SUPER-QMC: STRONG COUPLING PERTURBATION FOR LATTICE MODEL

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In collaboration with
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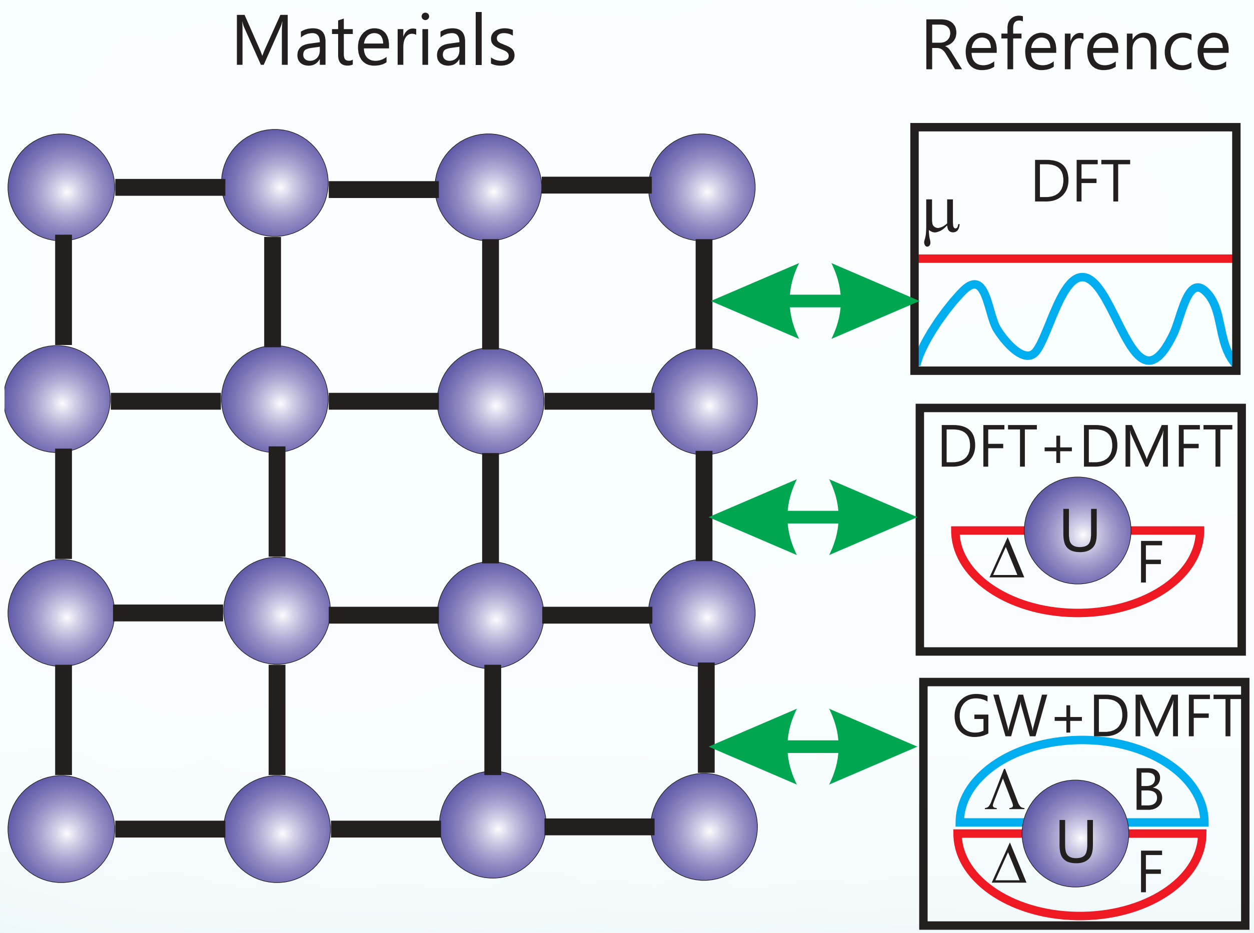
Outline

- Idea of Reference System
- Numerically Exact Lattice QMC
- DF-QMC Method

Reference Systems

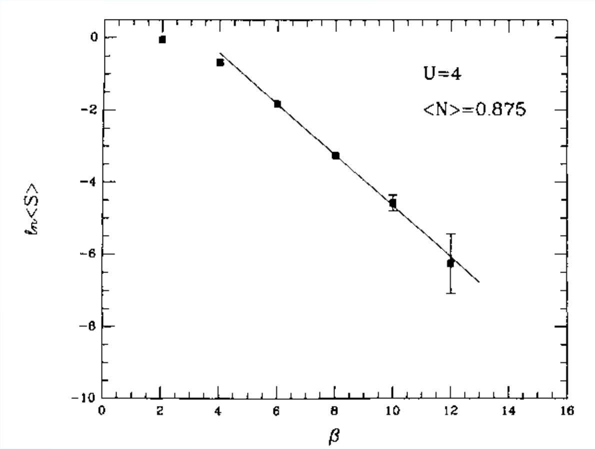


Many-Body: Peierls-Feynman-Bogoliubov variational principle:

$$F_1 \leq F_0 + \langle H_1 - H_0 \rangle_0$$

Fermionic QMC: sign problem vs. sign blessing

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

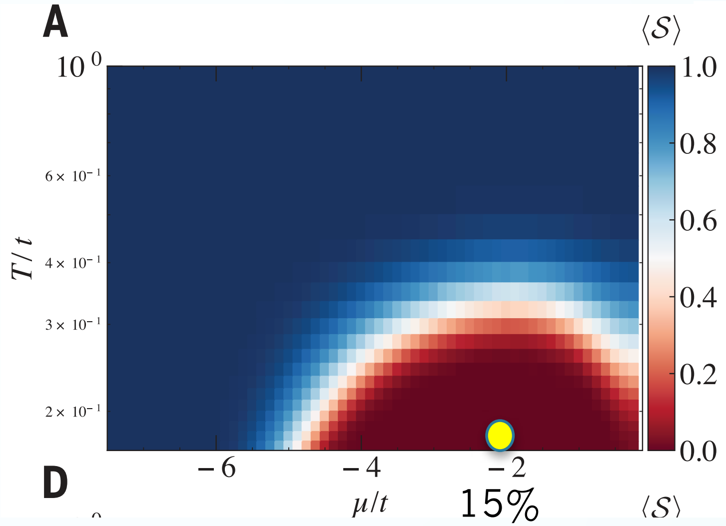


QMC „probability“ $\lessgtr$ 0

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

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

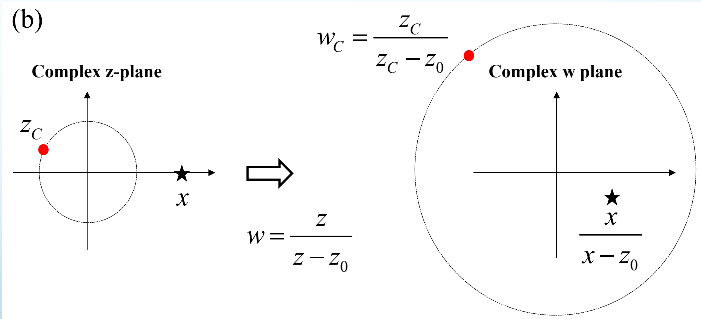
Sign is physical and related with QCP



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

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

Blessing: DiagMC and Cdet
Cancellation of high-order Feynman diagram
10-12 order is "converged" with "shifted-action" and conformal mapping

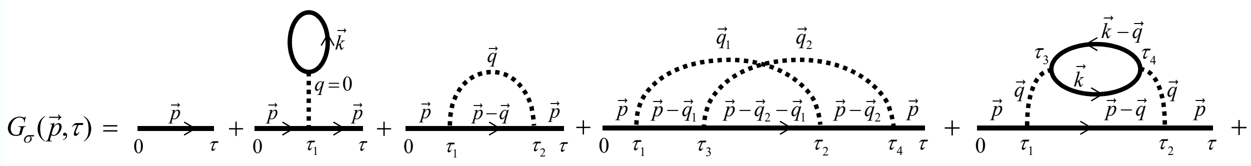


N. Prokof'ev "DiagMC" Jülich school 2019

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) for bosonic system

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

CT-QMC: CT-INT (”det G_0”) sign problem

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

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

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

Strong: U>>t complicated perturbation diagram –’diverge’

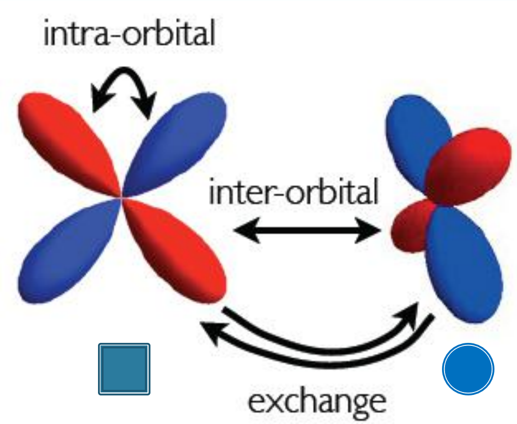
CT-QMC: CT-HYB (”det Δ”) – small system <6 and sign problem

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

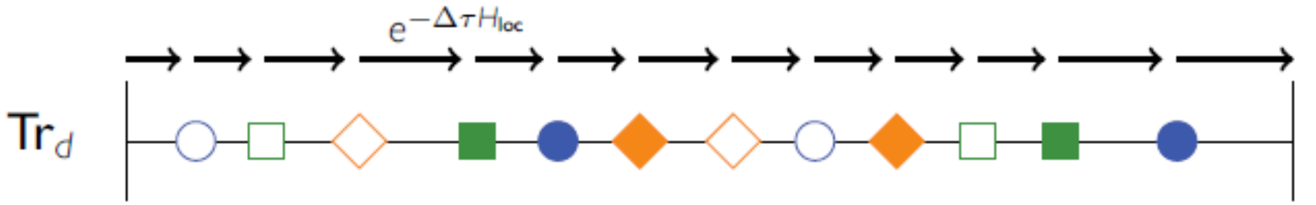
Multi-orbital impurity with general U

General Interaction:

$$U = \frac{1}{2} \sum_{\substack{ijkl \\ \sigma\sigma'}} \left\langle ij \left| \frac{1}{r_{12}} \right| kl \right\rangle d^{+}_{i\sigma} d^{+}_{j\sigma'} d_{l\sigma'} d_{k\sigma}$$



CT-HYB-QMC



$$\mathrm{Tr}_d\,[\ldots] = \mathrm{Tr}\left[e^{-(\beta-\tau_k)H_{loc}} O_k(\tau_k) e^{-(\tau_k-\tau_{k-1})H_{loc}} \ldots O_1(\tau_1) e^{-\tau_1 H_{loc}}\right]$$

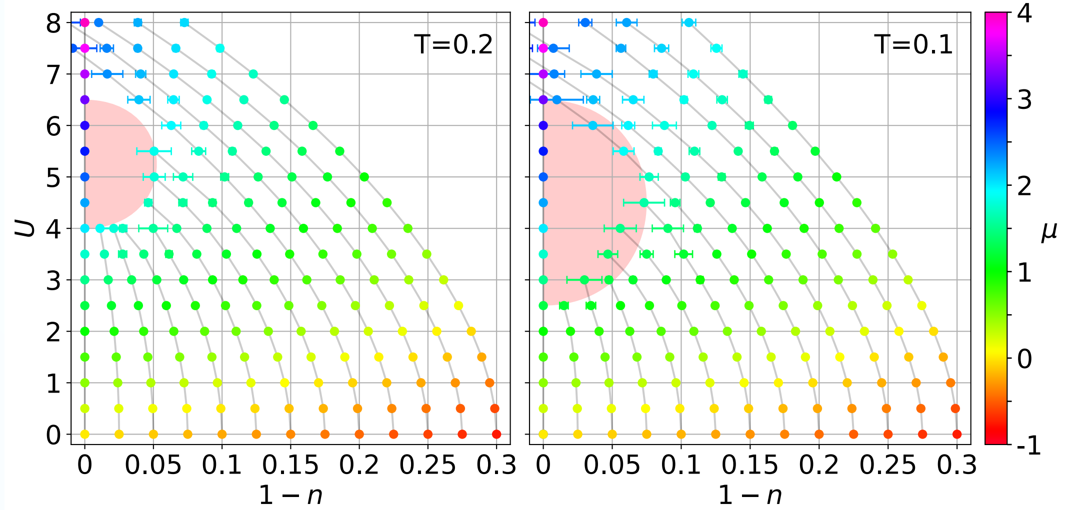
$$Z_{\mathrm{AIM}} = Z_{\mathrm{bath}} \sum_k \int d\tau_1 \cdots d\tau_k' \,\mathrm{Tr_d}\,[\ldots] \det \mathbf{\Delta}$$

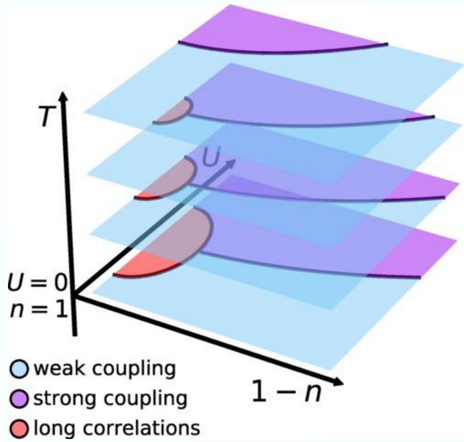
General multi-orbital system: strong sign-problem

E. Gull, A. Millis, A.L., A. Rubtsov, M. Troyer, Ph. Werner, Rev. Mod. Phys. **83**, 349 (2011)

Diag-MC CDet: State-of-the-Art

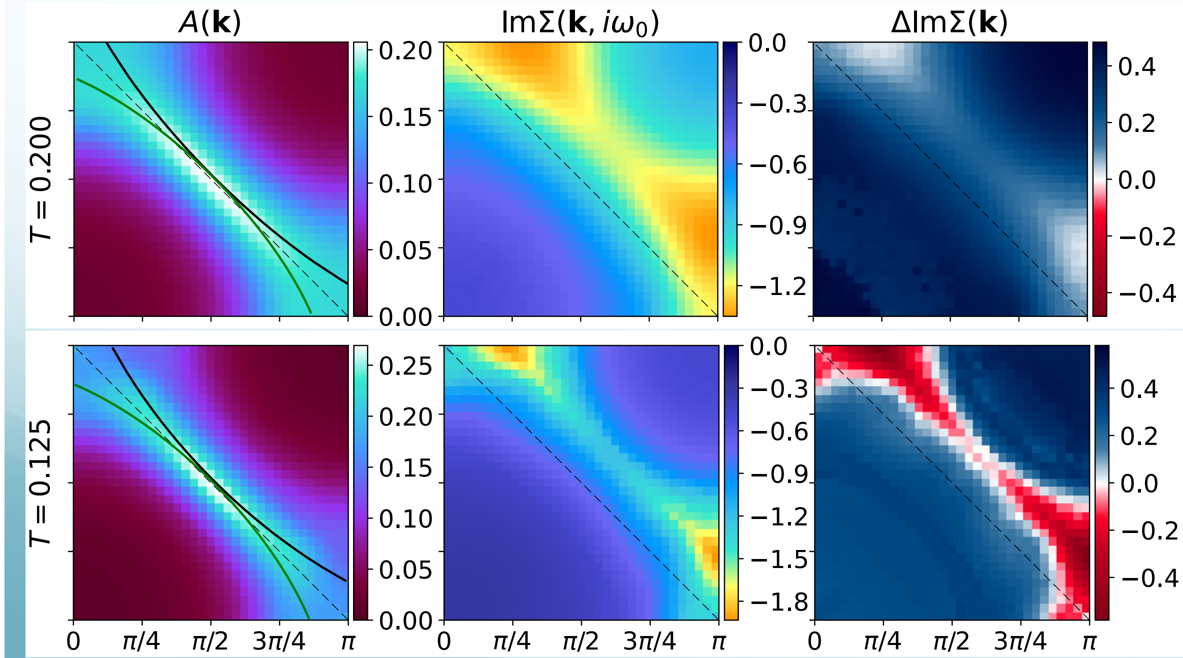
F. Šimkovic, R. Rossi, M. Ferrero, Phys. Rev. Res. 4, 043201 (2022)

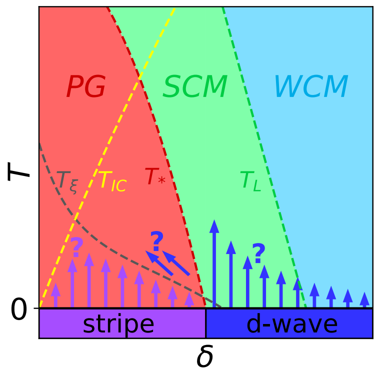


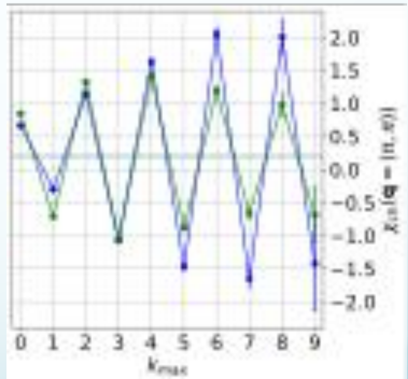


F. Šimkovic, R. Rossi, A. Georges, M. Ferrero, arXiv:2209.09237

Origin and fate of the pseudogap: 64x64 lattice







U=6.0 x=8.7% U=4.3 T=02

Strong PG
“shift”

