Collective modes of Hubbard model and phase diagram of cuprates

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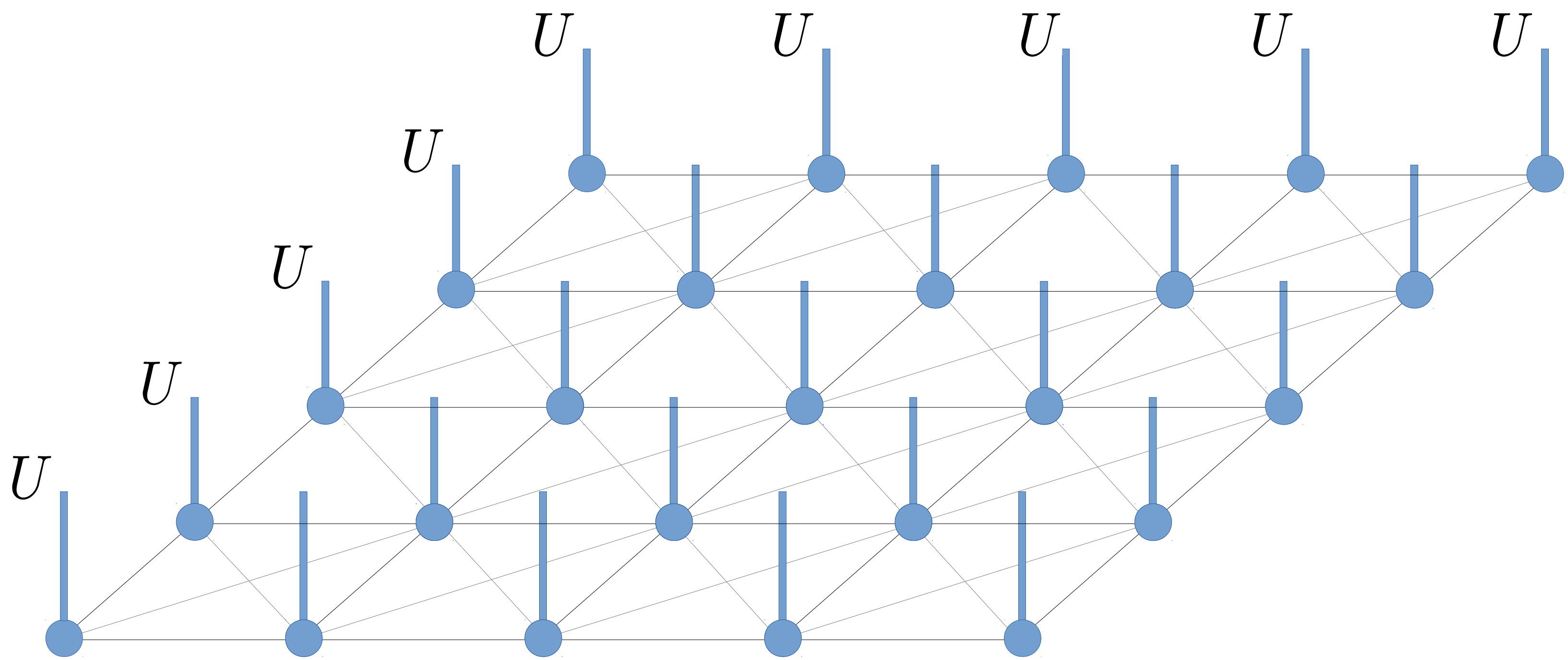
Kourovka 2020

"QUANTUM" = "INTERESTING"

Quantum materials:

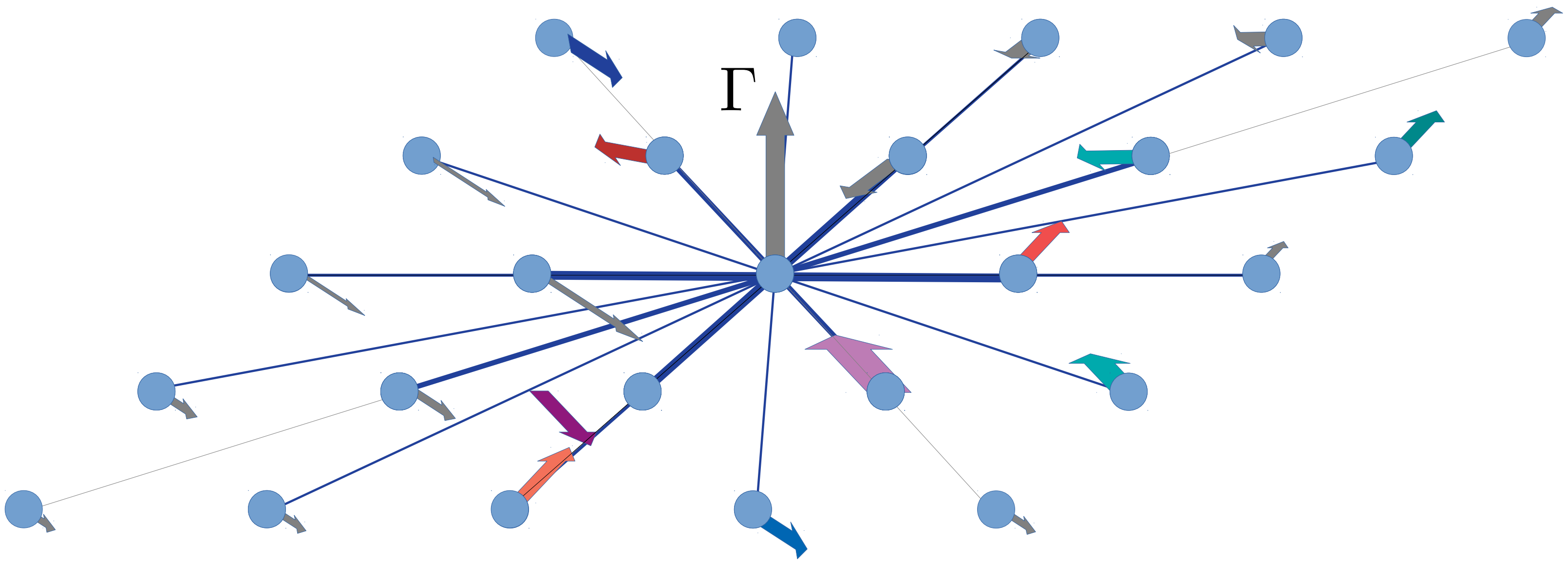
correlated, or topological, or Dirac, or whatever emergent



