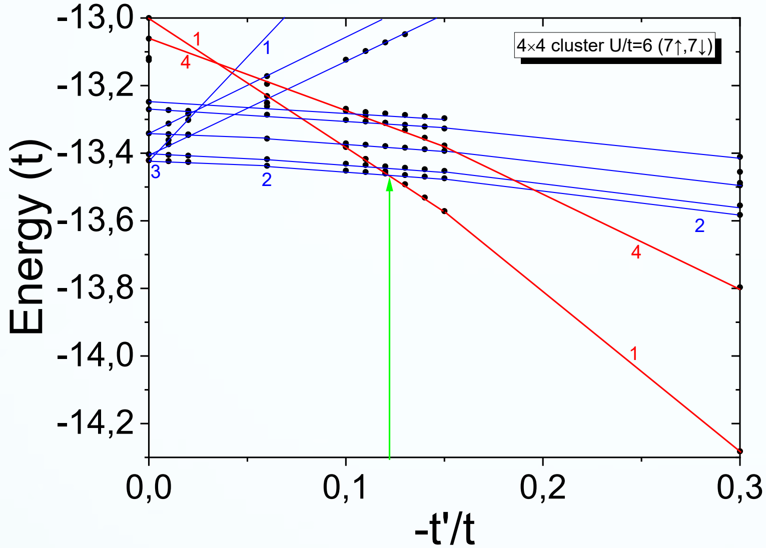
- DF-diagrammatic can be combined with Lattice DQMC to describe doped strongly correlated systems
- Importance of $t'$ for response on $d_{x^2-y^2}$ fields and $\mu$ dependence shows HTSC-physics

Collaborations with:

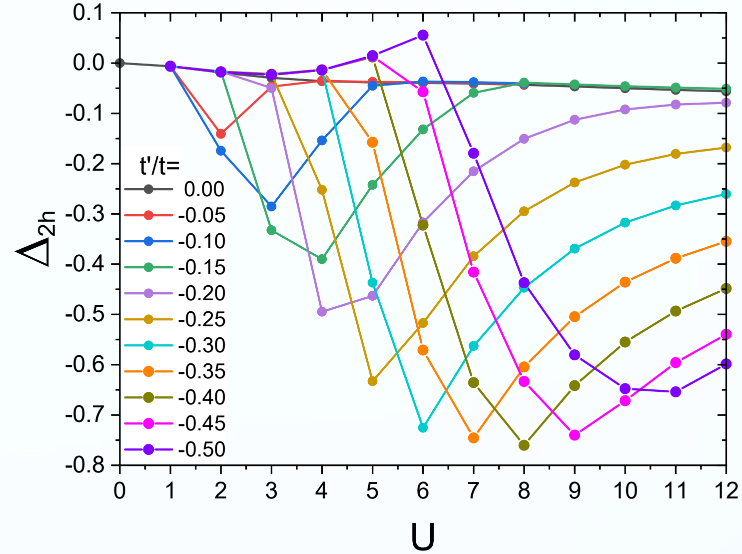
Sergei Iskakov (Michigan)
Evgeny Stepanov (Paris)
Mikhail Katsnelson (Nijmegen)