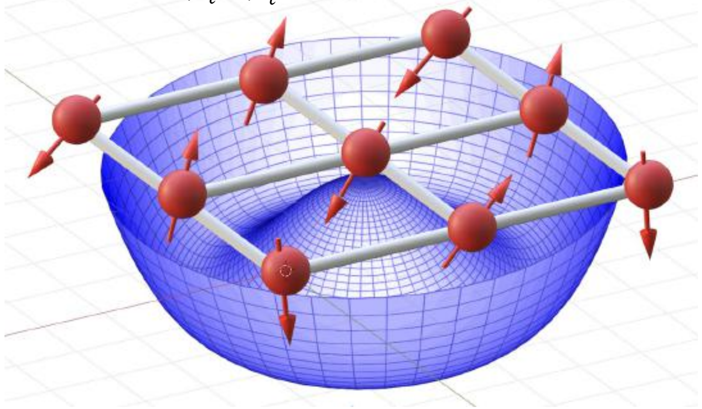
Emergent Magnetic Moment

$$\mathcal{S}_{\rm latt} = \int_0^\beta d\tau \Big\{ -\sum_{ij,\sigma\sigma'} c^*_{i\tau\sigma}\left[\delta_{ij}\delta_{\sigma\sigma'}(-\partial_\tau+\mu)-\varepsilon^{\sigma\sigma'}_{ij}\right]c_{j\tau\sigma'} + \sum_{i,\sigma\sigma'} U n_{i\tau\uparrow}n_{i\tau\downarrow} + \frac{1}{2}\sum_{ij,\varsigma}\rho^\varsigma_{i\tau}V^\varsigma_{ij}\rho^\varsigma_{j\tau}\Big\}$$

Correlated electrons lattice model

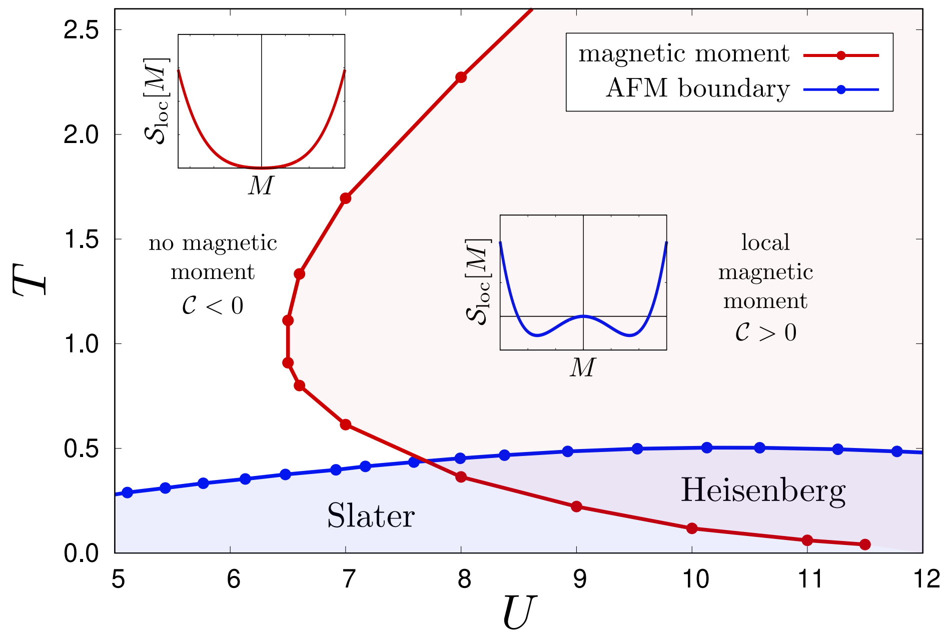
Criterium of Local Moment formation:

$$-\frac{\partial^2\mathcal{S}_{\rm loc}[\rho^s]}{\partial\rho^s_\tau\,\partial\rho^s_{\tau'}} = [\chi^s]^{-1}_{\tau\tau'} - J^{\rm loc}_{\tau\tau'}$$



Rotated local frame

$$R_{i\tau} = \begin{pmatrix} \cos(\theta_{i\tau}/2) & -e^{-i\varphi_{i\tau}}\sin(\theta_{i\tau}/2) \\ e^{i\varphi_{i\tau}}\sin(\theta_{i\tau}/2) & \cos(\theta_{i\tau}/2) \end{pmatrix}$$



E. Stepanov et al, PRB 105, 155151 (2022)

Effective bosonic action in the adiabatic limit

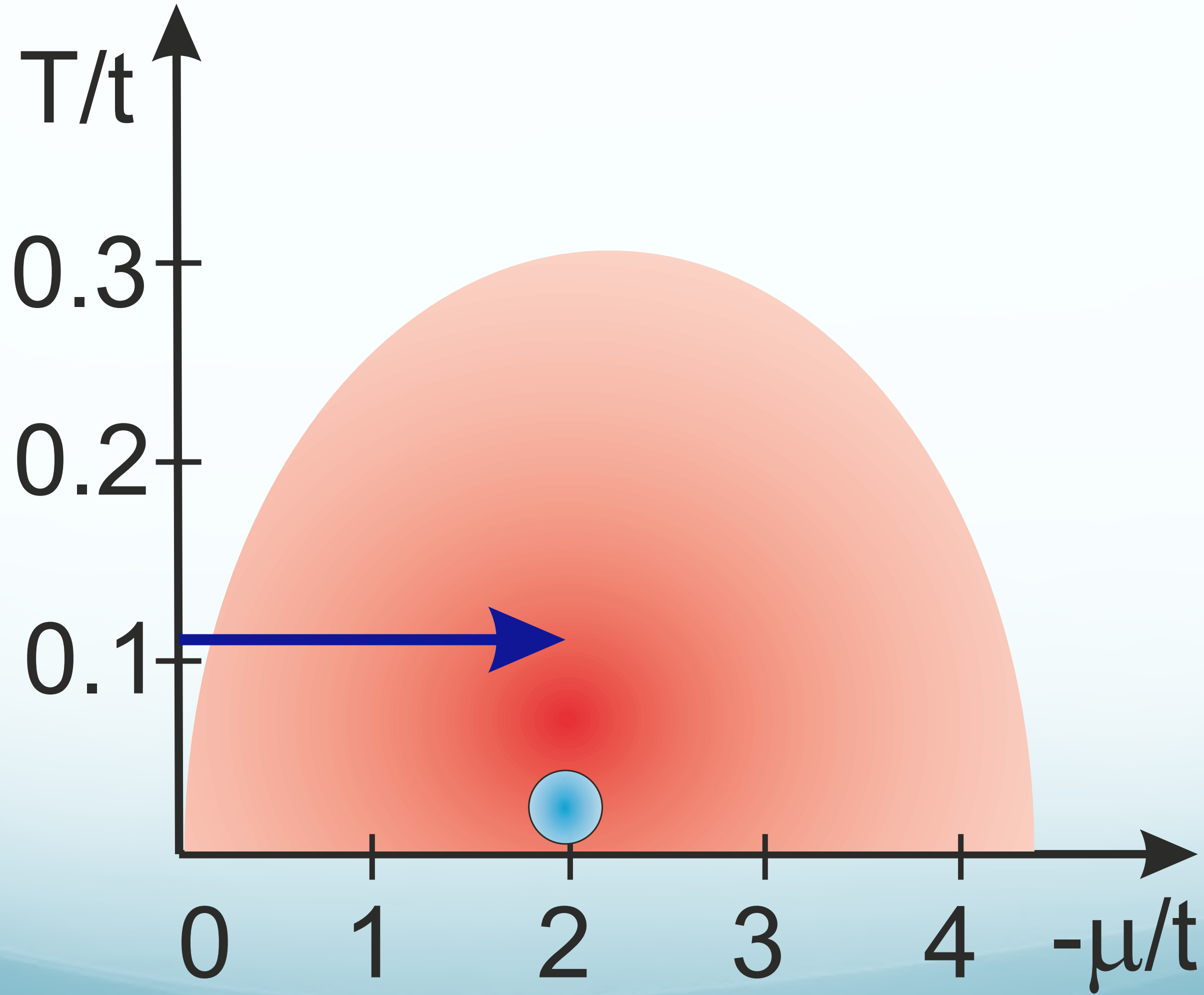
$$\mathcal{S} \simeq -\frac{1}{4}\int_0^\beta d\tau\, d\tau' \sum_{ij,\varsigma\varsigma'}\rho^\varsigma_{i\tau}\mathcal{I}^{\varsigma\varsigma'}_{ij,\tau\tau'}\rho^{\varsigma'}_{j\tau'} + \int_0^\beta d\tau \sum_i A^z_{i\tau}M_{i\tau}$$

kinetic term (spin precession)

$$-\frac{1}{2}\int_0^\beta d\tau\, d\tau' \sum_i \left\{\rho^c_{i\tau}\chi^{c\,-1}_{\tau\tau'}\rho^c_{i\tau'} + M_{i\tau}\chi^{z\,-1}_{\tau\tau'}M_{i\tau'}\right\}$$

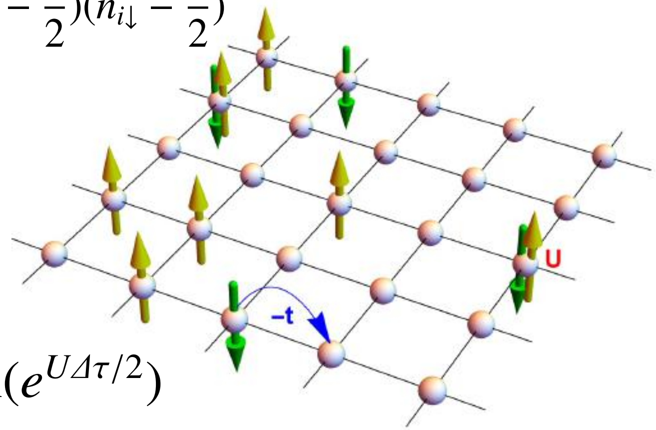
longitudinal (Higgs) fluctuations

Can we “shift μ“?



Numerically Exact Lattice DQMC: Hirsch-Fye

Hubbard model: $N_x \times N_y$ 2D-space $\hat{H}_\alpha = -\sum_{i,j,\sigma} t_{ij}^{\alpha} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} U(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})$



Discrete Hirsch-Hubbard-Stratanovich transformation

$$e^{-U\Delta\tau[n_{i\uparrow}n_{i\downarrow}-(n_{i\uparrow}+n_{i\downarrow})/2]} = \frac{1}{2}\sum_{s_i=\pm 1} e^{\lambda s_i(n_{i\uparrow}-n_{i\downarrow})}$$

$$\lambda = \operatorname{arccosh}(e^{U\Delta\tau/2})$$

D+1 Gaussian Action: $S[c^*, c] = -\sum_{i,j,\sigma} c_{i\sigma}^{*}\, G_{ij\sigma}^{-1}\, c_{j\sigma}$

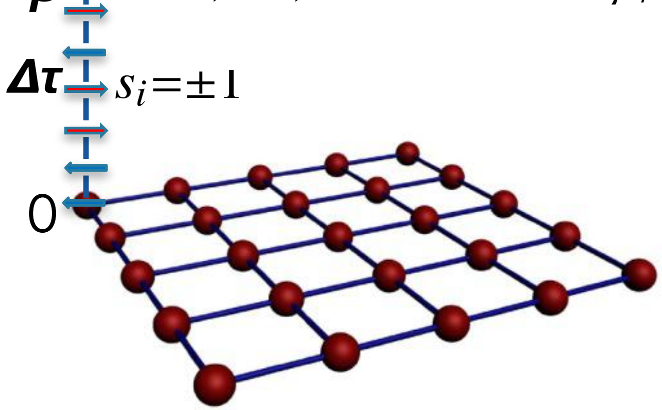
D+1 QFT: $i \equiv (\mathbf{r}, \tau)$

Imaginary time mesh

$$\tau = l * \Delta\tau$$

$l = 0, \cdots, L-1$ and $\Delta\tau = \beta/L$

$$G_{ij\sigma}^{-1}(s) = \mathcal{G}_{ij\sigma}^{-1} - \delta_{i,j}\lambda s_i \sigma$$



Partition function: $Z = \frac{1}{2^{NL}}\sum_{s}\prod_{\sigma}\det[G_{\sigma}^{-1}(s)]$

Green's Function: $g_{ij}^{\sigma} = \frac{1}{Z}\sum_{s} P(s)\, G_{ij}^{\sigma}(s)$

P(s)>0 for N=1 $P(s) = \det[G_{\uparrow}^{-1}(s)] \cdot \det[G_{\downarrow}^{-1}(s)]$ "Rule of thumb" $U\Delta\tau/2 \lesssim 1$.

Details of DQMC: discrete GF

Antiperiodic fermionic $\delta_{i,j'}$ in time space:

$$\delta_{l,l'+1} \quad \begin{aligned} &= 1 \quad \text{if} \quad l = l'+1, l = 2, \ldots, L-1 \\ &= -1 \ \text{if} \ l = 1, \ l' = L \end{aligned}$$

Inverse GF in time-space:

$$G_\sigma^{-1}(s) = \begin{pmatrix} 1 & 0 & \cdots & 0 & B(s_L) \\ -B(s_1) & 1 & \cdots & \cdots & 0 \\ 0 & -B(s_2) & 1 & \cdots & \cdots \\ \cdots & \cdots & \cdots & 1 & 0 \\ \cdots & \cdots & \cdots & -B(s_{L-1}) & 1 \end{pmatrix}$$

$$B(\sigma s) \equiv \exp[-\Delta\tau \mathscr{H}^0] \exp[V^\sigma(s)]$$

Simple example for L=3

$$G_\sigma^{-1}(s) = \begin{pmatrix} 1 & 0 & B_3 \\ -B_1 & 1 & 0 \\ 0 & -B_2 & 1 \end{pmatrix}$$

$$G_{ij}^\sigma(s) = \begin{pmatrix} \{1+B_3B_2B_1\}^{-1} & -B_3B_2\{1+B_1B_3B_2\}^{-1} & -B_3\{1+B_2B_1B_3\}^{-1} \\ B_1\{1+B_3B_2B_1\}^{-1} & \{1+B_1B_3B_2\}^{-1} & -B_1B_3\{1+B_2B_1B_3\}^{-1} \\ B_2B_1\{1+B_3B_2B_1\}^{-1} & B_2\{1+B_1B_3B_2\}^{-1} & \{1+B_2B_1B_3\}^{-1} \end{pmatrix}$$

CT-QMC: Interaction Expansion

Interaction expansion CT-INT: A. Rubtsov and A. L., JETP Lett (2004) $i \equiv (\mathbf{r}_k, \tau_k)$

$$Z = \int \mathcal{D}[c^*, c]\, e^{-S_0[c^*,c]} \sum_{k=0}^{\infty} \frac{(-U)^k}{k!} \int_0^\beta d\tau_{1\ldots k}\, c^*_{i_1\uparrow} c_{i_1\uparrow}\, c^*_{i_1\downarrow} c_{i_1\downarrow} \ldots c^*_{i_k\uparrow} c_{i_k\uparrow}\, c^*_{i_k\downarrow} c_{i_k\downarrow}$$

So is Gaussian action, then we get (kxk) determinant of $\mathcal{G}^\sigma$

$$Z = Z_0 \sum_{k=0}^{\infty} (-U)^k \int_0^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^\beta d\tau_k \prod_\sigma \det \mathcal{G}_k^\sigma$$

Metropolis Monte-Carlo with probability $P(k \to k+1) = \min\left(1, \frac{\beta U}{k+1} \prod_\sigma \frac{(\det \mathcal{G}_{k+1}^\sigma}{\det \mathcal{G}_k^\sigma}\right)$

Green's Function: $g_{ij}^\sigma = \mathcal{G}_{ij}^\sigma - \sum_{k,k'} \mathcal{G}_{ik}^\sigma \cdot M_{k,k'}^\sigma \cdot \mathcal{G}_{k'j}^\sigma$

where: $M=\mathcal{G}^{-1}$

numerical complexity: $O(N^2K^2 \log(K))$.
For 8x8 system at β = 10 the average K ~ 700