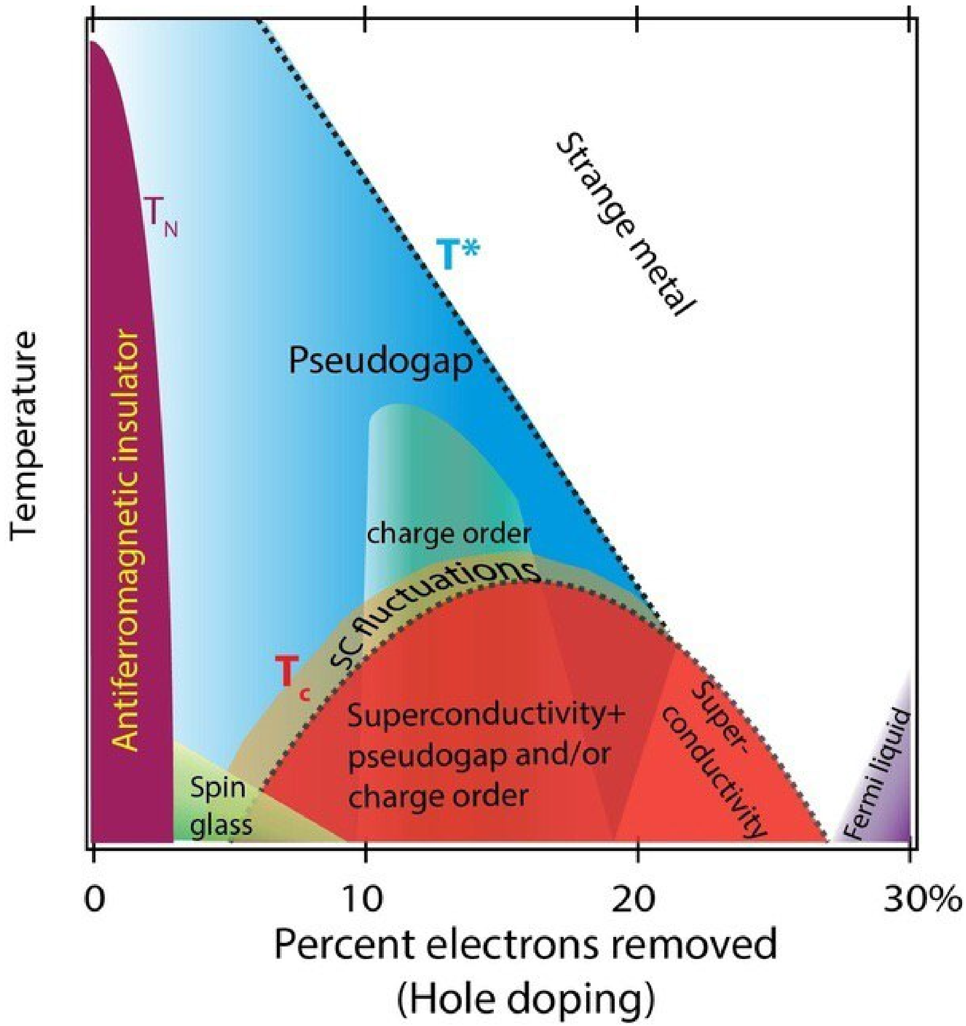
“ULTRA QUANTUM” = “VERY INTERESTING”

Ultraquantum materials:

Long-range correlated with complex low-energy physics



Theoretical challenges

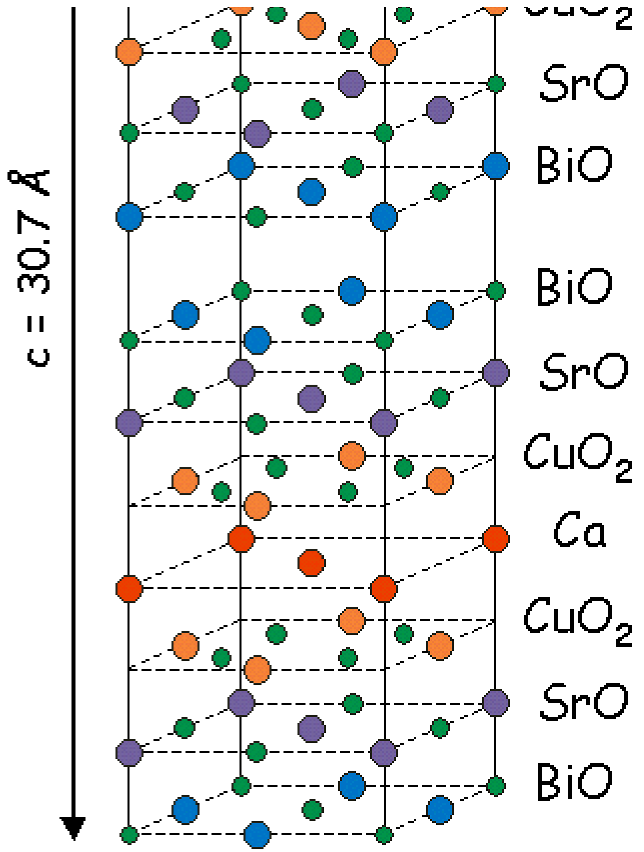


- Hard to solve
- Many scales
- Rich phase diagram

- A method controlling relevant lengths and energies is needed

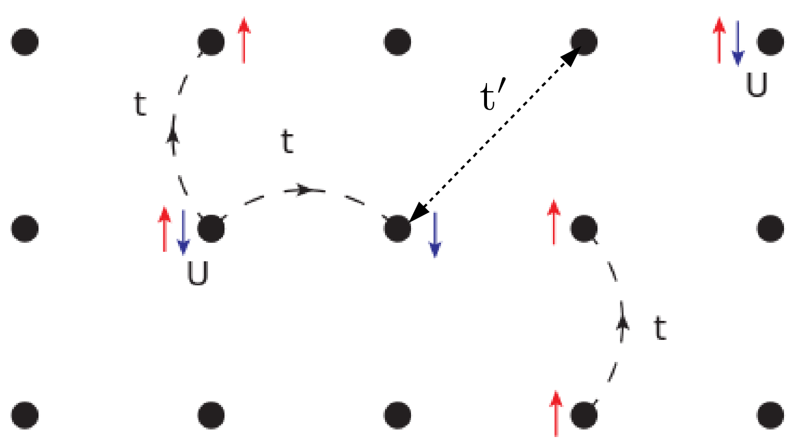
BSCCO structure & Hubbard model

$Bi_2Sr_2CaCu_2O_{8+x}$



picture from http://hoffman.physics.harvard.edu

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



! reach physics at different scales !

What has been done so far...

- DMRG 4x32, Tohyama 2018

  T=0 SC

- DCA 4x4, Maier 2005

  SC dome

- Parquet 6x6, Tam 2013

  No SC

- DF, Otsuki 2014

  SC, no dome

- DΓA, DMFT+FLEX, Kitatani 2018

  SC dome

- FRG

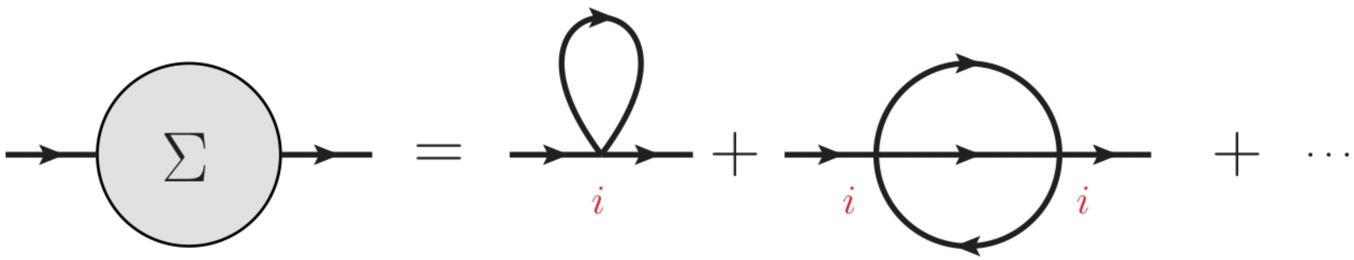
  SC dome

Teaser for our method

- We assume that high-energy part of correlations is local

  and threat local phenomena exactly.
- We suppose that non-local correlations are related with low-energy collective fluctuations. Mutual interactions of different collective modes is kept through parquet formalism.
- Trade-off: neglecting high-frequency non-local correlations allowed for higher momentum resolution (parquet equations are solved for up to 32x32 lattices).