# Effects of t’ on 4x4 cluster

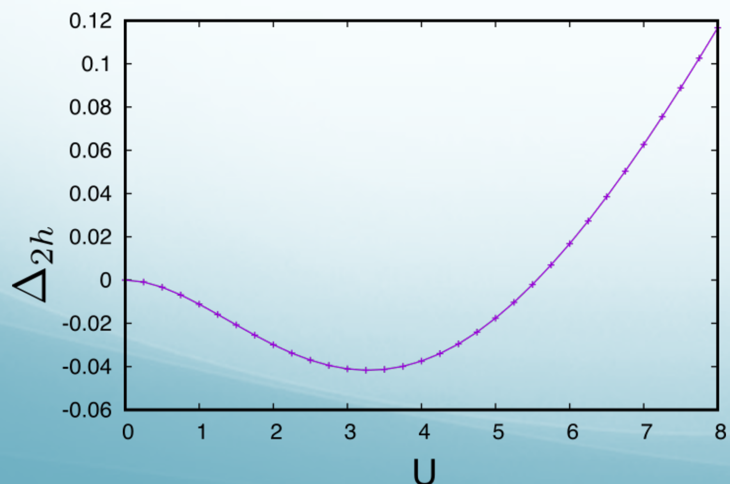
## Ground State crossing



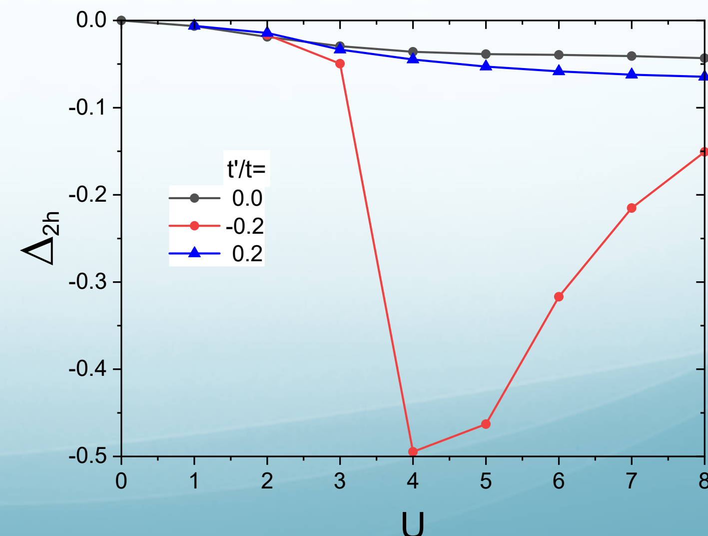

## Large pair-binding for negative t‘/t



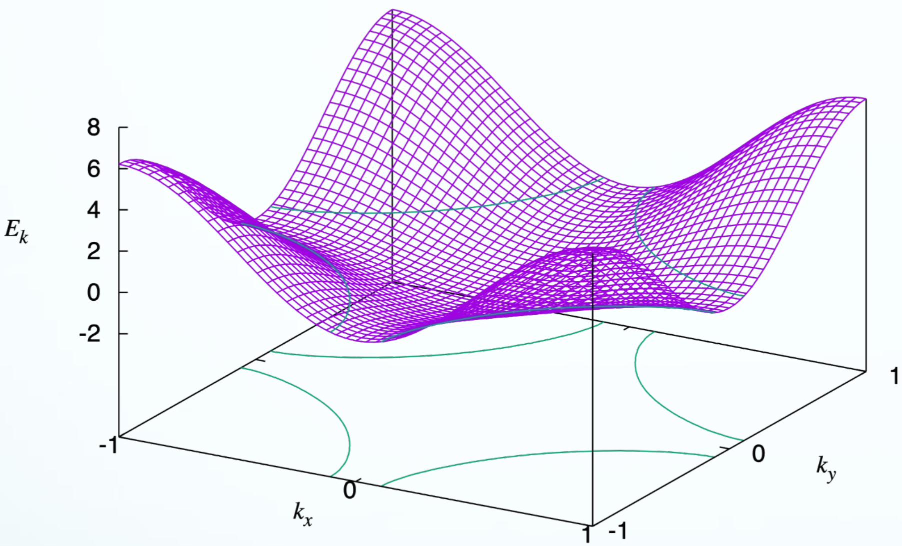

## Small pair-binding for 2x2 cluster

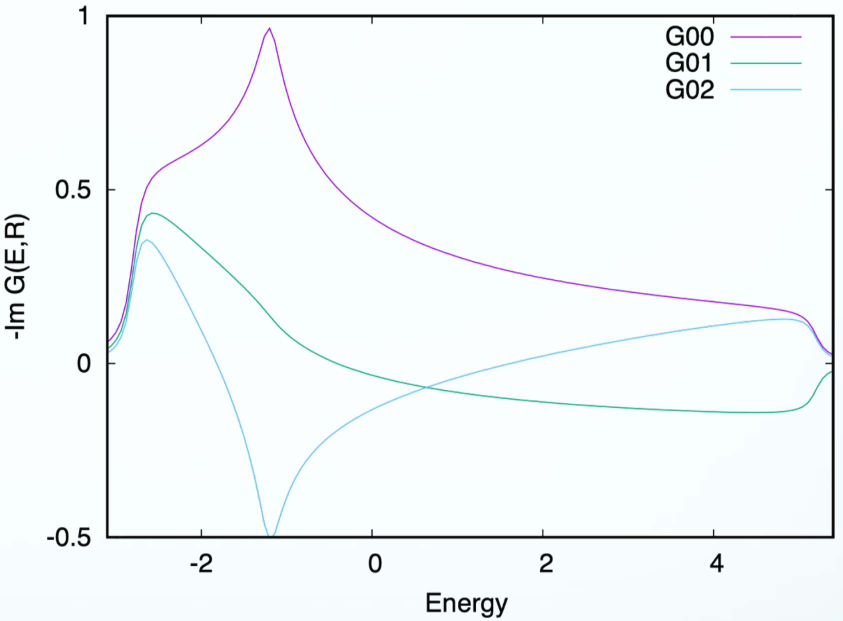