E. Gull, A. Millis, A.L., A. Rubtsov, M. Troyer, Ph. Werner, Rev. Mod. Phys. **83**, 349 (2011)

CT-INT: random walks in the *det(k×k)* space

$Z = \ldots Z_{k-1} + Z_k + Z_{k+1} + \ldots.$

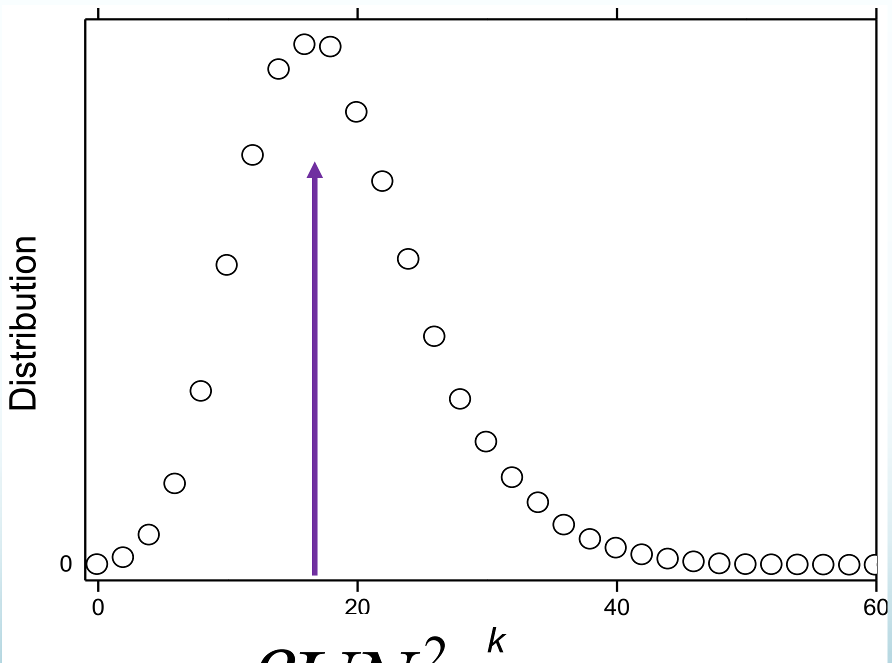
k-1 *k*+1

Acceptance ratio

decrease

Step *k*-1

$$\frac{k}{|w|}\,\frac{D^{k-1}}{D^{k}}$$



increase

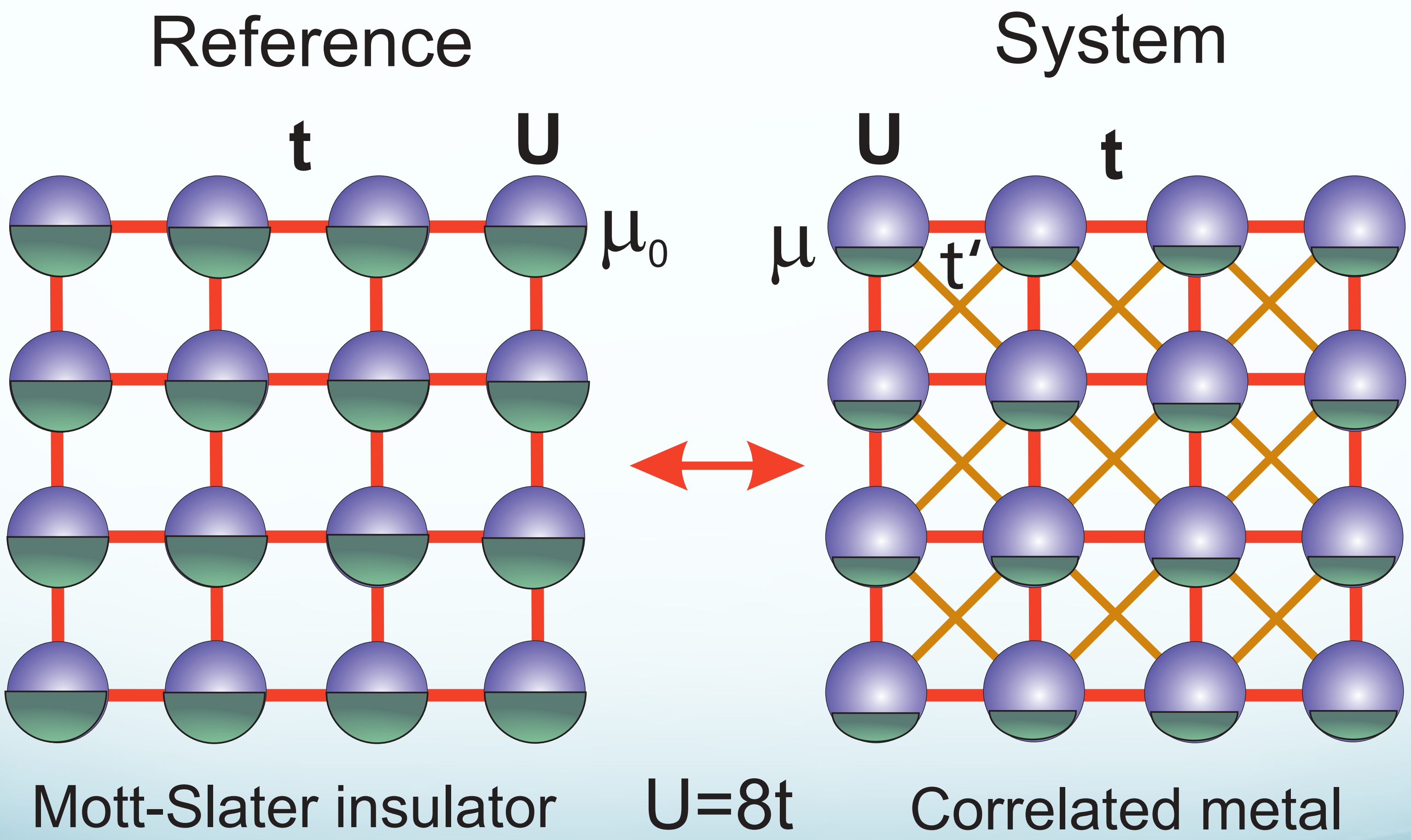
Step *k*+1

$$\frac{|w|}{k+1}\,\frac{D^{k+1}}{D^{k}}$$

Maximum at $\beta U N^2$

Super-perturbation: DF-QMC

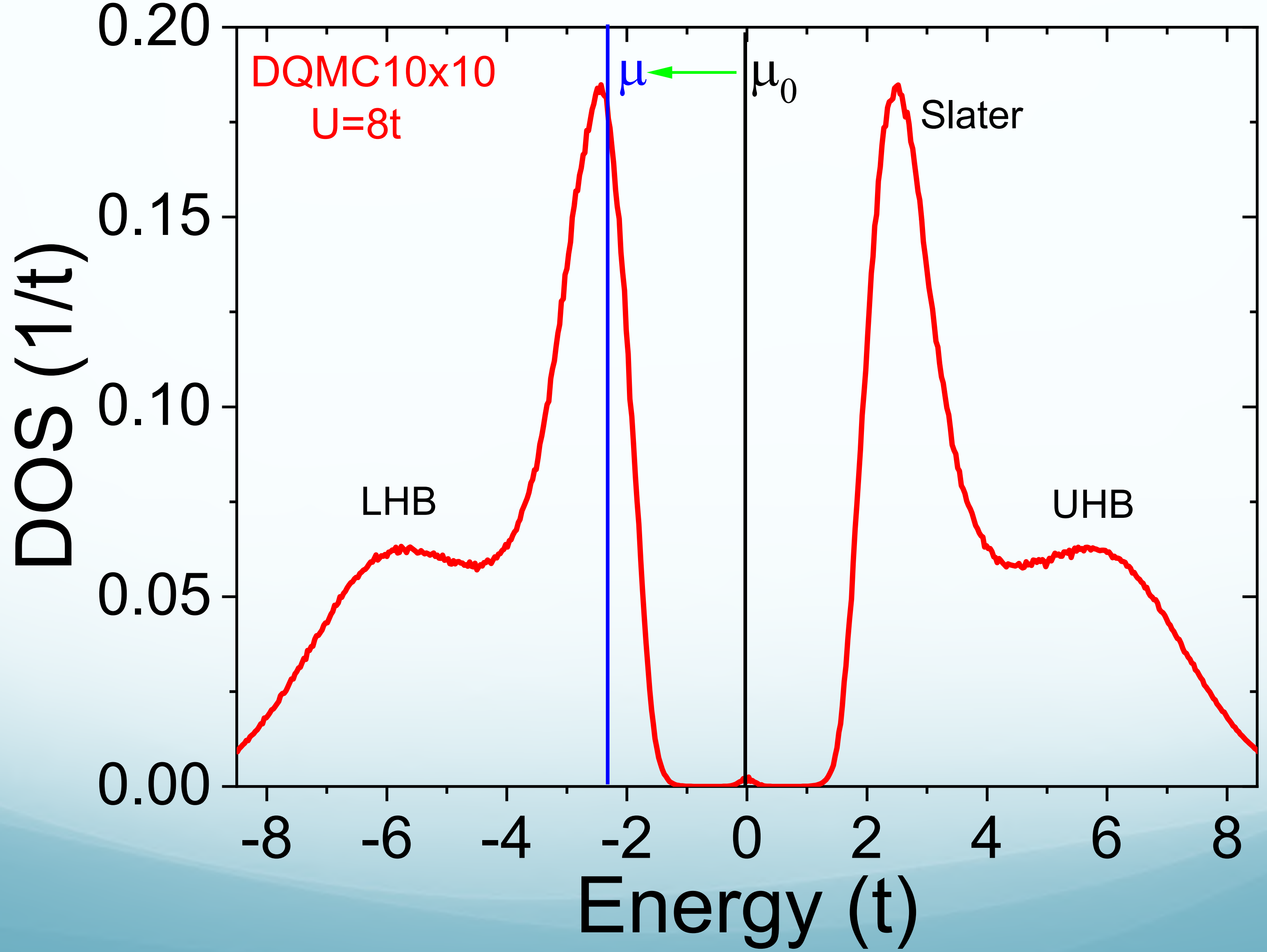
- Controllable perturbative solution of doped Hubbard model for HTSC
- Developed DF expansion around DQMC for N=1, t'=0



DQMC – no sign problem

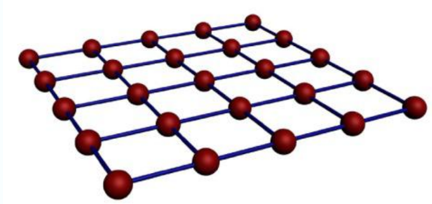
DF QMC super-perturbation

DOS for Reference System



Dual Fermion scheme

General Lattice Action $Z_\alpha = \int \mathcal{D}[c^*, c] \exp(-S_\alpha[c^*, c])$

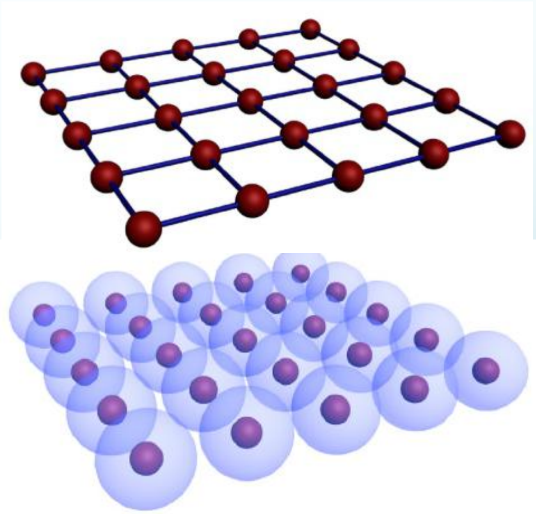


$$S_\alpha[c^*, c] = -\sum_{1,2} c_1^* \, (\mathcal{G}_\alpha)^{-1}_{12} \, c_2 + \frac{1}{4} \sum_{1234} U_{1234} c_1^* c_2^* c_4 c_3$$

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

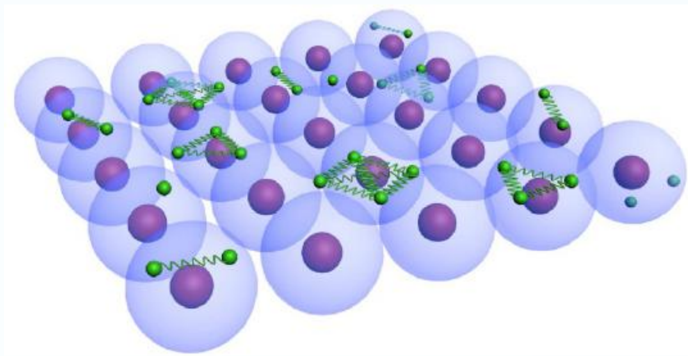
Connection between Reference and System:

$$S[c^*, c] = S_0[c^*, c] + \sum_{12} c_1^* \tilde{t}_{12} c_2$$



A. Rubtsov, et al, PRB **77**, 033101 (2008)

Dual Transformation

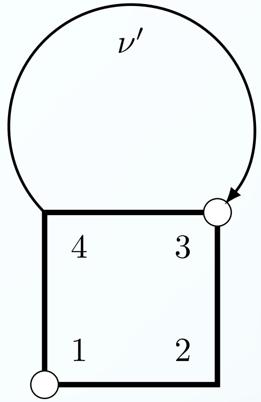


Gaussian path-integral

$$e^{-c_1^* \, \tilde{t}_{12} \, c_2} = Z_t \int \mathcal{D}[d^*, d] \, e^{d_1^* \, \tilde{t}_{12}^{-1} \, d_2 + d_1^* c_1 + c_1^* d_1}$$

with $Z_t = \det[-\tilde{t}\,]$

new Action:



$$\tilde{S}[d^*, d] = -\sum_{12\,\nu\sigma} d_{1\nu\sigma}^* \, (\tilde{G}_\nu^0)_{12}^{-1} \, d_{2\nu\sigma} + \frac{1}{4} \sum_{1234} \gamma_{1234} d_1^* d_2^* d_4 d_3$$

Diagrammatic 1-st order correction:

$$\longrightarrow \quad \tilde{G}_{12}^0 = \left[\tilde{t}^{-1} - \hat{g} \right]_{12}^{-1}$$

$$\tilde{\Sigma}_{12}^{(1)} = \sum_{s-QMC} \sum_{3,4} \gamma_{1324}^d(s) \tilde{G}_{43}^0$$

$$\square \quad \gamma_{1234} = \langle c_1 c_2 c_3^* c_4^* \rangle_0 - \langle c_1 c_4^* \rangle_0 \langle c_2 c_3^* \rangle_0 + \langle c_1 c_3^* \rangle_0 \langle c_2 c_4^* \rangle_0$$

$$\gamma_{1234}^d = \gamma_{1234}^{\uparrow\uparrow\uparrow\uparrow} + \gamma_{1234}^{\uparrow\uparrow\downarrow\downarrow}$$

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

Dual Fermion Action: Details

Lattice partition function with DF-transformation

$$Z = Z_0 Z_t \int \mathcal{D}[d^*, d]\, e^{d_1^* \tilde{t}_{12}^{-1} d_2} \left\langle e^{d_1^* c_1 + c_1^* d_1} \right\rangle_0$$

Where average over So:

$$\langle \ldots \rangle_0 = \frac{1}{Z_0} \int \mathcal{D}[c^*, c] \; \ldots \; e^{-S_0[c^*, c]}$$

Now: integrate-out original c-Fermions and get the Cumulants expansion

$$\left\langle e^{d_1^* c_1 + c_1^* d_1} \right\rangle_0 = \exp\left[\sum_{n=1}^{\infty} \frac{(-1)^n}{(n!)^2} \gamma^{(2n)}_{1 \cdots n, n' \cdots 1'} d_1^* \cdots d_n^* d_{n'} \cdots d_{1'} \right]$$

Dual potential related with Cumulants or connected correlators:

$$\gamma^{(2n)}_{1 \cdots n, n' \cdots 1'} = (-1)^n \langle c_1 \cdots c_n c_{n'}^* \cdots c_{1'}^* \rangle_{0c}$$

Green function n=1: $$g_{12} = -\langle c_1 c_2^* \rangle_0 = \frac{-1}{Z_0} \int \mathcal{D}[c^*, c]\; c_1 c_2^* \; e^{-S_0[c^*, c]}$$

First interacting term n=2: $$\langle c_1 c_2 c_3^* c_4^* \rangle_0 = \frac{1}{Z_0} \int \mathcal{D}[c^*, c]\; c_1 c_2 c_3^* c_4^* \; e^{-S_0[c^*, c]}$$

$$\gamma_{1234} = \langle c_1 c_2 c_3^* c_4^* \rangle_0 - \langle c_1 c_4^* \rangle_0 \langle c_2 c_3^* \rangle_0 + \langle c_1 c_3^* \rangle_0 \langle c_2 c_4^* \rangle_0$$

Dual and Lattice Green's Functions

Exact connection between Real and Dual GF:

$$G_{12} = \frac{\delta \ln Z}{\delta \tilde{t}_{21}} = -\tilde{t}_{12}^{-1} + \tilde{t}_{13}^{-1} \tilde{G}_{34} \tilde{t}_{42}^{-1}$$

Definition of exact Dual Green's function:

$$\tilde{G}^{-1} = \tilde{G}_0^{-1} - \tilde{\Sigma}$$

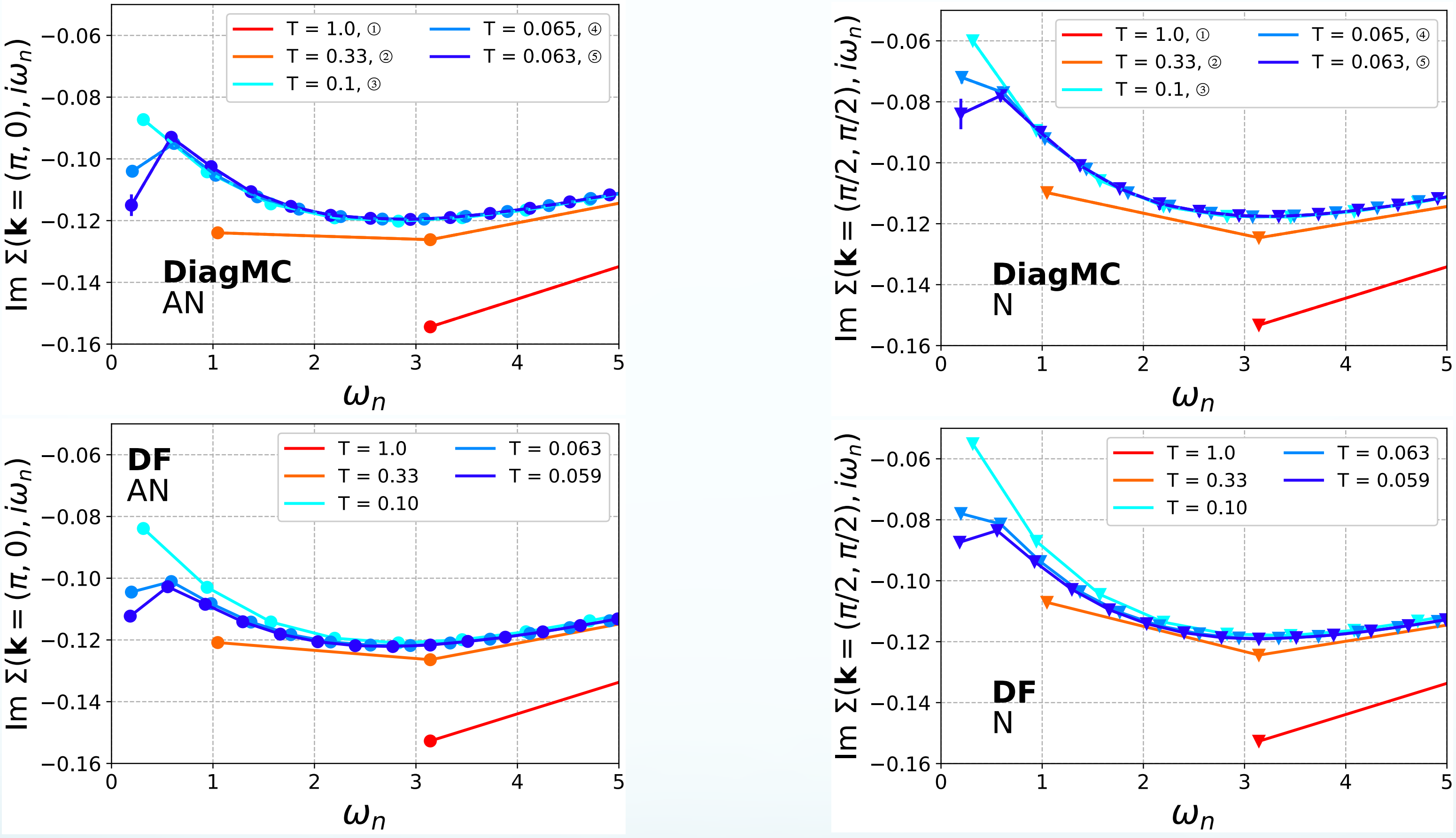
Expression of Green functions in Dual Theory:

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

Dual self-energy is similar to T-matrix like quantity: G=(g+gTg)