Local correlations



- Single-particle properties are mostly affected by local correlations

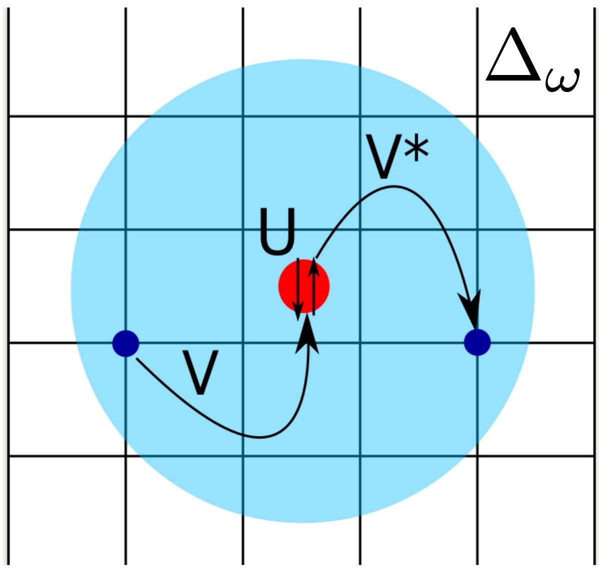
$$G^{(0)} = \frac{1}{\omega - \varepsilon_k - \Sigma_\omega}$$

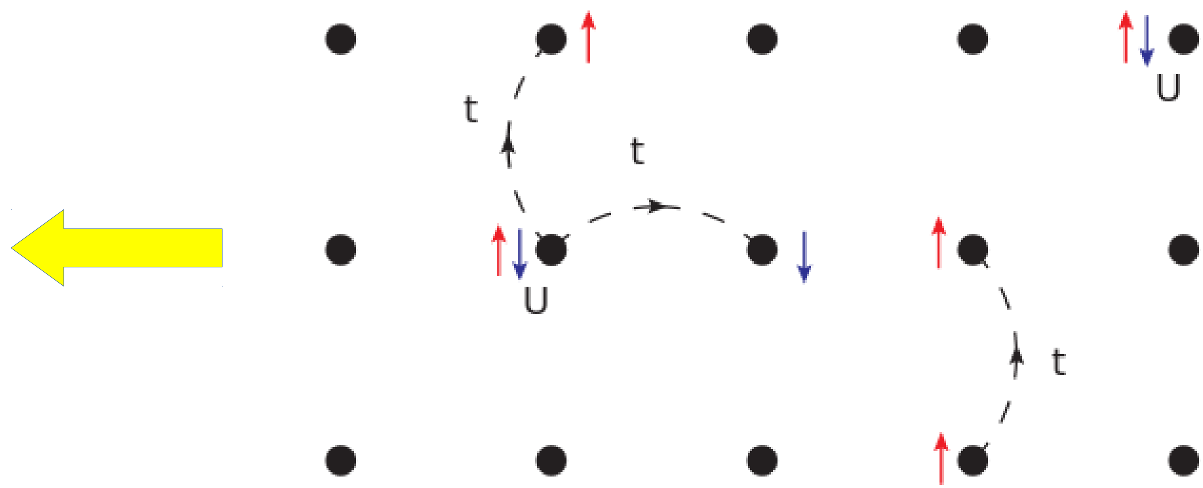
- The main effect is DOS-effective mass renormalization

$$G^{(0)}_{\omega\to 0} = \frac{Z}{\omega - Z\varepsilon_k}, \quad Z = \frac{1}{1 - \partial_\omega \Sigma_{\omega\to 0}}$$

Dynamical Mean Field Theory

$$S = S_{at}[c^\dagger, c] + \iint_0^\beta \Delta_{\tau-\tau'} c^\dagger_\tau, c_{\tau'} d\tau d\tau'$$



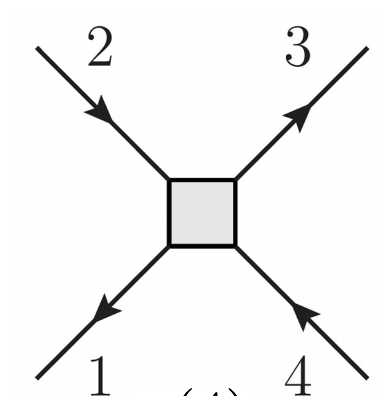


Diagrammatics around local approximation (dual fermions)

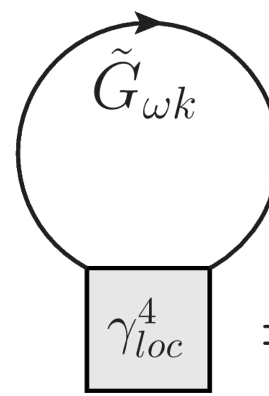
$$S[c,c^\dagger] = \sum_{\omega k\sigma}(-i\omega + \epsilon_k - \mu)c^\dagger_{\omega k\sigma}c_{\omega k\sigma} + U\sum_i \int_0^\beta n_{i\uparrow\tau}n_{i\downarrow\tau}$$

$$S[f,f^\dagger] = \sum_{\omega k\sigma} \underbrace{g_\omega^{-2}\left((\Delta_\omega - \epsilon_k)^{-1} + g_\omega\right)}_{-\tilde{G}_0^{-1}} f^\dagger_{\omega k\sigma}f_{\omega k\sigma} + \sum_n \gamma^{(n)}_{\mathrm{loc}}$$

$$\frac{1}{G_0^{-1}(\omega,k) - \Sigma_\omega} - g_\omega$$



$\gamma^{(4)}_{\mathrm{loc}}$

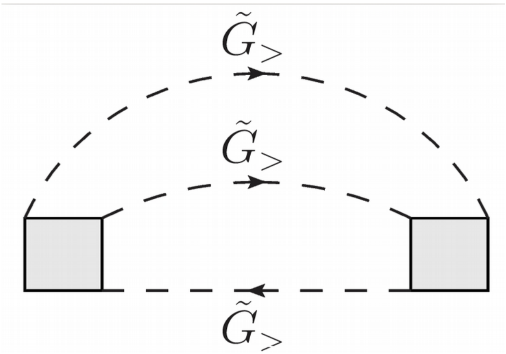


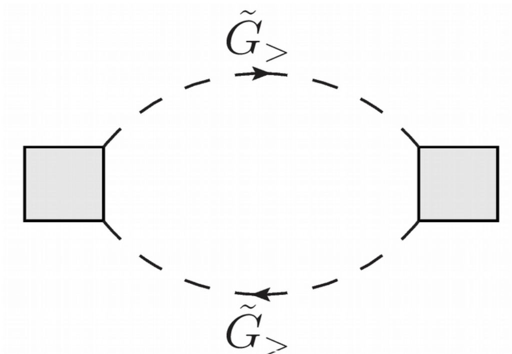
$= 0$

Low-energy action

$$S[f^\dagger, f] = \sum_{\omega k \sigma} -\tilde{G}_0^{-1} f^\dagger_{\omega k \sigma} f_{\omega k \sigma} + \sum_n \gamma^{(n)}_{\text{loc}}$$

$$S_< = -\sum \mathcal{G}_{12}^{-1} f^\dagger_{1<} f_{2<} + \sum \mathcal{J}_{1234} f^\dagger_{1<} f_{2<} f^\dagger_{3<} f_{4<}$$