## Small pair-binding for positive t‘/t



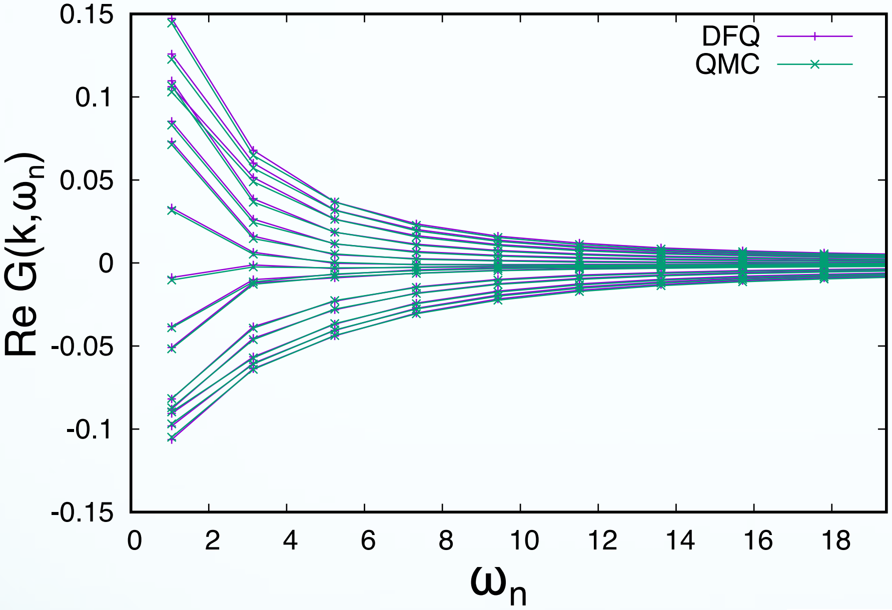
# TB-Model: HTSC

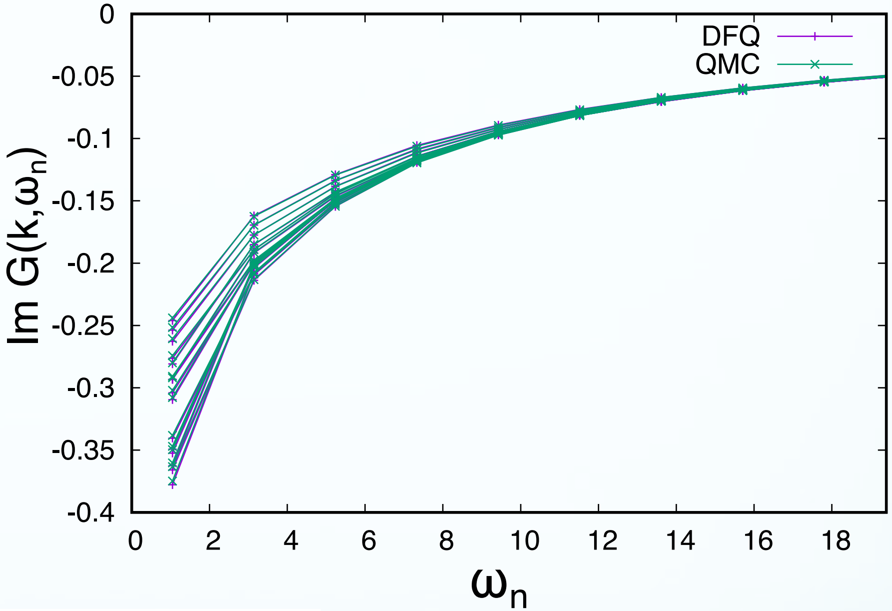



From DFT-calculations: t'/t=-0.3

# 8x8 test DF-QMC vs. DQMC

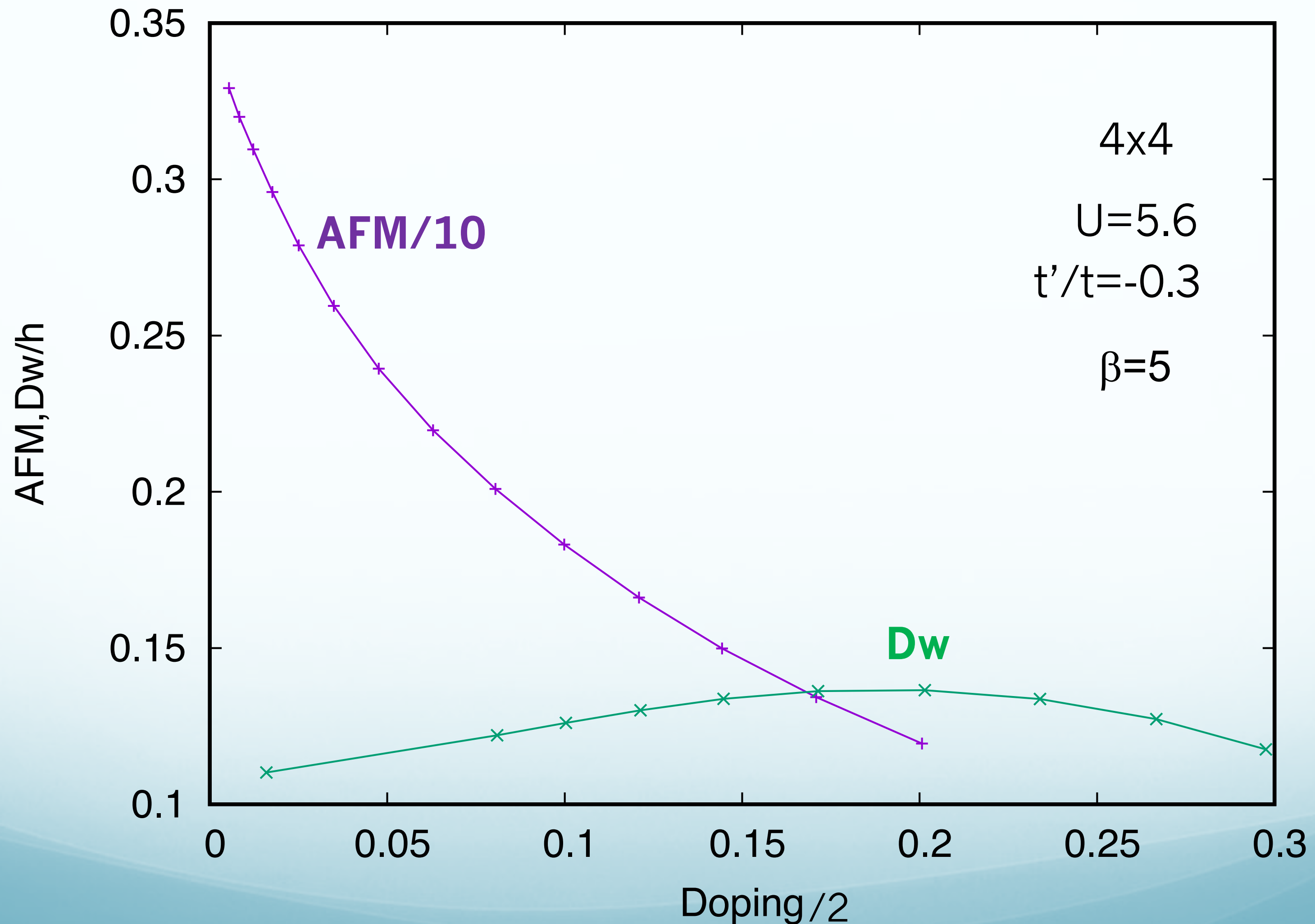



$\beta$=3
U=5.56
t'/t=-0.15
$\mu$=-0.5

Hirsch-Fye DQMC

# AFM vs. Dw



0.35
0.3
0.25
0.2
0.15
0.1
AFM,Dw/h
0
0.05
0.1
0.15
0.2
0.25
0.3
Doping/2
AFM/10
Dw
4x4
U=5.6
t'/t=-0.3
β=5

# From DFT to var-QMC

M. Schmid,...,M. Imada, Phys. Rev. X 13, 041036 (2023)