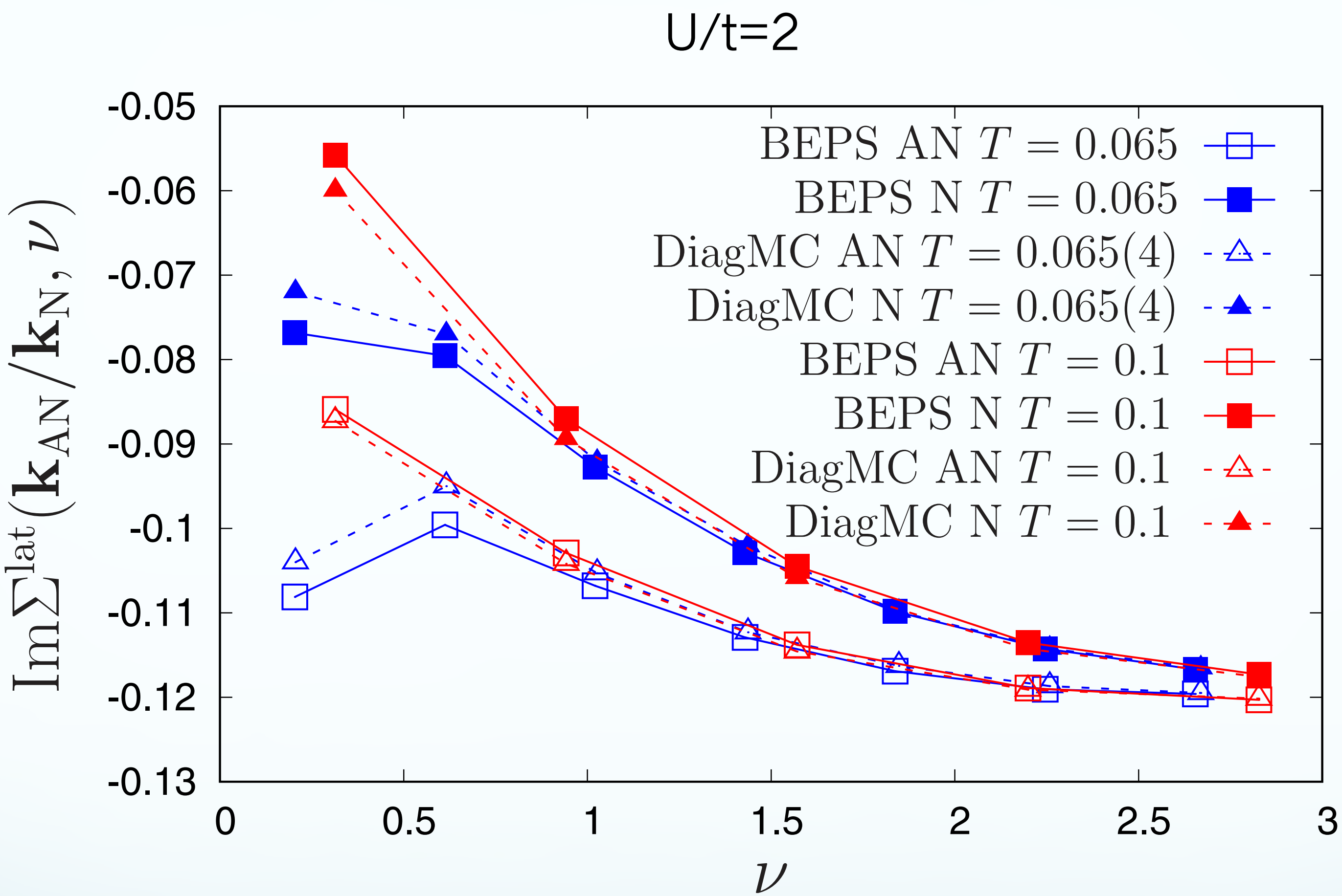
DF-Ladder vs. DiagMC

U/t=2



DF: James LeBlanc (openDF-code)
DiagMC: Fedor Šimkovic
from Phys. Rev. X 11, 011058 (2021)

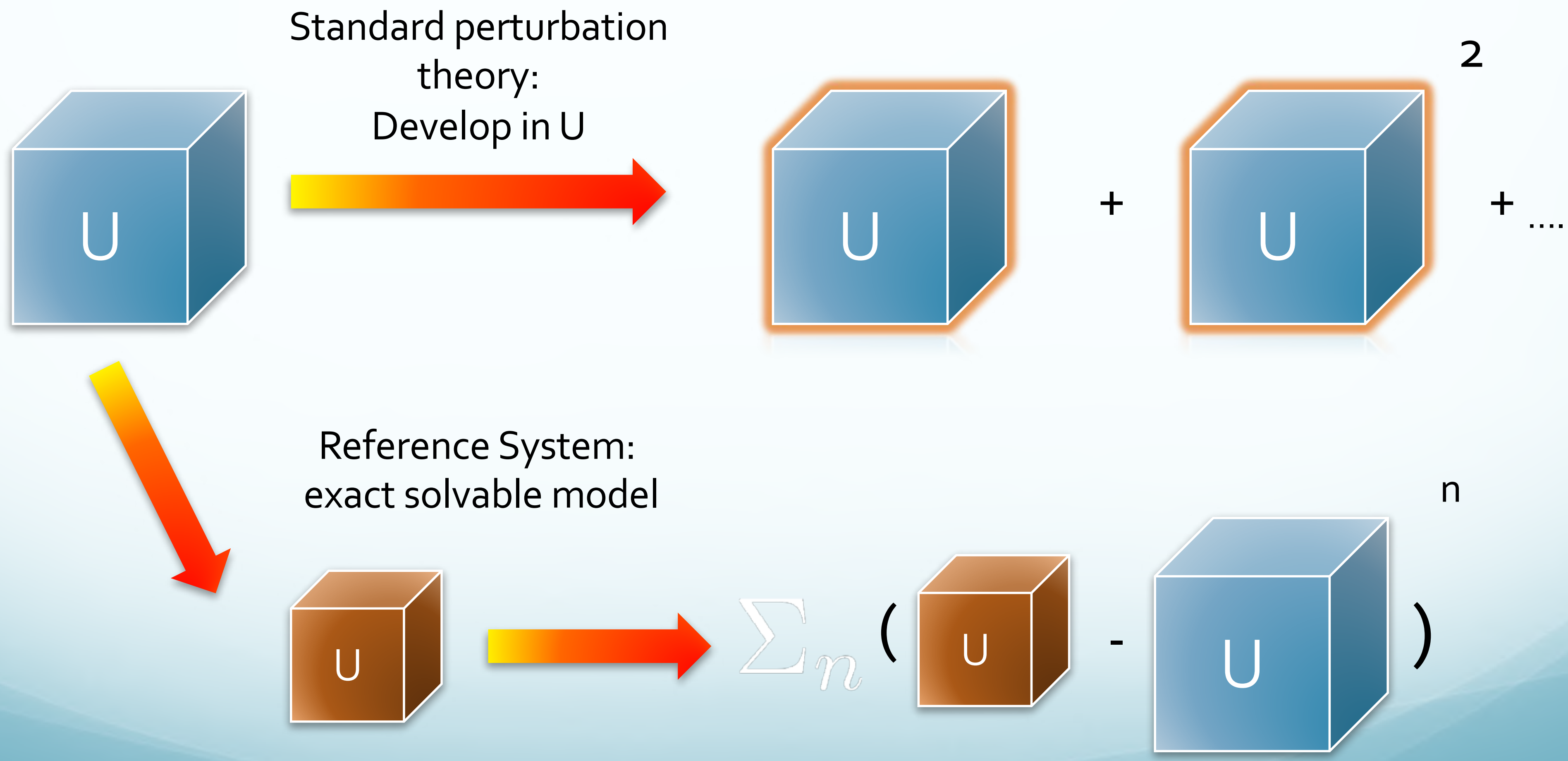
DF-Parquet vs. DiagMC



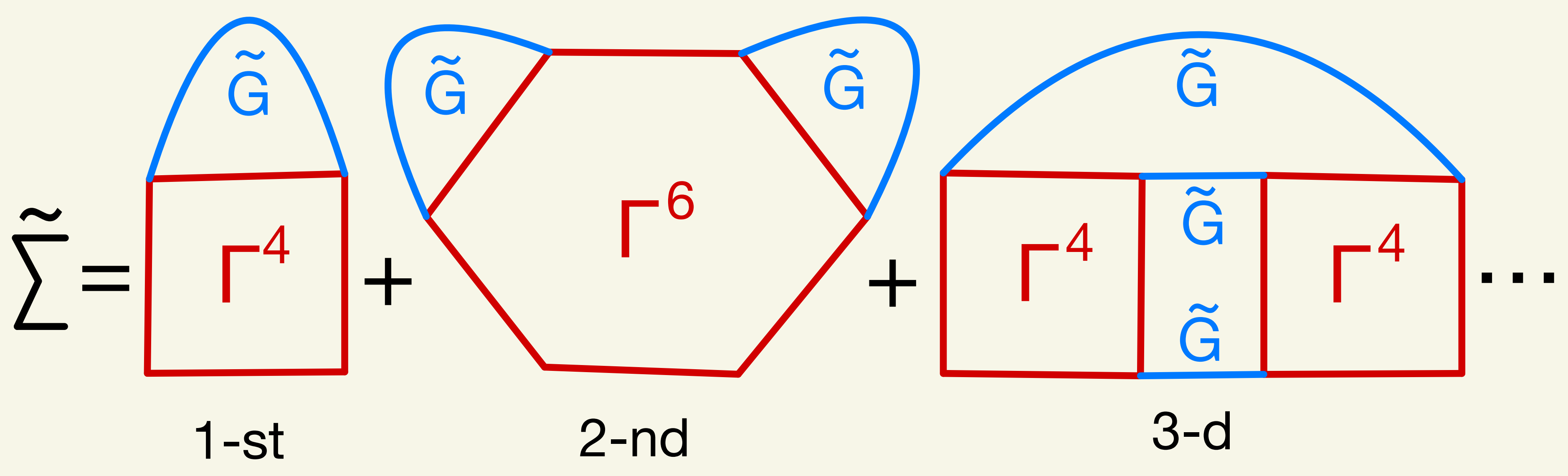
BEPS = boson exchange parquet solver in DF-space
F. Krien, et al Phys. Rev. B 102, 235133 (2020)

DiagMC: Fedor Šimkovic
from Phys. Rev. X 11, 011058 (2021)

Super-perturbation



DF-exact diagrammatics

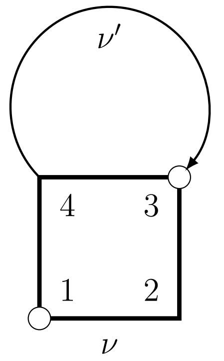


A. Rubtsov, M. Katsnelson, and A.L., PRB 77, 033101 (2008)
S. Brener, E. Stepanov, A. Rubtsov, M. Katsnelson, and A.L., Ann. Phys. 422, 168310 (2020)

Similar “strong-coupling” cumulant expansion:

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

1-st order diagram for dual self-energy



$$\widetilde{\Sigma}^{(1)i}_{12}(\nu) = \sum_{\nu',3,4} \gamma^{d}_{1234}(\nu,\nu',0)\, \widetilde{G}^{ii}_{43}(\nu')$$

Density (d) and Magnetic (m) Vertices:

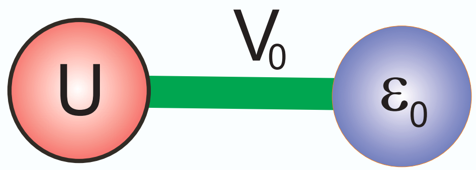
$$\gamma^{d/m}_{1234}(\nu,\nu',\omega) = \gamma^{\uparrow\uparrow}_{1234}(\nu,\nu',\omega) \pm \gamma^{\uparrow\downarrow}_{1234}(\nu,\nu',\omega)$$

Connected 2-particle GF:

$$\gamma^{\sigma\sigma'}_{1234}(\tau_1,\tau_2,\tau_3,\tau_4) = -\left\langle c_{1\sigma}c^{*}_{2\sigma}c_{3\sigma'}c^{*}_{4\sigma'}\right\rangle_{\Delta} + g^{\sigma}_{12}g^{\sigma'}_{34} - g^{\sigma}_{14}g^{\sigma}_{32}\delta_{\sigma\sigma'}$$

Two site test

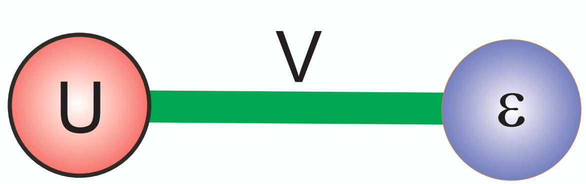
$U=2,\ \varepsilon_0=0$ $\quad V_0=0.5$



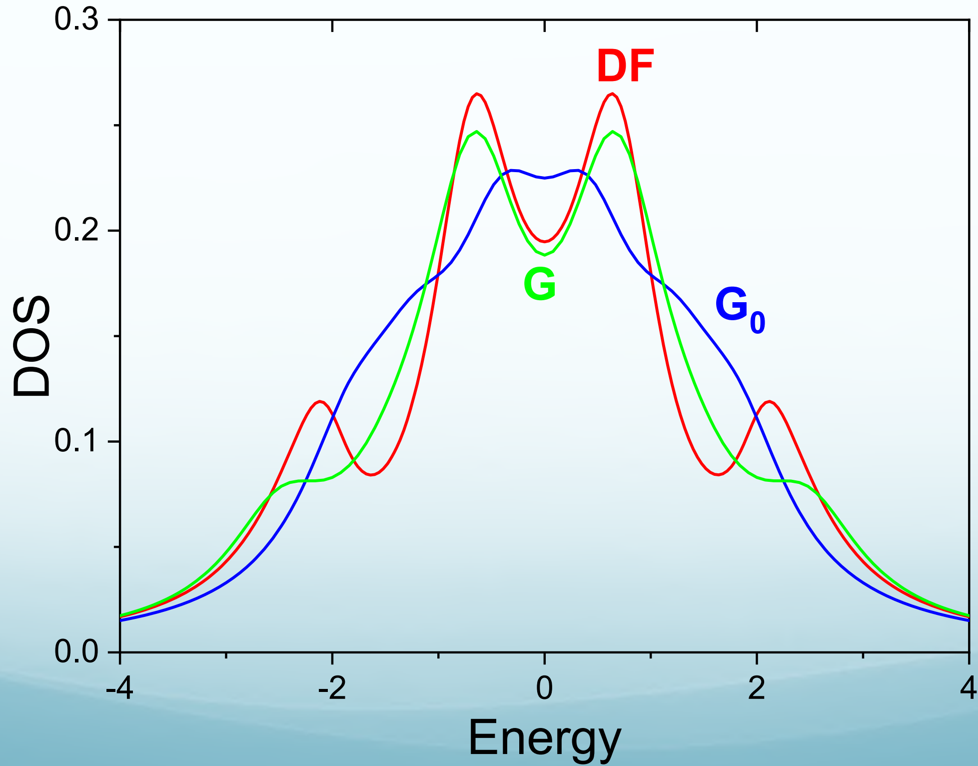
Ref.

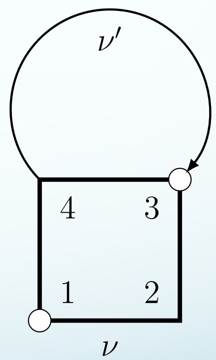
Fixed

$V=1.5V_0$



Sys.





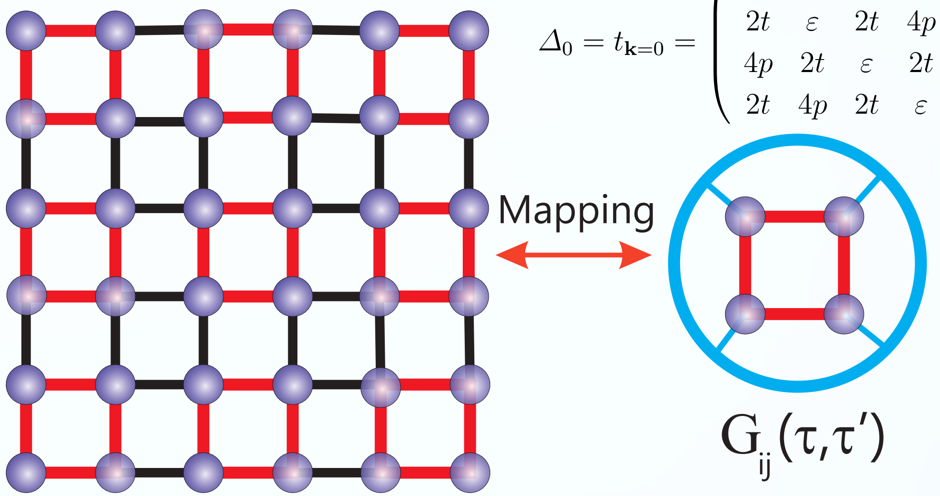
Plaquette DF-perturbation

$$t_{\mathbf{k}} = \begin{pmatrix} \varepsilon & tK^{0+} & pL^{-+} & tK^{-0} \\ tK^{0-} & \varepsilon & tK^{-0} & pL^{--} \\ pL^{+-} & tK^{+0} & \varepsilon & tK^{0-} \\ tK^{+0} & pL^{++} & tK^{0+} & \varepsilon \end{pmatrix}$$