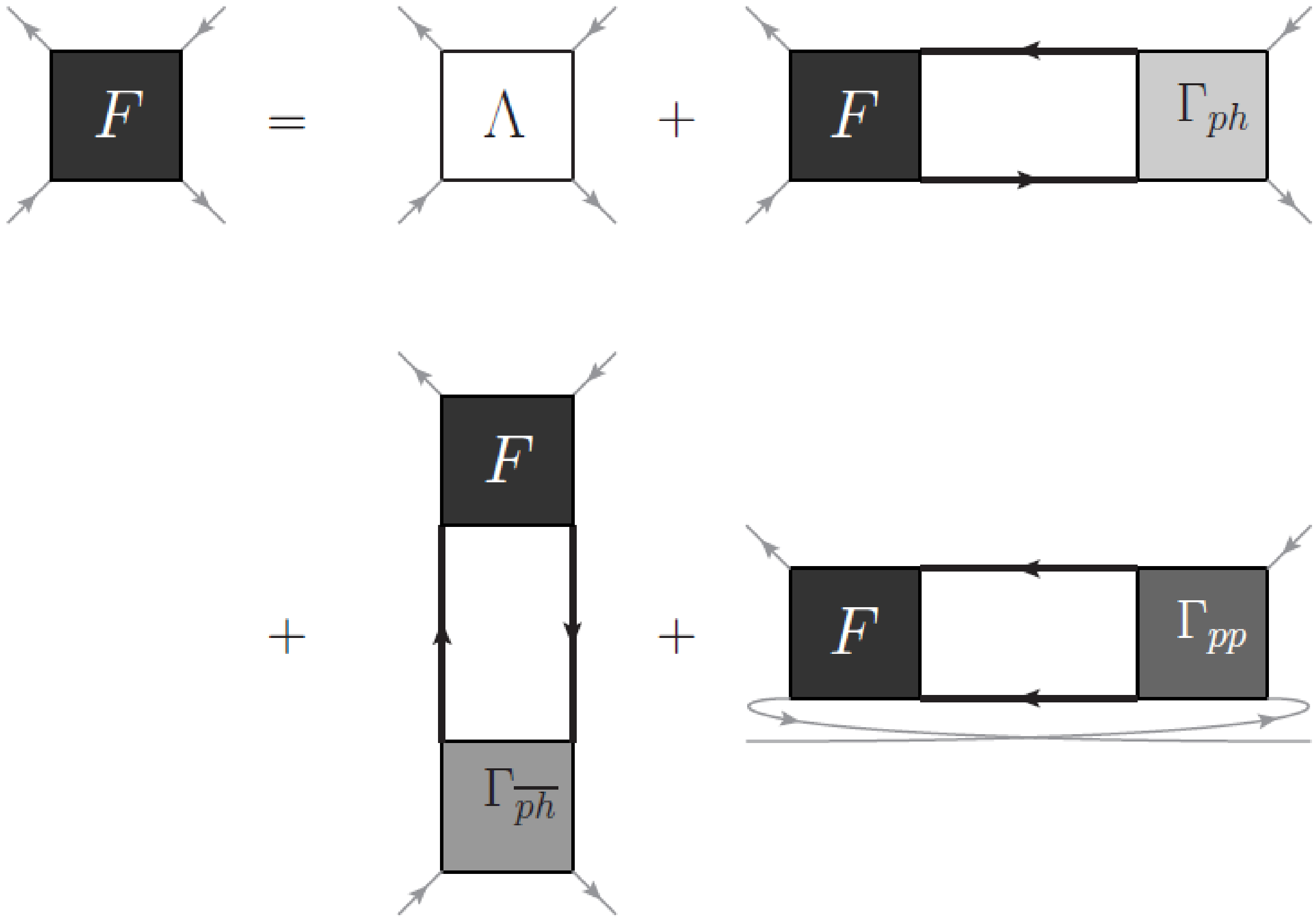




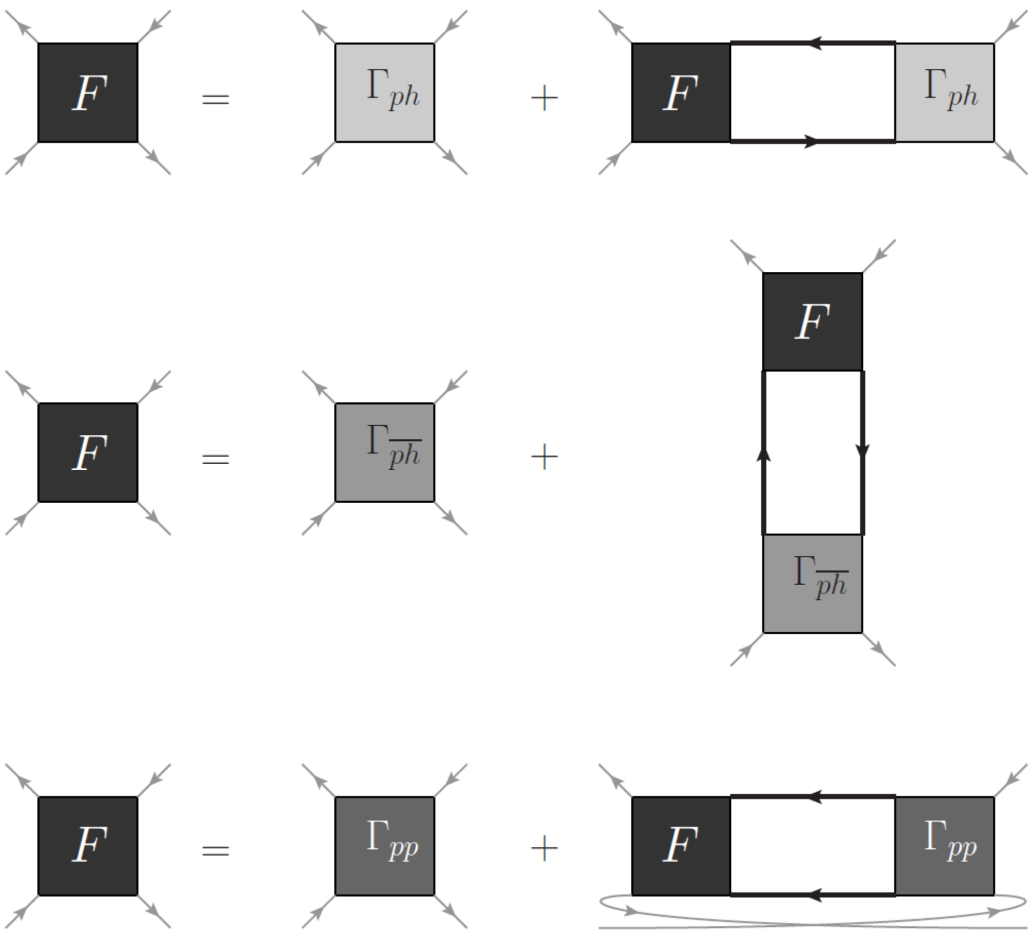
$$f = f_< + f_>$$

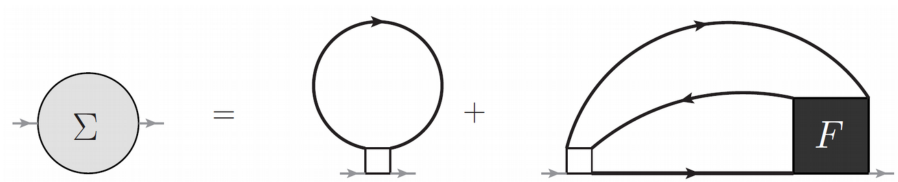
$$f^{(\dagger)}_< = \begin{cases} f^{(\dagger)}_{\omega k \sigma}, & \text{for } |\omega| = \pi T \\ 0, & \text{for } |\omega| > \pi T \end{cases}$$

Parquet formalism

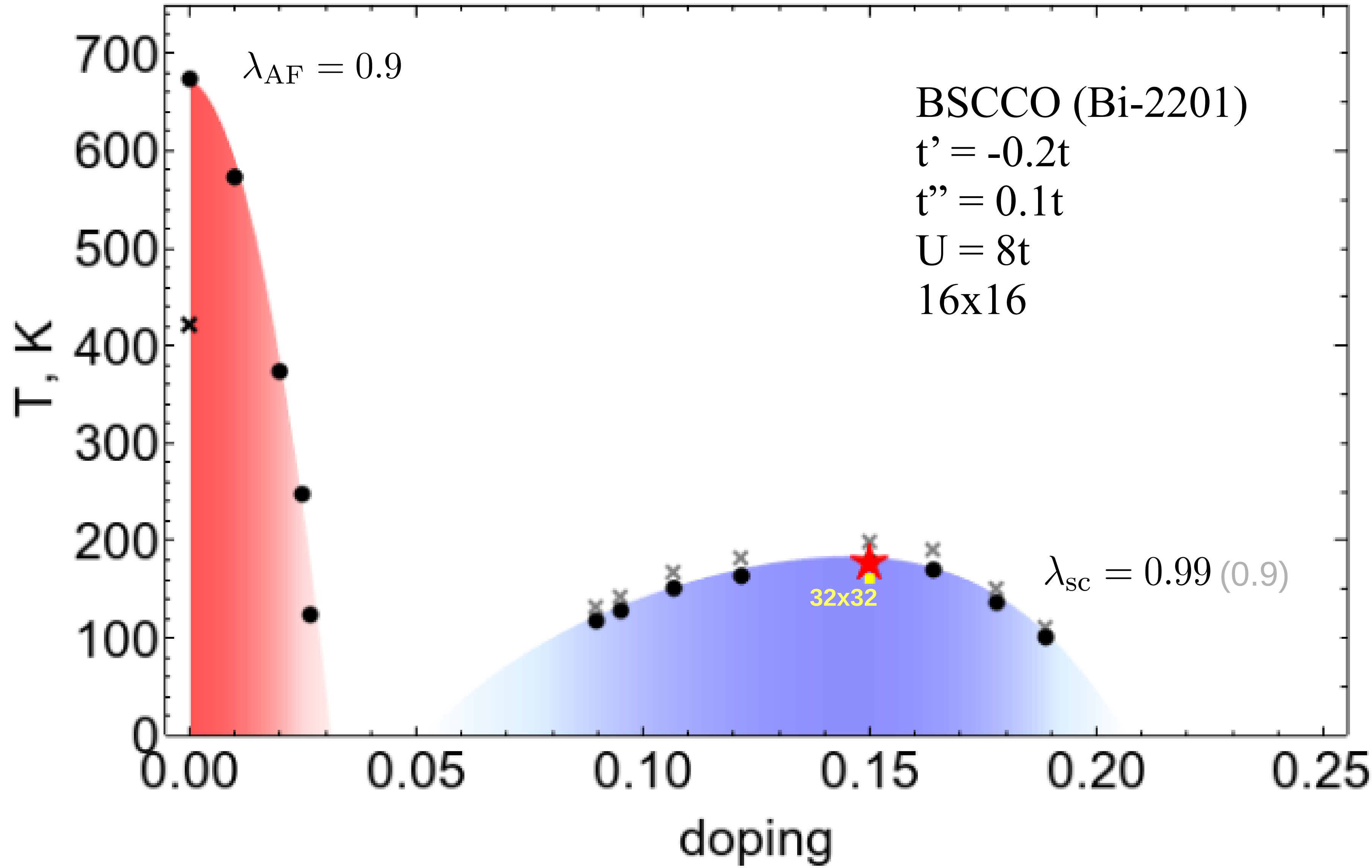


Bethe-Salpeter & Dyson equations



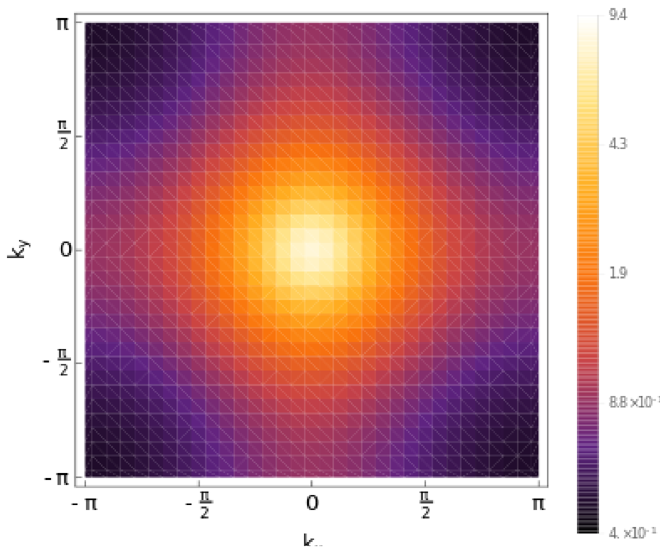


Phase diagram

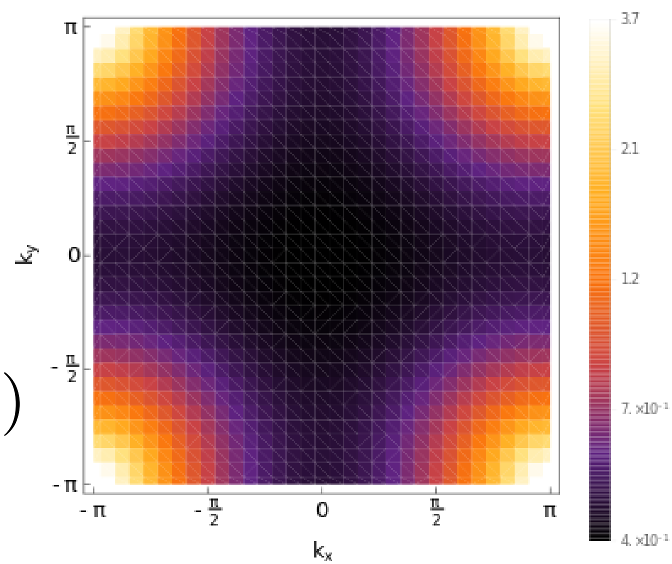


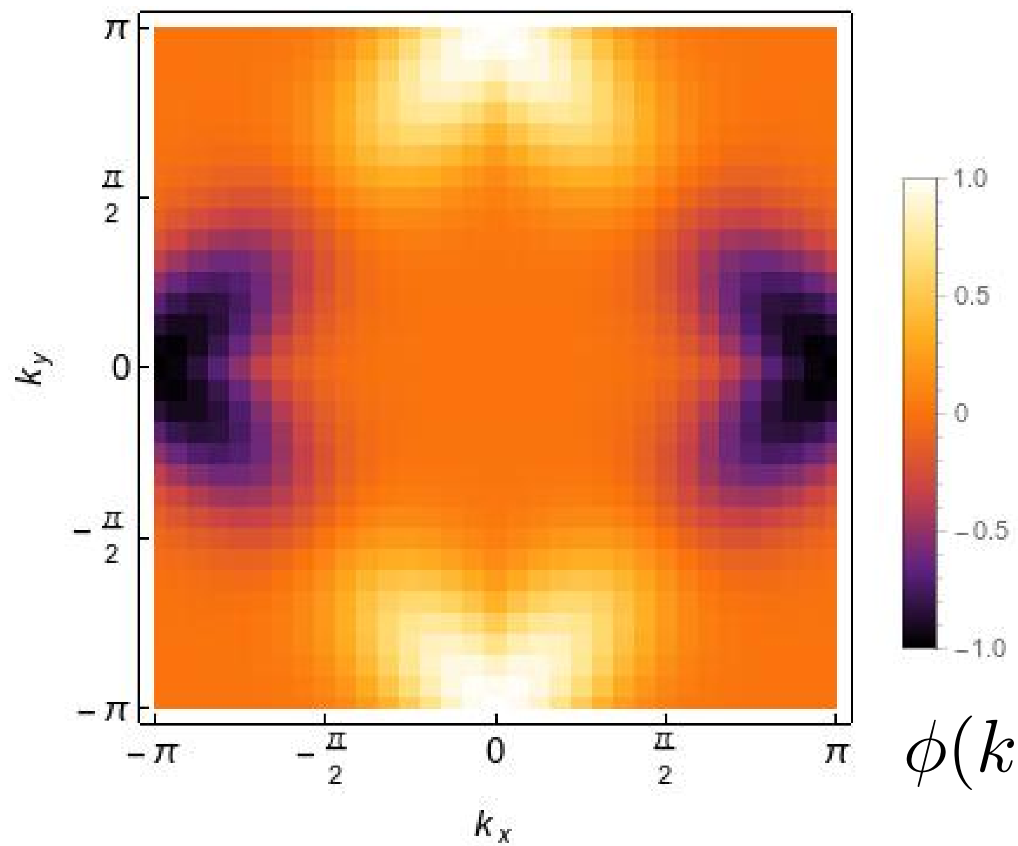
D-wave superconductivity and antiferromagnetism, 32x32 lattice