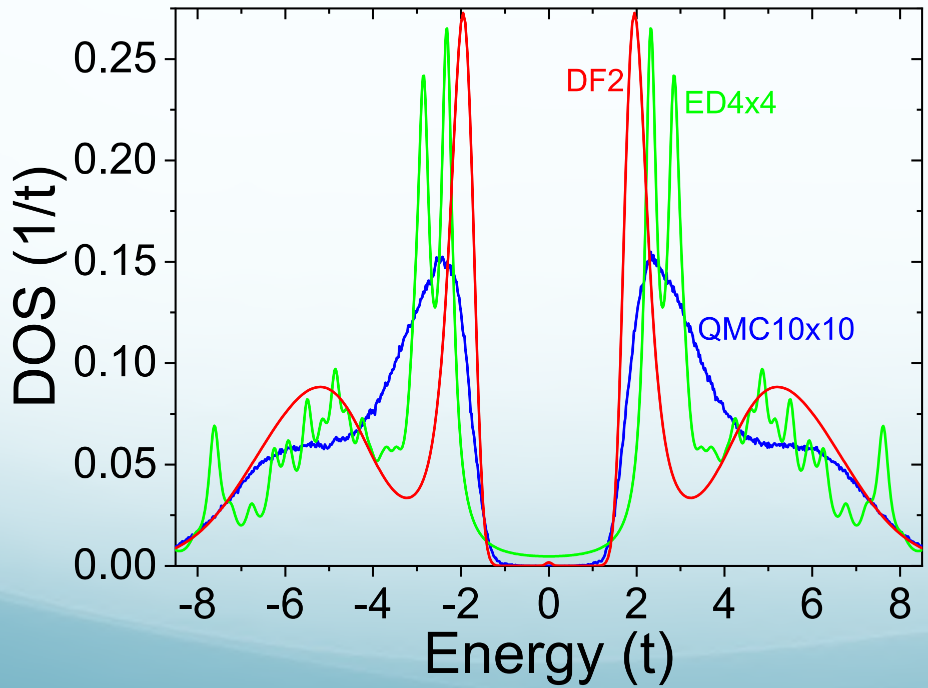
$$\begin{aligned} K_{\mathbf{k}}^{mn} &= 1 + e^{i(mk_x+nk_y)} \\ L_{\mathbf{k}}^{mn} &= 1 + e^{i(mk_x+nk_y)} + e^{imk_x} + e^{ink_y} \end{aligned}$$

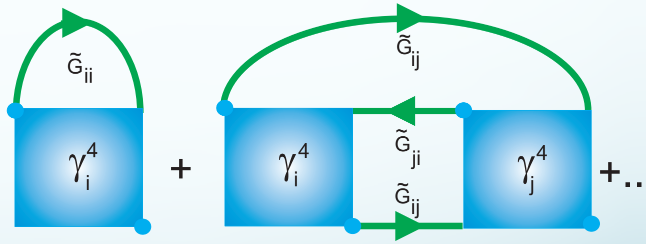
$$[m(n)] = -(1), 0, +(1)$$

$$\Delta_0 = t_{\mathbf{k}=0} = \begin{pmatrix} \varepsilon & 2t & 4p & 2t \\ 2t & \varepsilon & 2t & 4p \\ 4p & 2t & \varepsilon & 2t \\ 2t & 4p & 2t & \varepsilon \end{pmatrix}$$

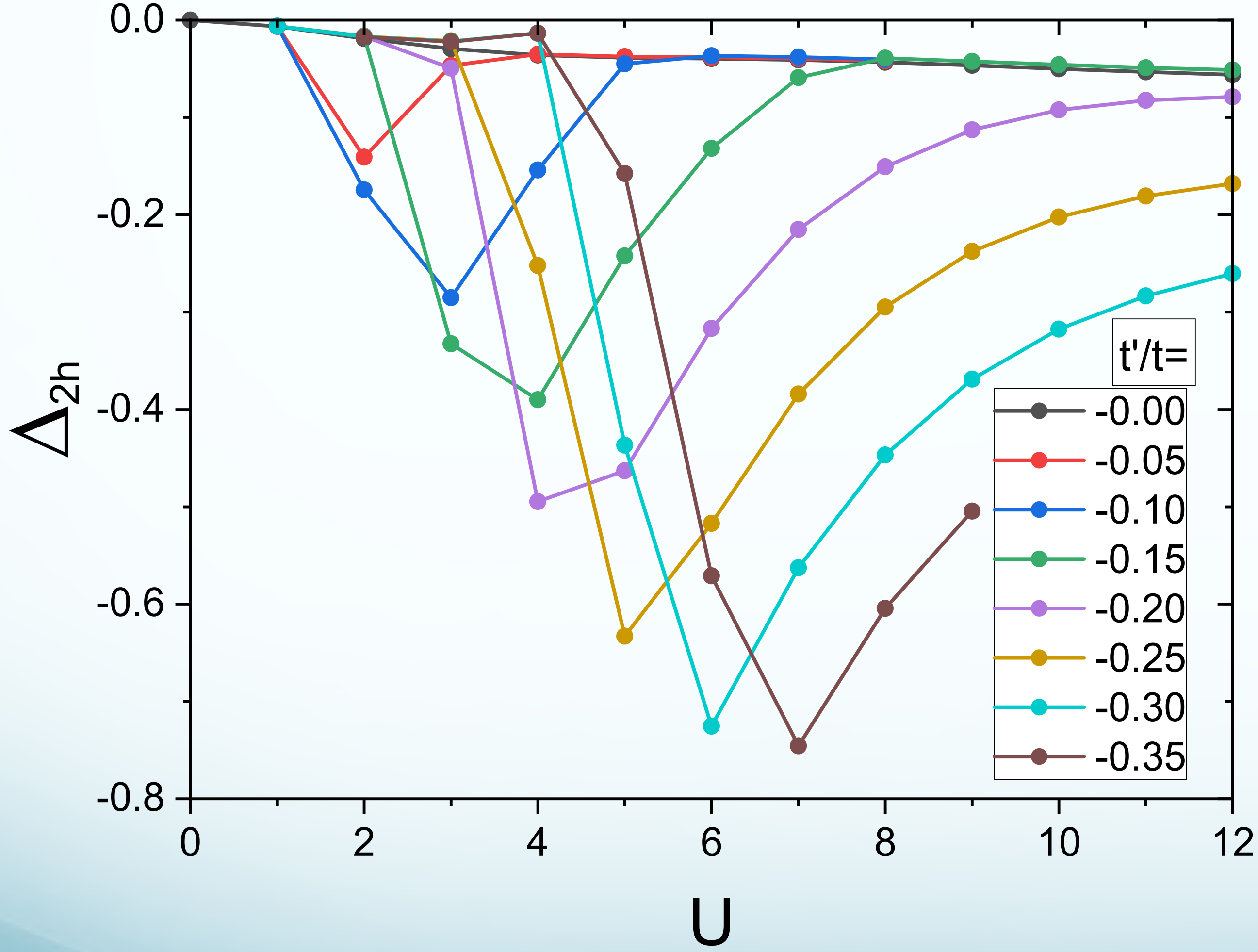


U=8
t=1
T=t/5





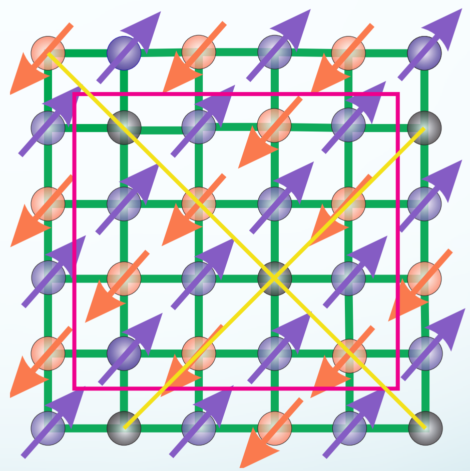
ED 4x4 cluster: Local Pairs



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

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

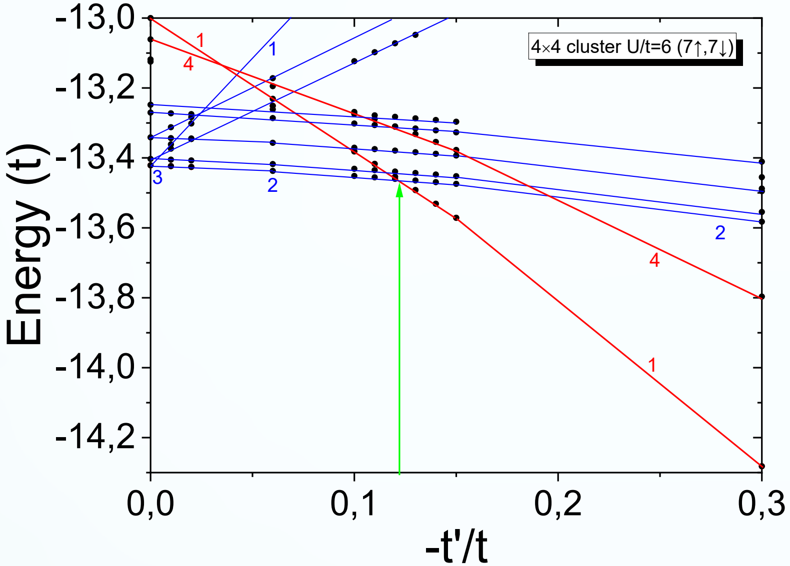
Δ_{2h}=0.7t=3000 K



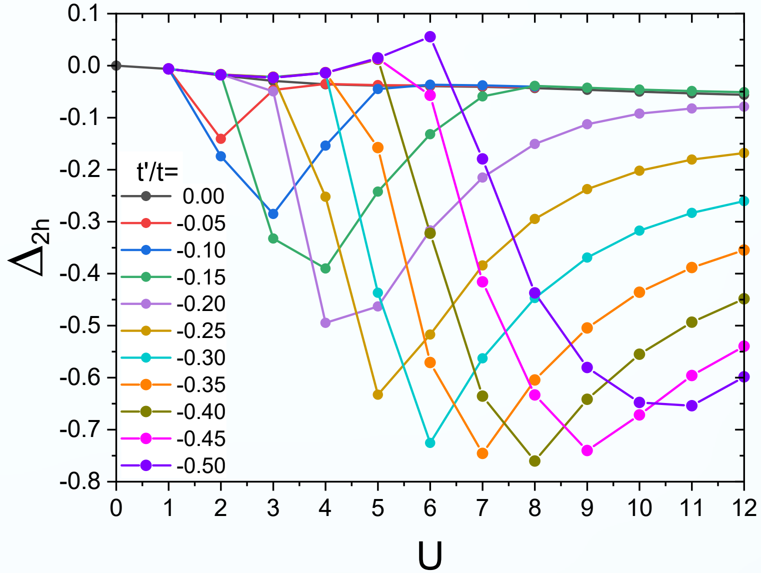
M. Danilov, E.G.C.P. van Loon, S. Brener, S. Iskakov, M. Katsnelson, A.L.
npj Quantum Materials **7,** 50 (2022)

Effects of t’ on 4x4 cluster

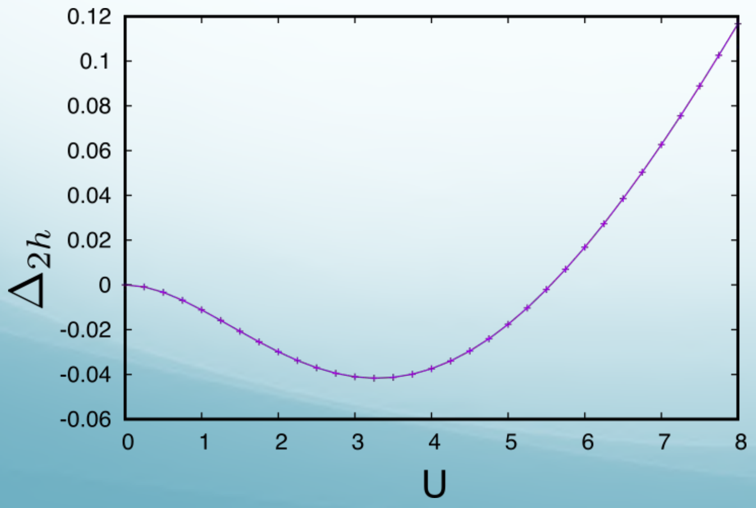
Ground State crossing



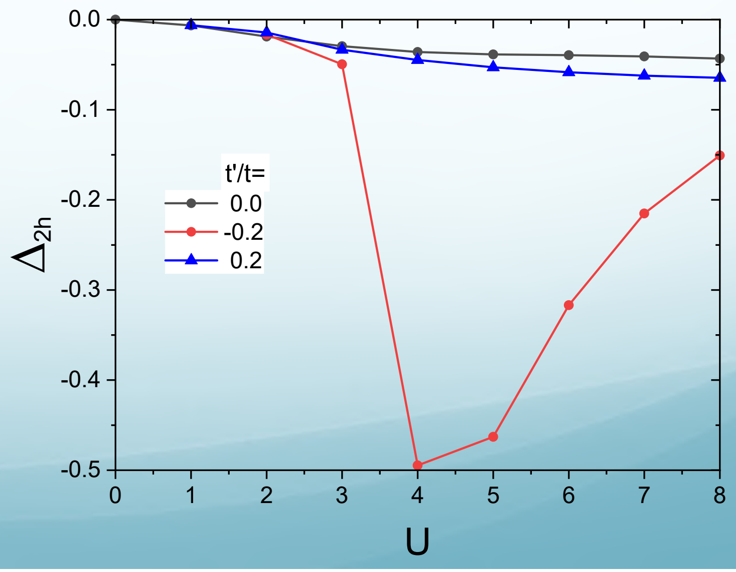
Large pair-binding for negative t‘/t



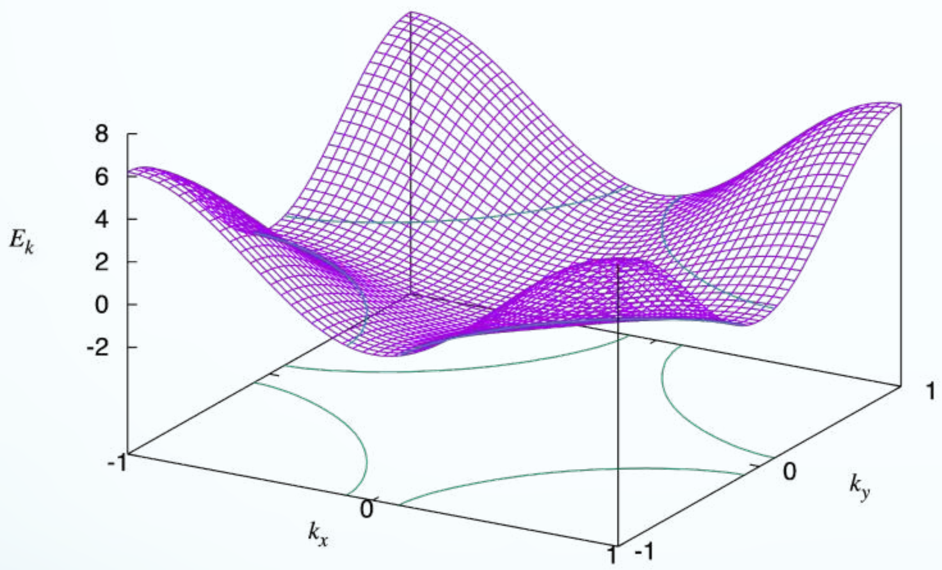
Small pair-binding for 2x2 cluster

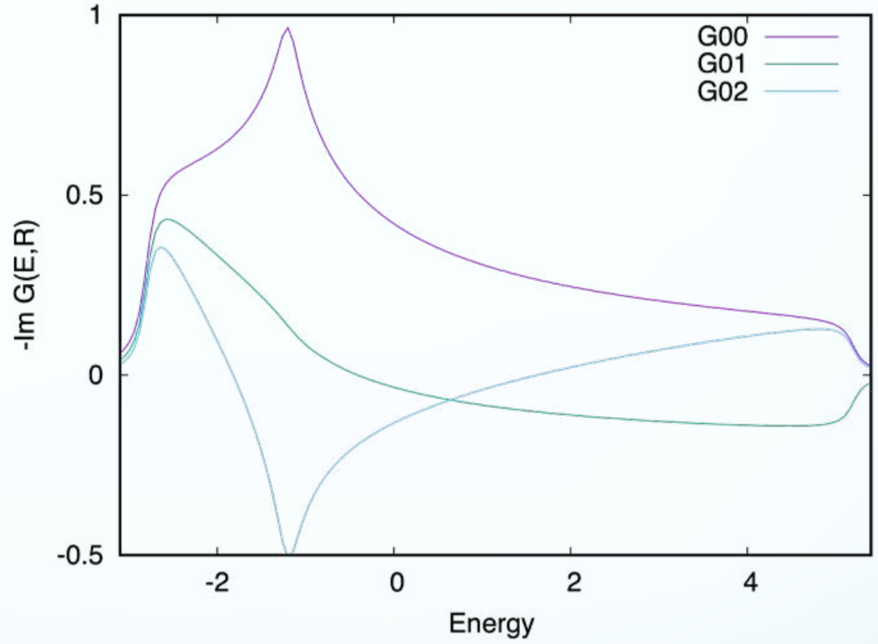


Small pair-binding for positive t‘/t



TB-Model: HTSC





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

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:

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

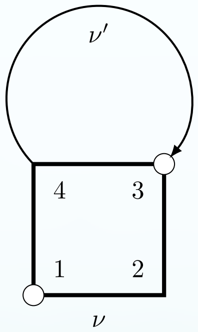
Dual GF: $\tilde{G}^0_{12} = \left[\tilde{t}^{-1} - \hat{g}\right]^{-1}_{12}$