$\chi_{\mathrm{SC}}(k)$



$\chi_{\mathrm{AF}}(k)$

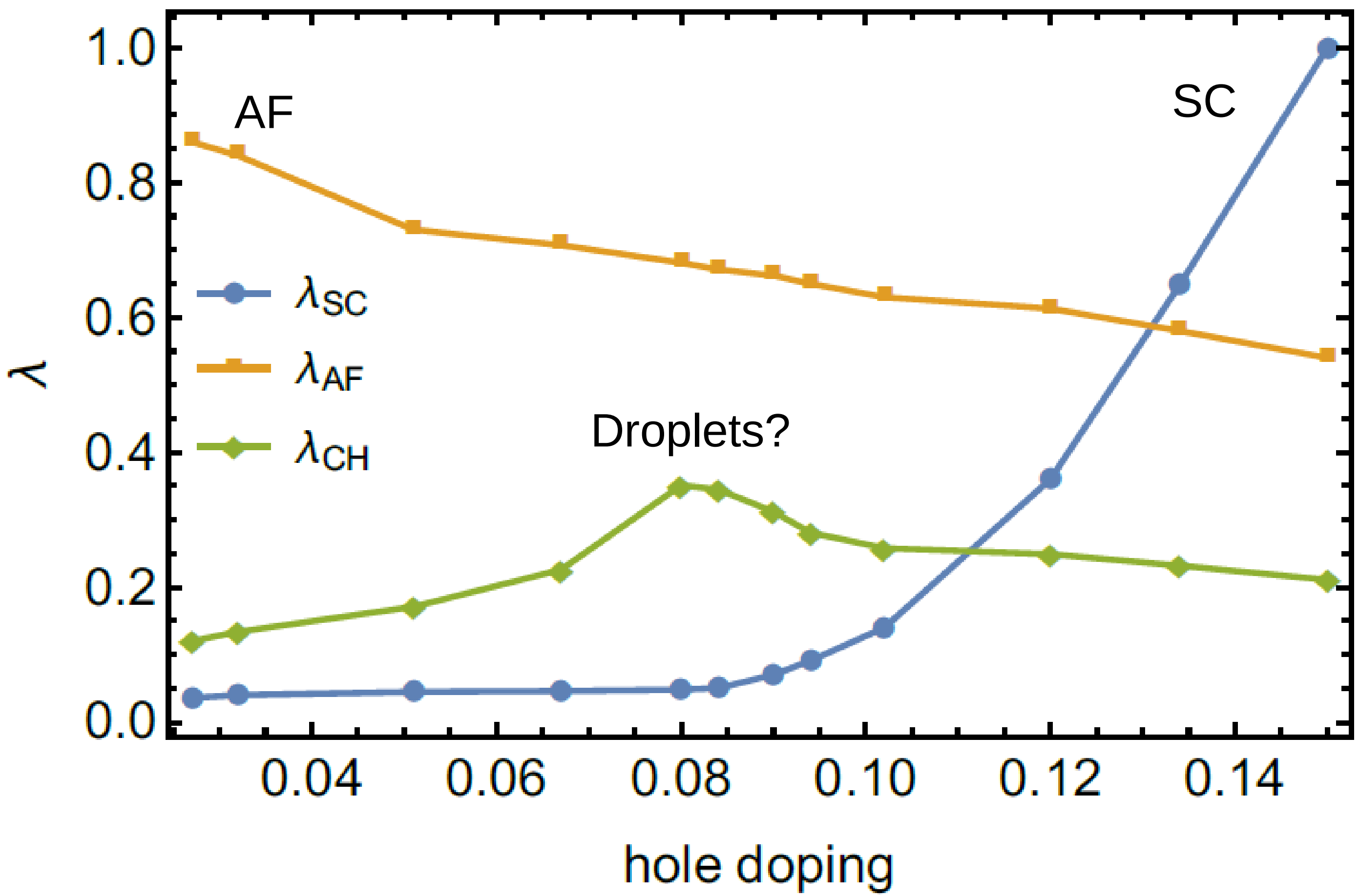


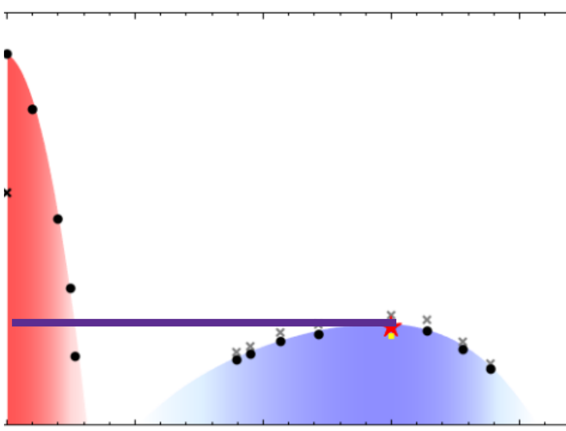


$\phi(k)$

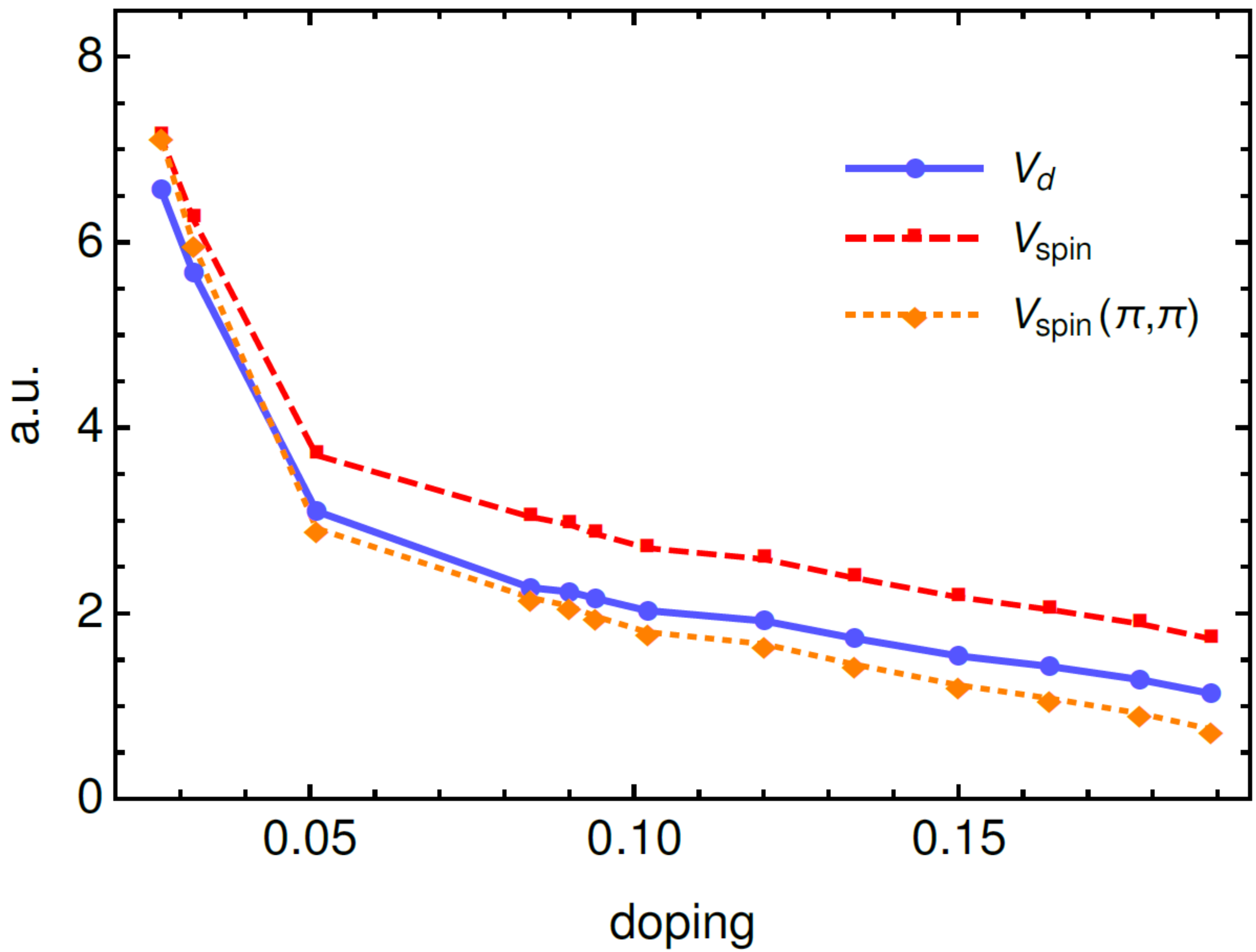
$$(-\chi^0_{\mathrm{pair}}\Gamma^{pp})\phi \; = \lambda_{SC}\phi$$