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

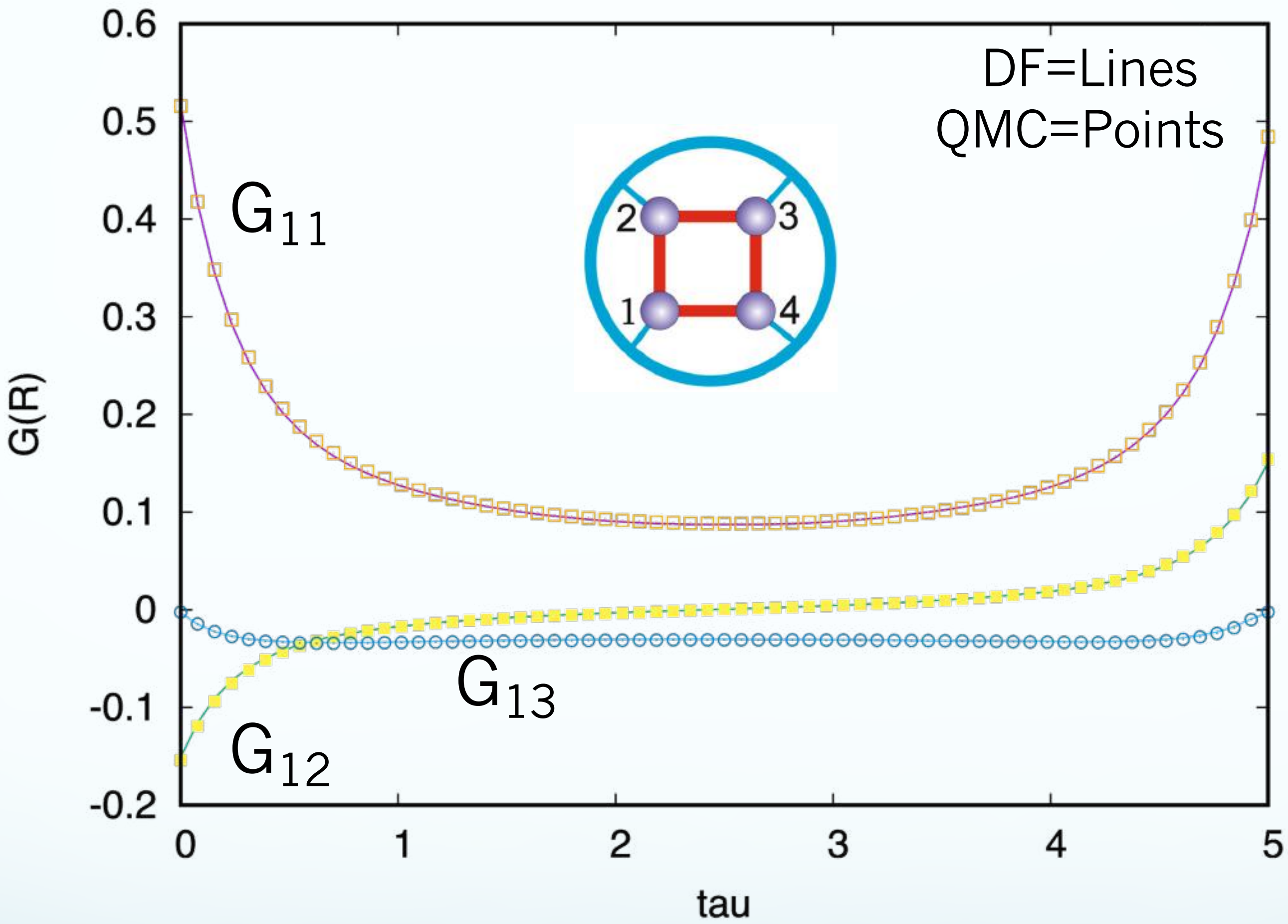
Final GF:

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

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 test DQMC-Hirsch-Fye



DF-pert:

μ=-0.3

t'=0

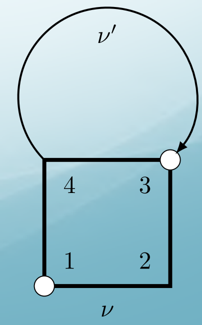
U=5.56

β=5

L=64

(ℓ =1,L)

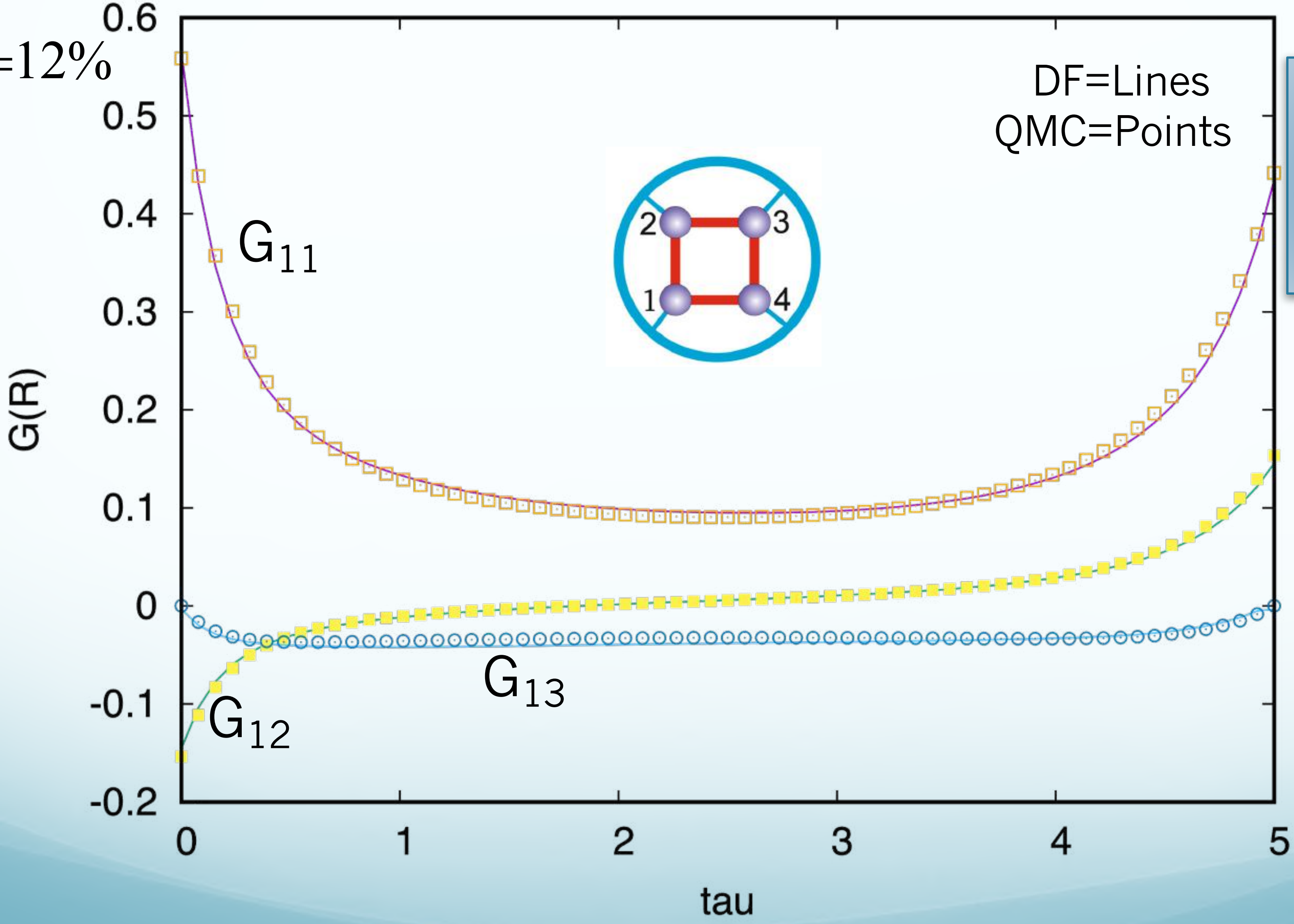
$$\Sigma_{12} \sim \frac{1}{Z}\operatorname*{Tr}_{\{s\}} \langle c_1 c_2^* c_3 c_4^* \rangle_{\{s\}} \tilde{G}_{43} \qquad 1 \equiv (i, \ell, \sigma)$$



$$\langle c_1 c_2^* c_3 c_4^* \rangle_{\{s\}} = \langle c_1 c_2^* \rangle_{\{s\}} \langle c_3 c_4^* \rangle_{\{s\}} - \langle c_1 c_4^* \rangle_{\{s\}} \langle c_3 c_2^* \rangle_{\{s\}}$$

Super-DF-QMC 2x2 compare with exact QMC

δ=12%



DF-pert:

μ=–1.3

t'/t=-0.15

U=5.56

β=5

L=64

(ℓ =1,L)

DF-QMC scheme: K - Space

Action in Fourier-space $\tilde{S}[d^*, d] = -\sum_{\mathbf{k}\,\nu\sigma} d^*_{\mathbf{k}\nu\sigma}\, \tilde{G}^{-1}_{0\mathbf{k}\nu}\, d_{\mathbf{k}\nu\sigma} + \frac{1}{4}\sum_{1234} \gamma_{1234} d_1^* d_2^* d_3 d_4$

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

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

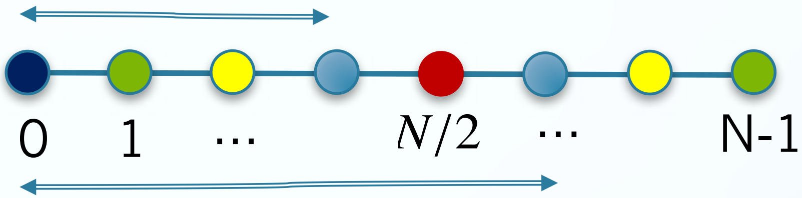
Periodization

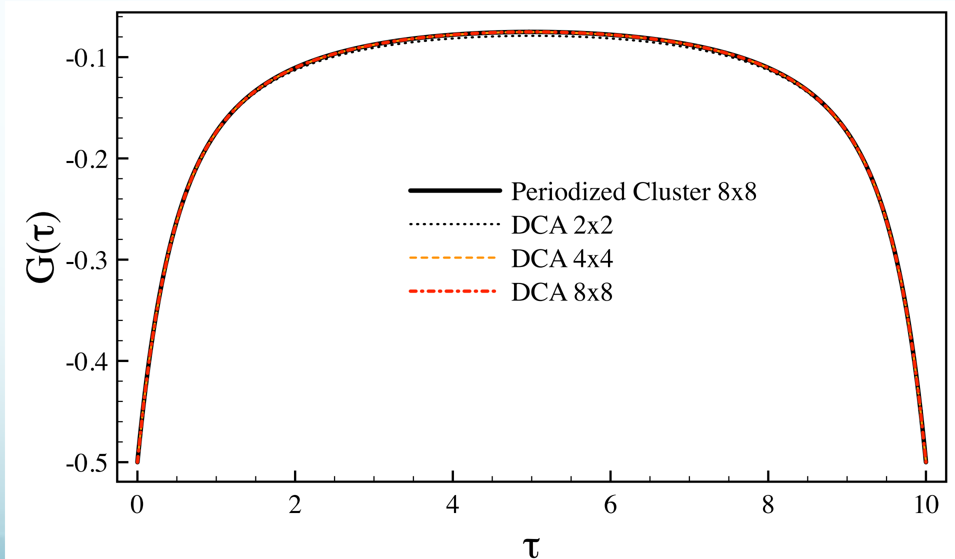
Simple 1-d theory: $\mathcal{G}_{ij}(\nu_n)$ with (i,j=0,N-1)

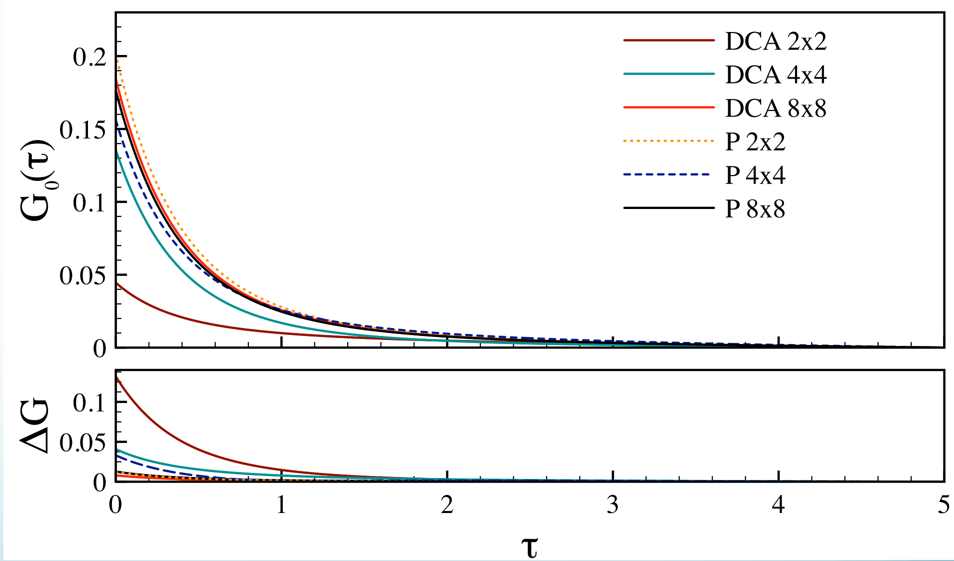
Step-1: average $\mathcal{G}_{0,n}$ and $\mathcal{G}_{0,N-n}$