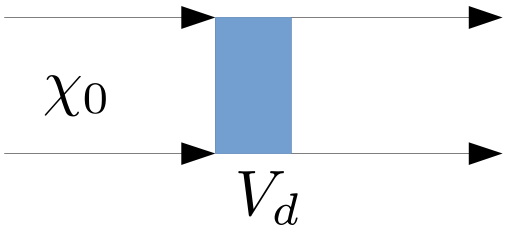
Leading eigenvalues in different channels, fixed T

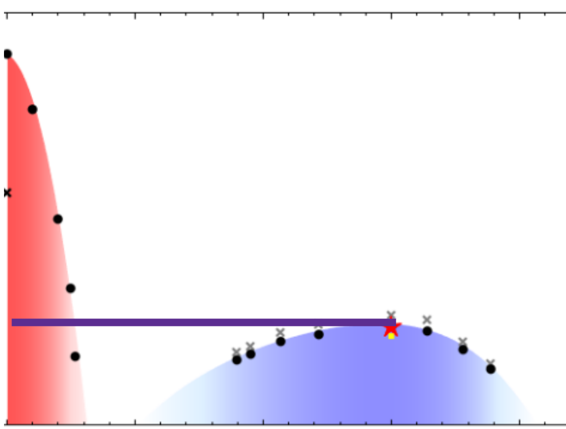




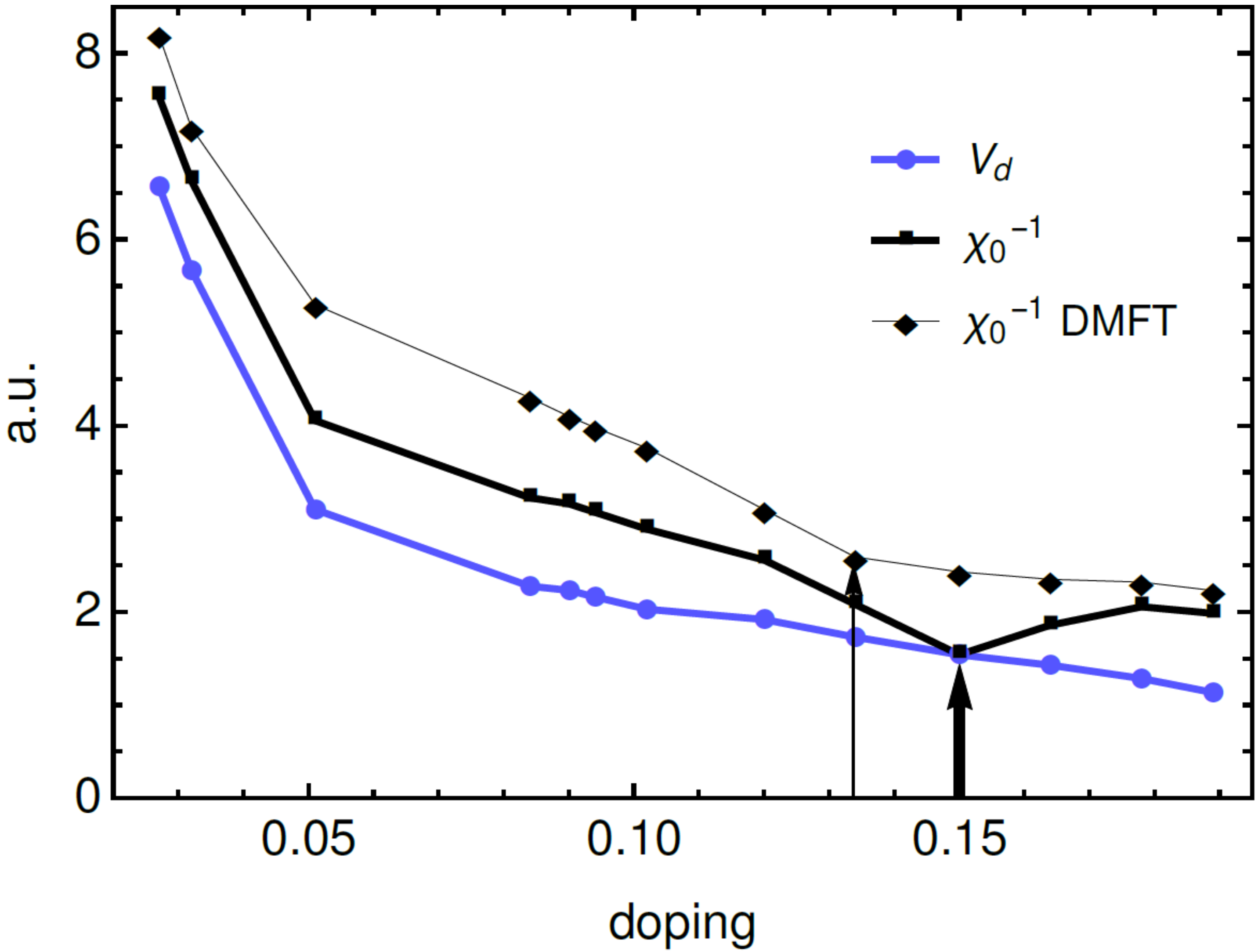
Efective interaction, fixed T