Step-2: double FFT $\mathcal{G}_{ij}$ to $\mathcal{G}_{kk'}$

Step-3: periodic part: $\mathcal{G}_k\delta_{kk'}$

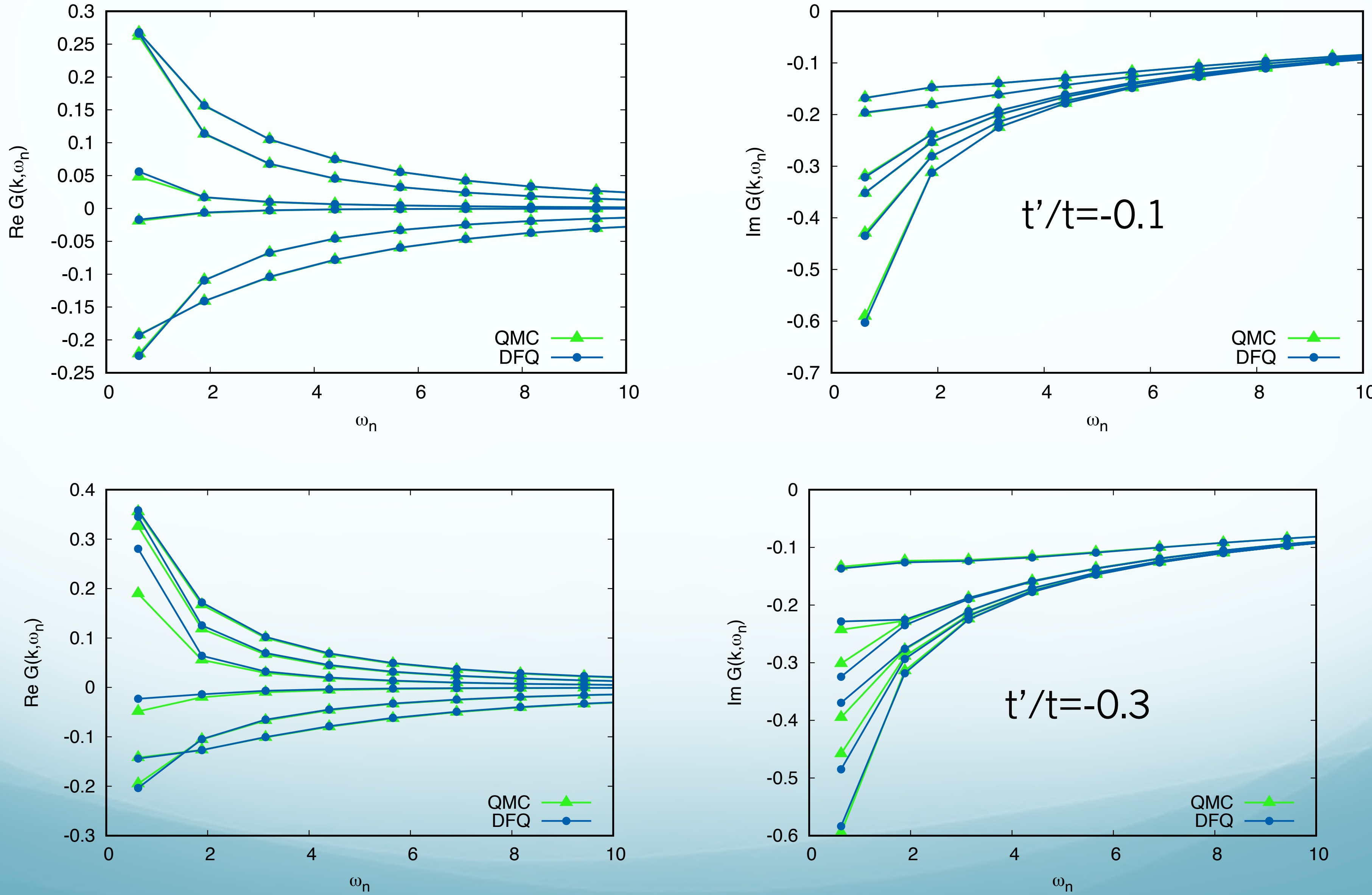






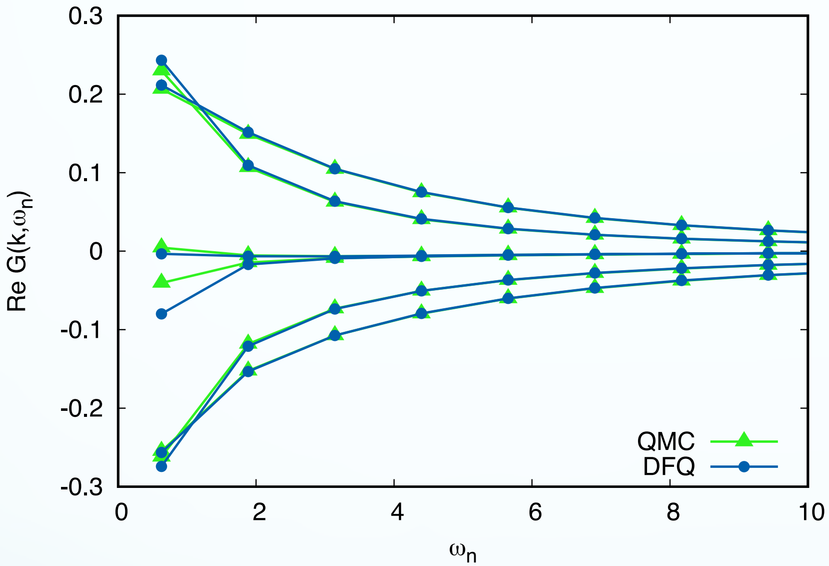
K-space test 4x4 system

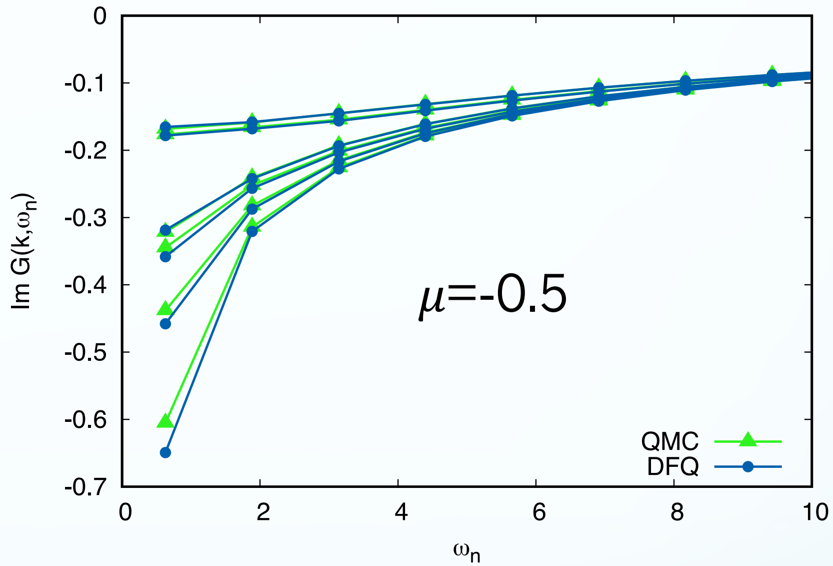
U/t=5.56 T/t=0.2



K-space test 4x4 system

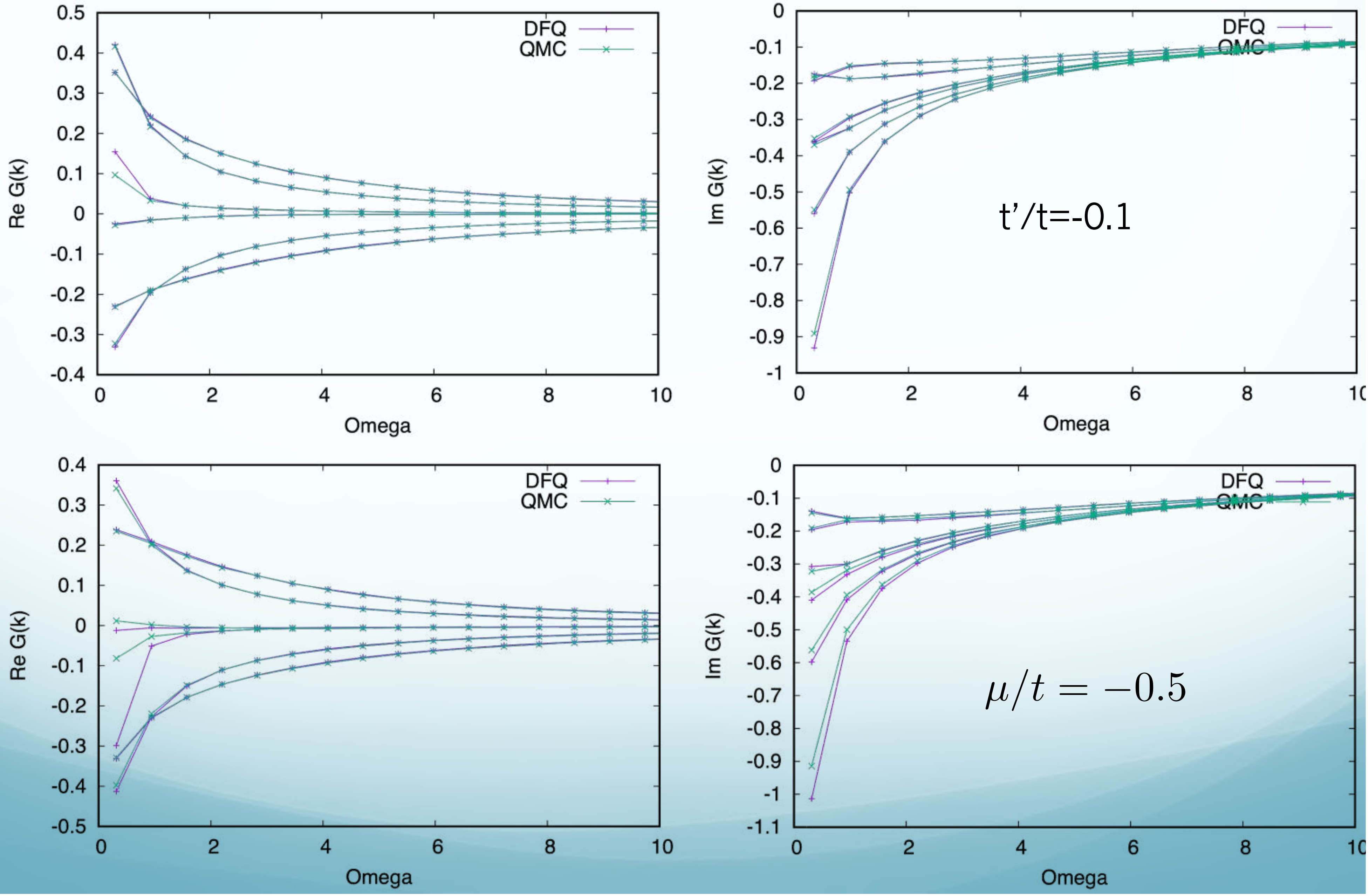
U/t=5.56 T/t=0.2





K-space test 4x4 system

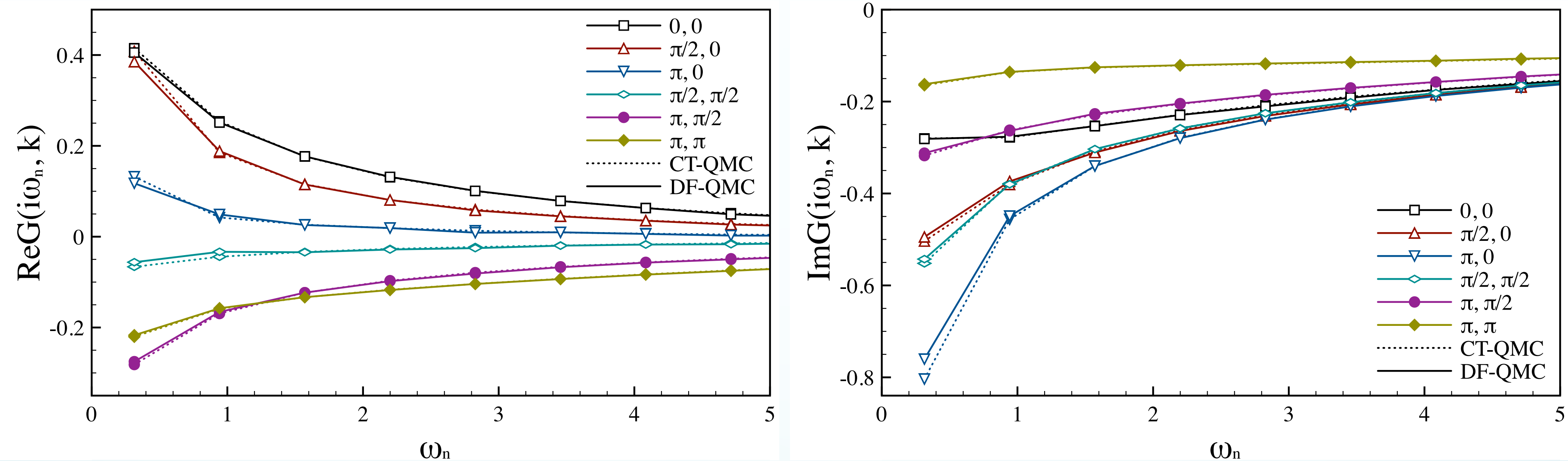
U/t=5.56 T/t=0.1



K-space test 4x4 system CT-INT

U/t=5.56 T/t=0.1

μ=-0.5
t'/t=-0.3



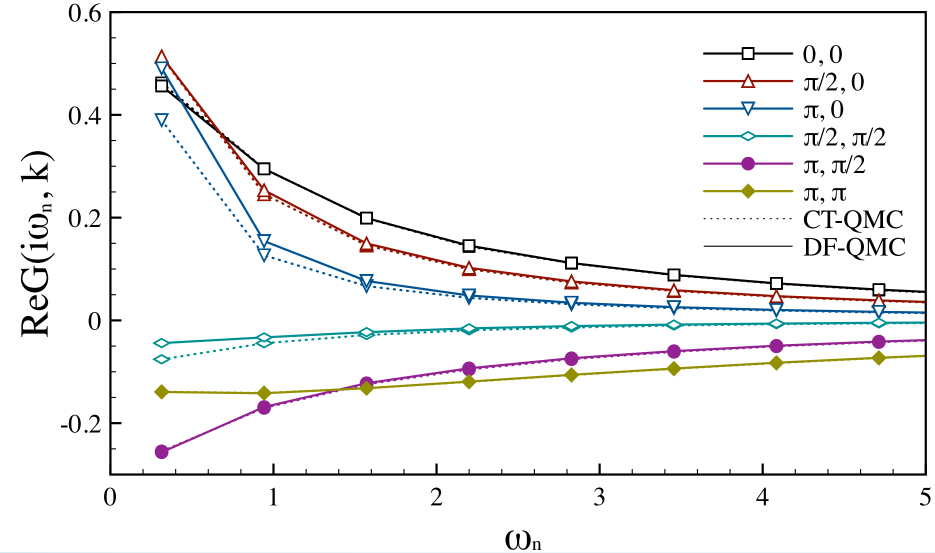
K-space test 4x4 system CT-INT

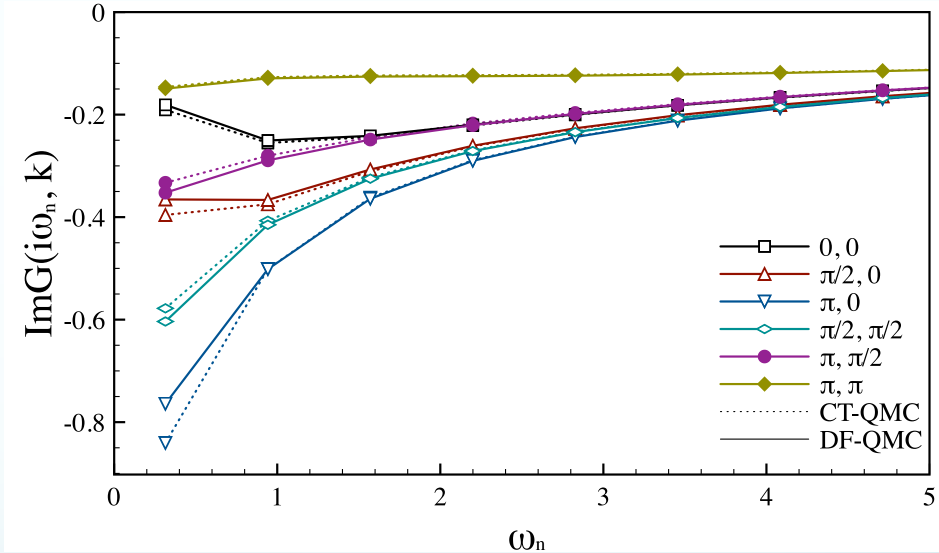
U/t=5.56 T/t=0.1

μ=0
t'/t=-0.3

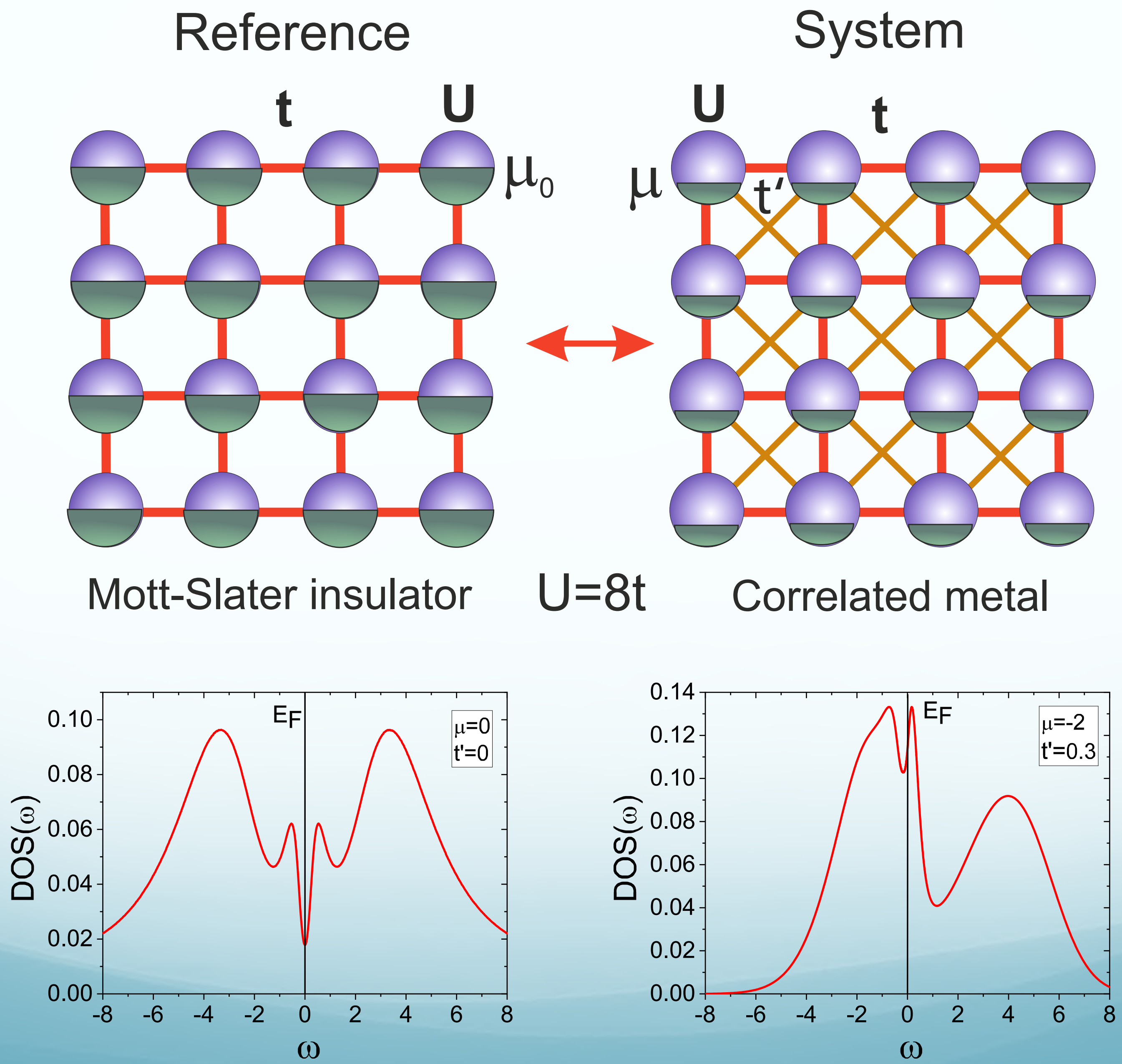
From Reference:

μ=0
t'/t=-0.1

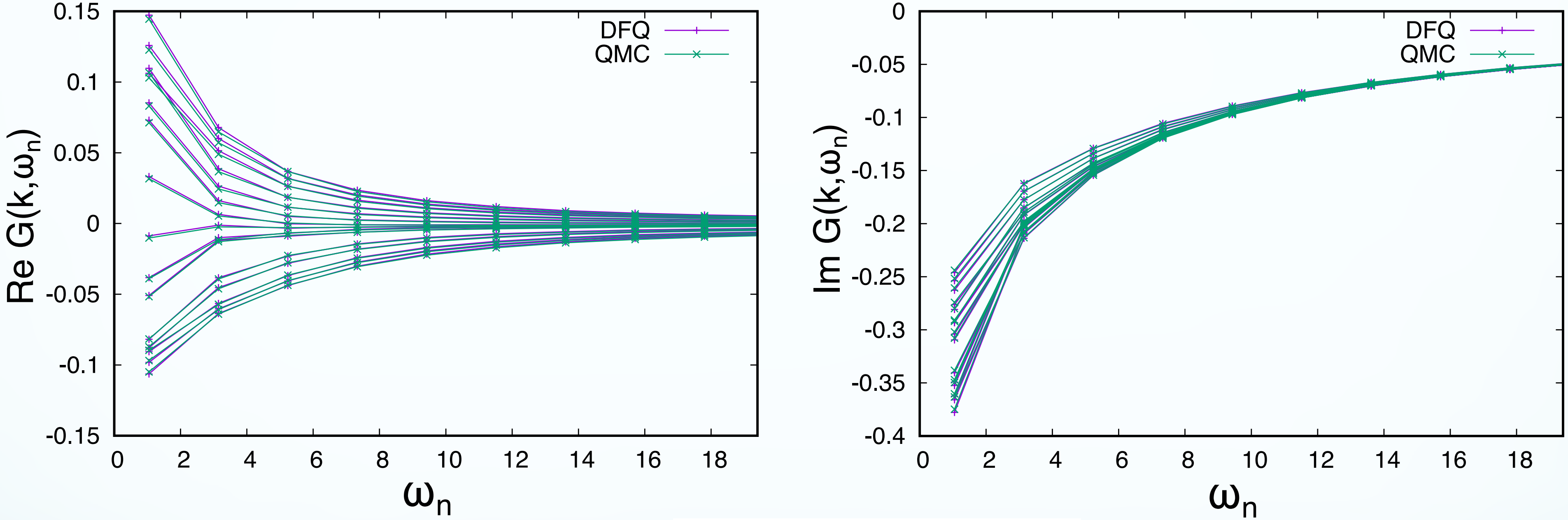




DF-QMC 8x8 CT-INT



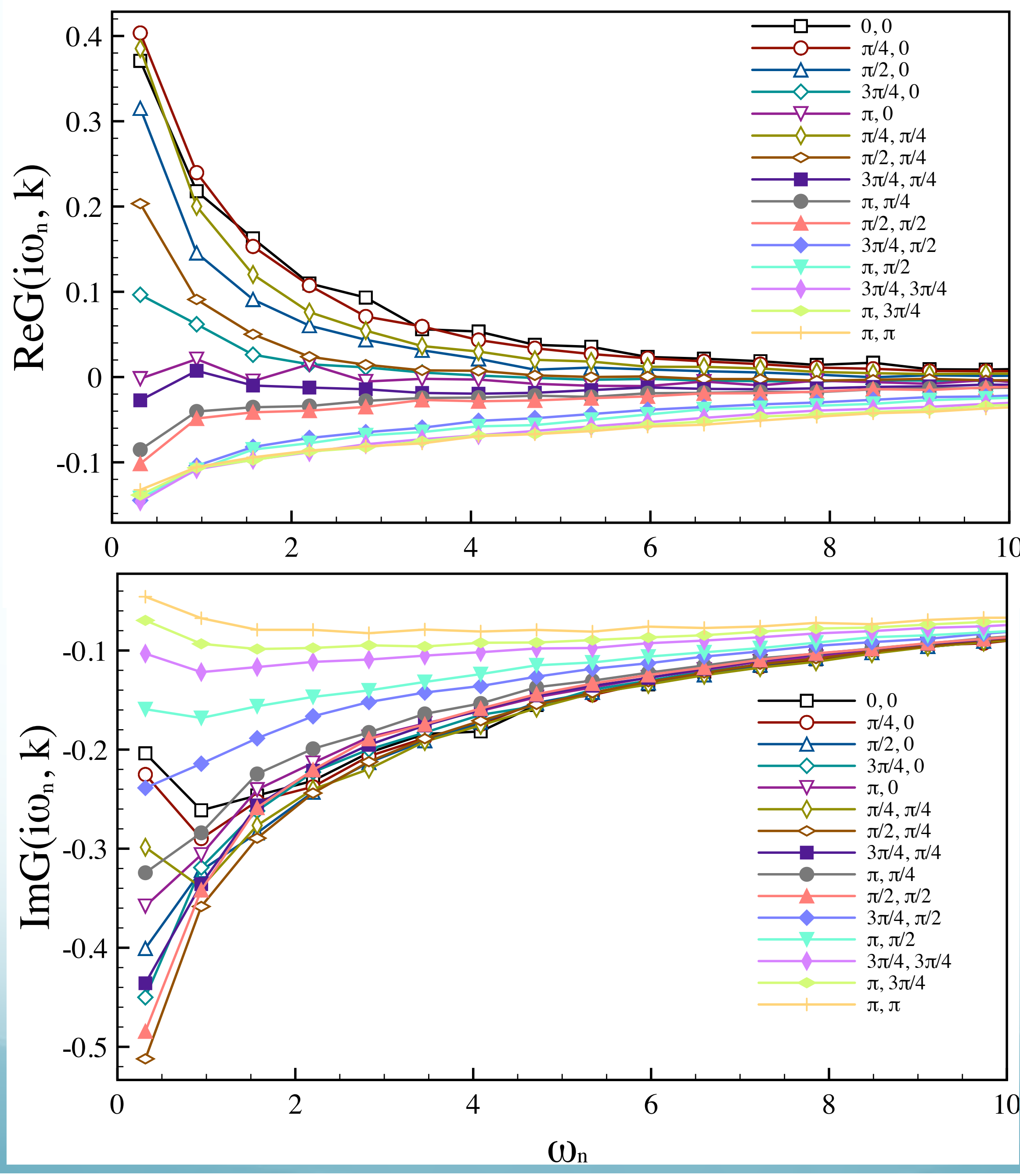
8x8 test DF-QMC vs. DQMC



β=3
U=5.56
t'/t=-0.15
μ=-0.5

Hirsch-Fye DQMC

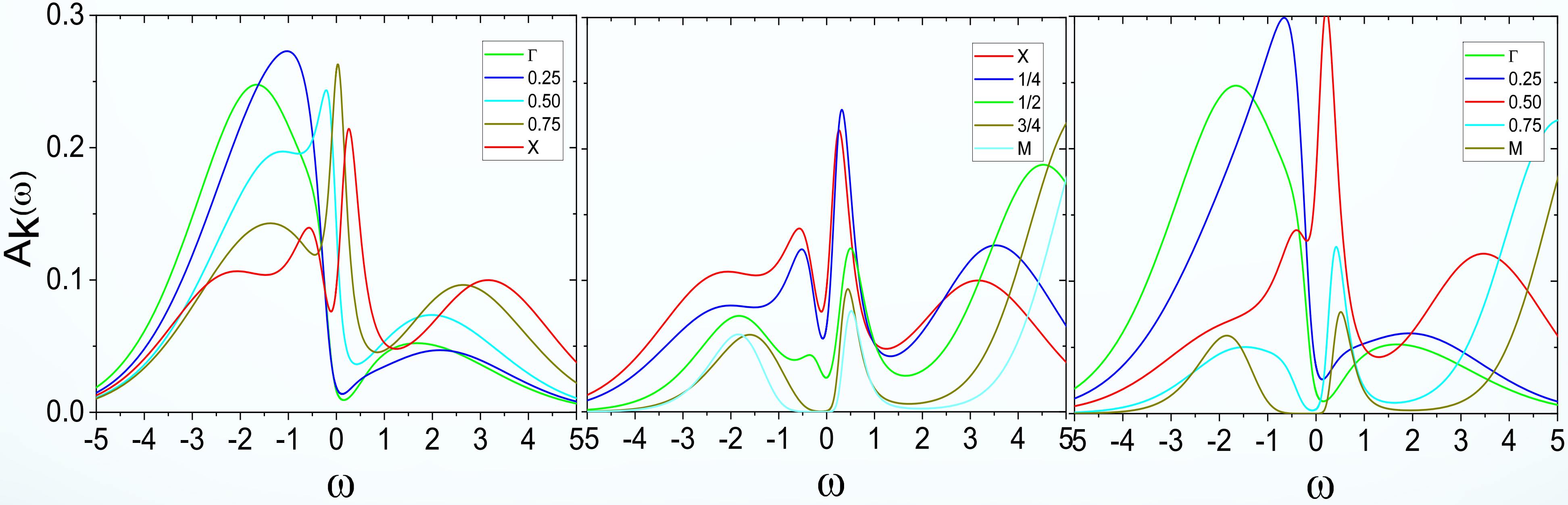
Matsubara Green's Function

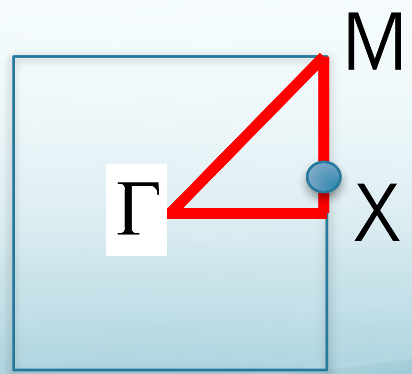


β=10
U=8
t'/t=-0.3
μ=-2
x=16%

CT-INT
Sergey
Iskakov

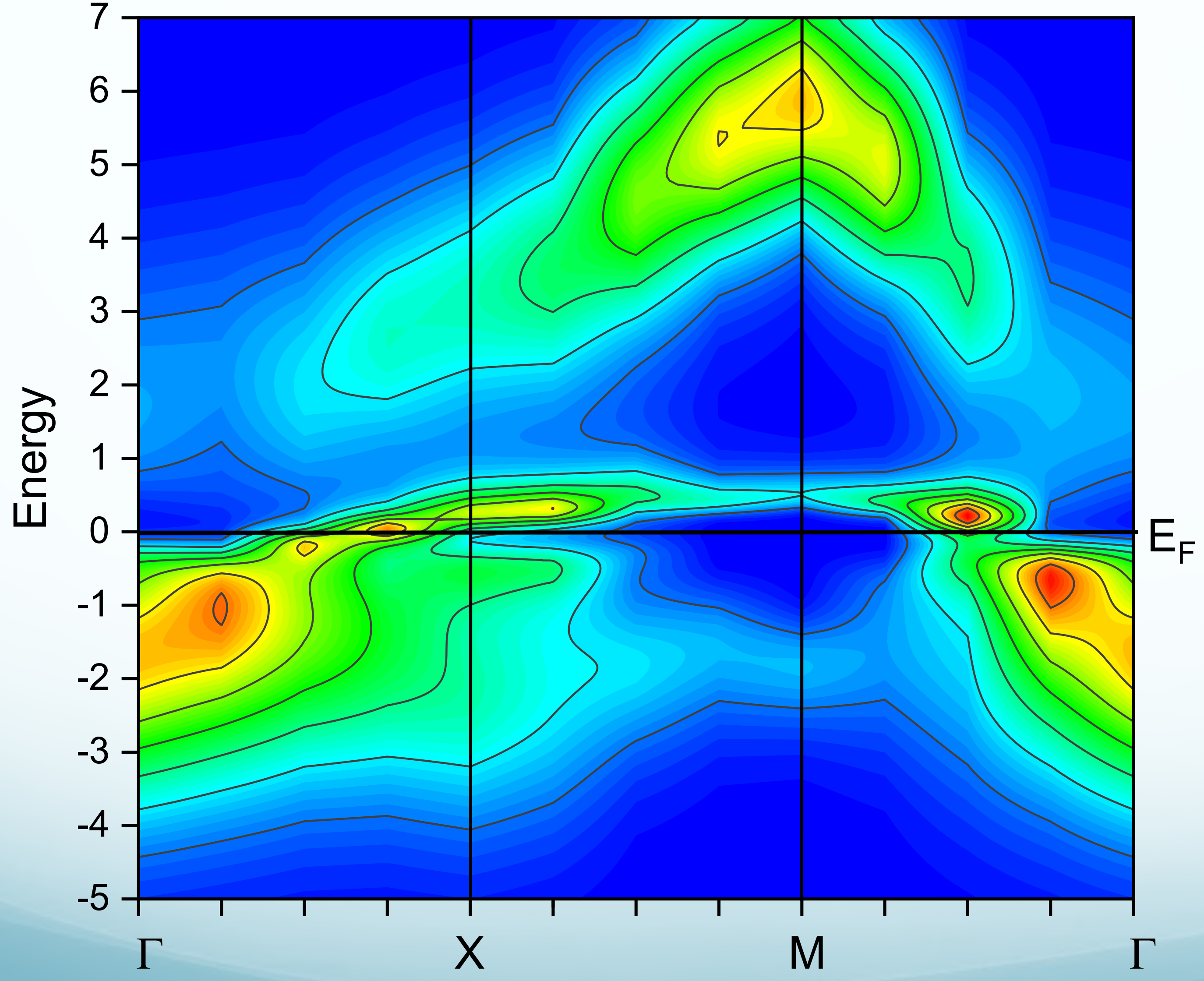
Spectral Function





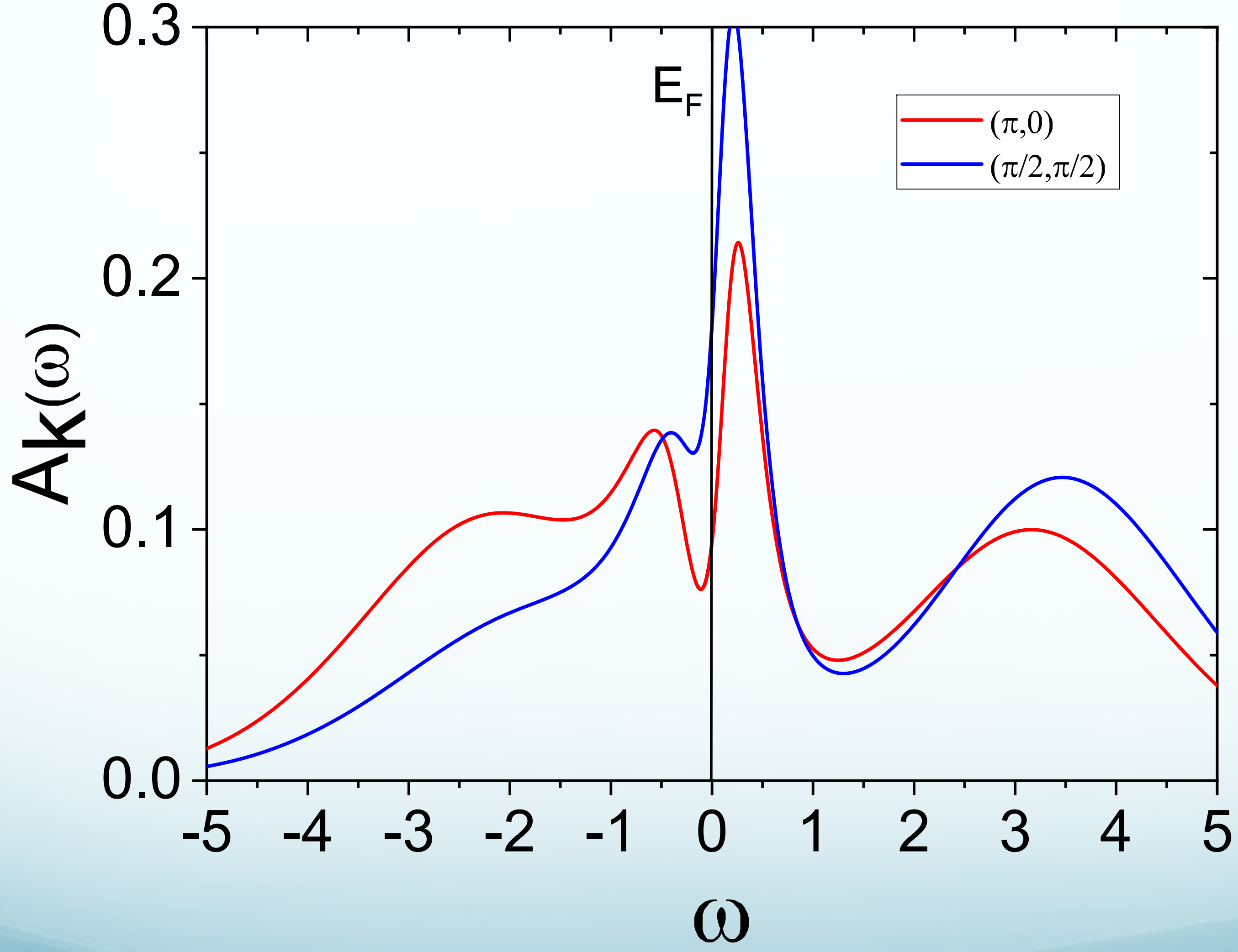
Strong PG
"shift" c.f.
F. Šimkovic, R. Rossi,
A. Georges, M. Ferrero,
arXiv:2209.09237

DF-QMC for 8x8: Spectral Function

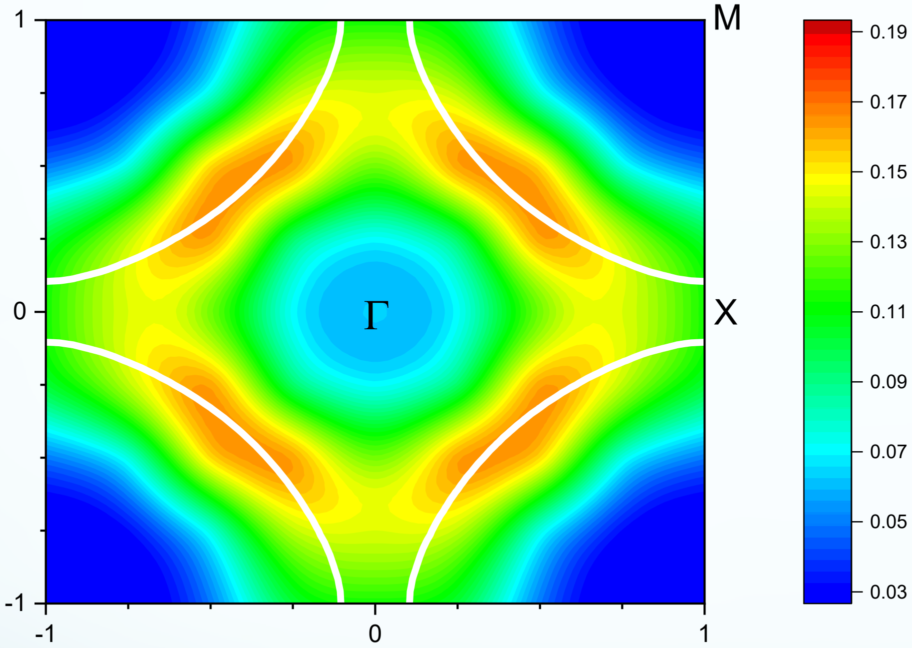


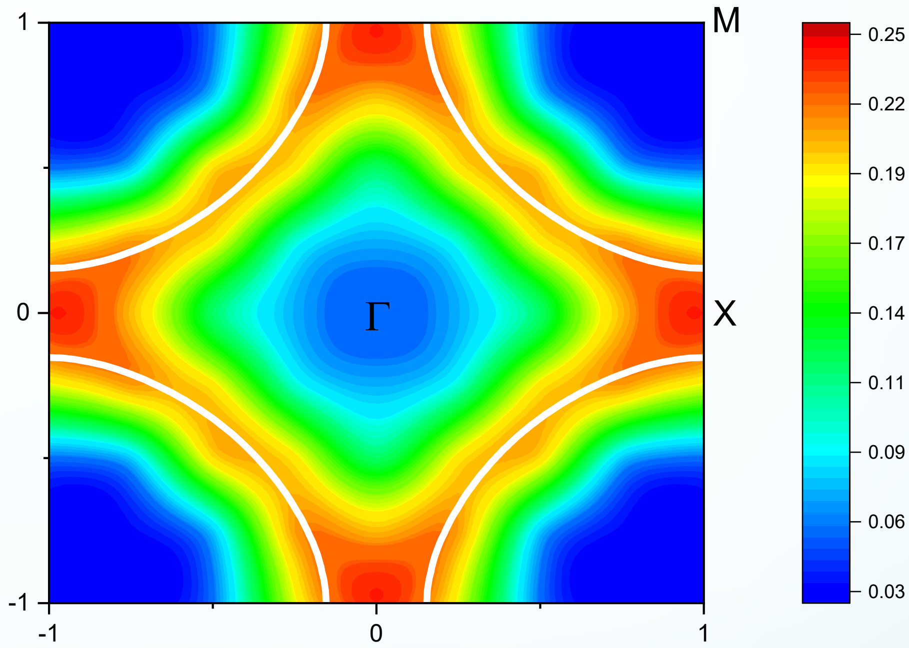
T=t/10
t'/t=-0.3
U=8
β=10
μ=-2
x=167%

Nodal-Antinodal dichotomy



Fermi Surface





U=8
t'/t=-0.3

U=5.6
t'/t=-0.3

Conclusions

- DF-diagram can be combined with Lattice DQMC to describe doped strongly correlated materials
- 1-st order response as function of doping and t’

Collaborations with:

Sergei Iskakov (MSU, Michigan)
Evgeny Stepanov (EPL, Paris)
Mikhail Katsnelson (RU, Nijmegen)