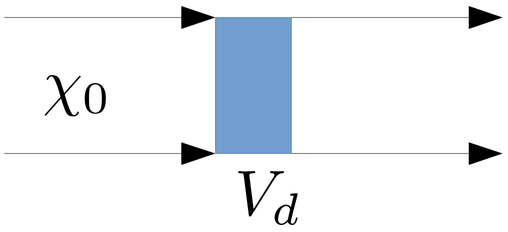


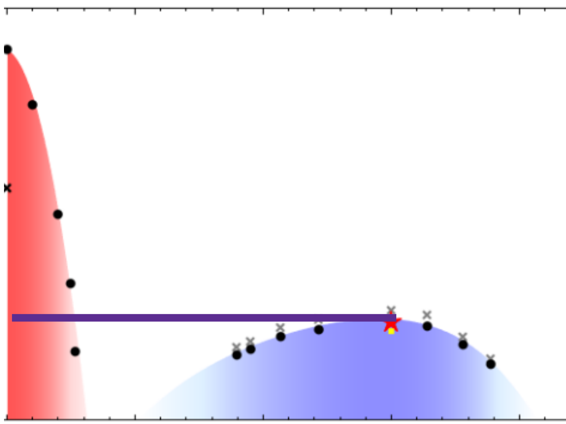




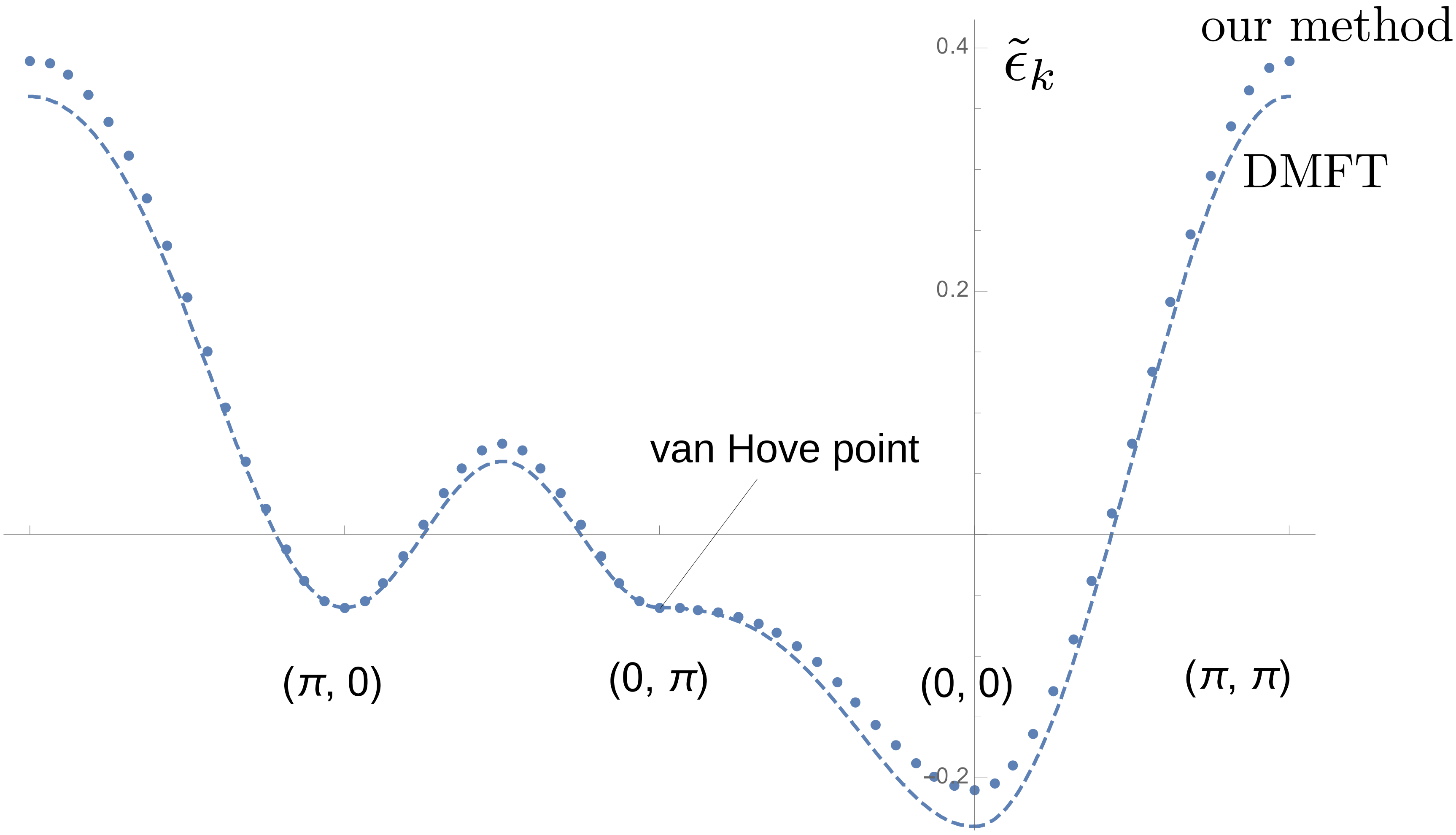
P-p buble vs effective interaction, fixed T



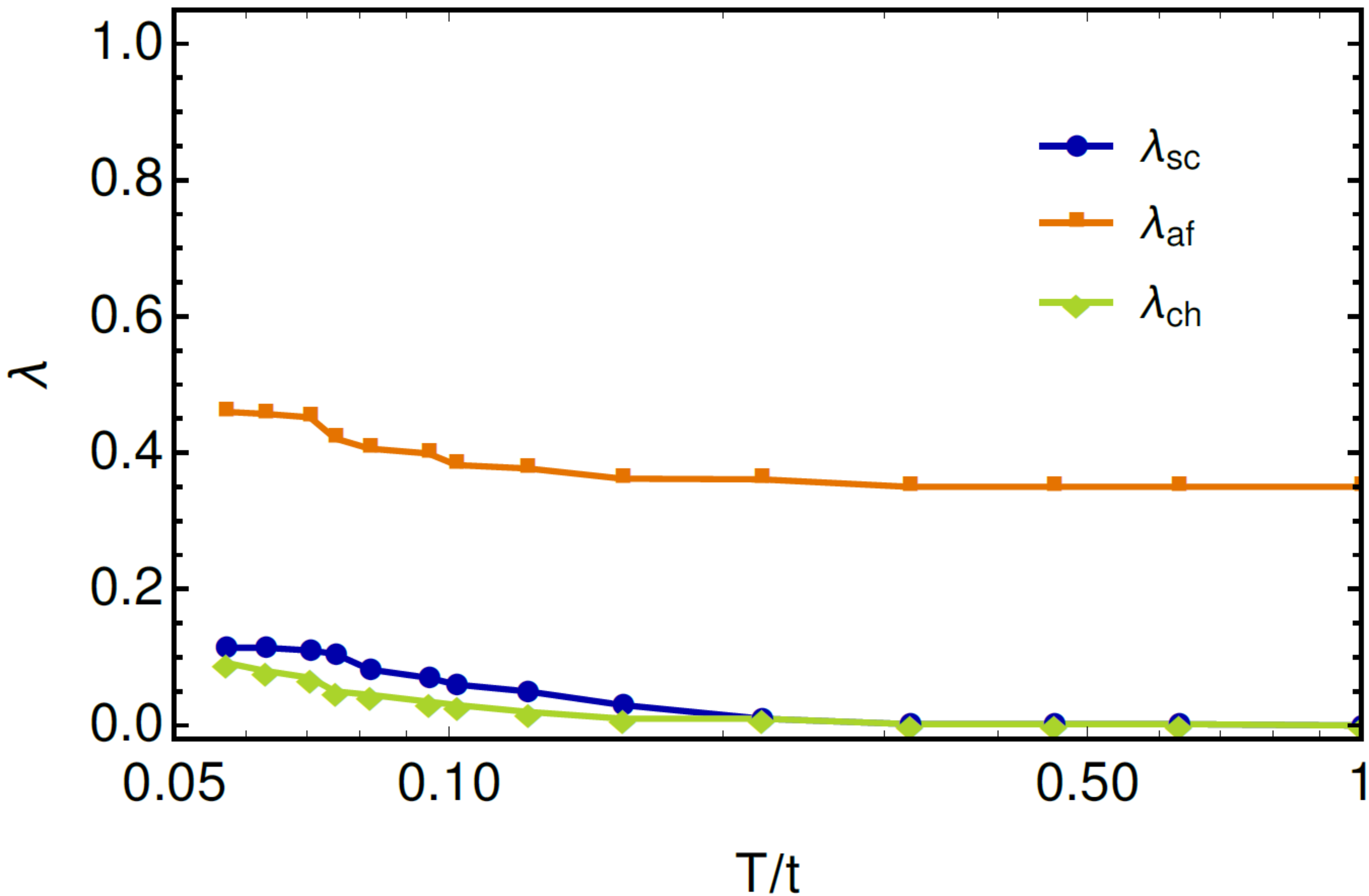




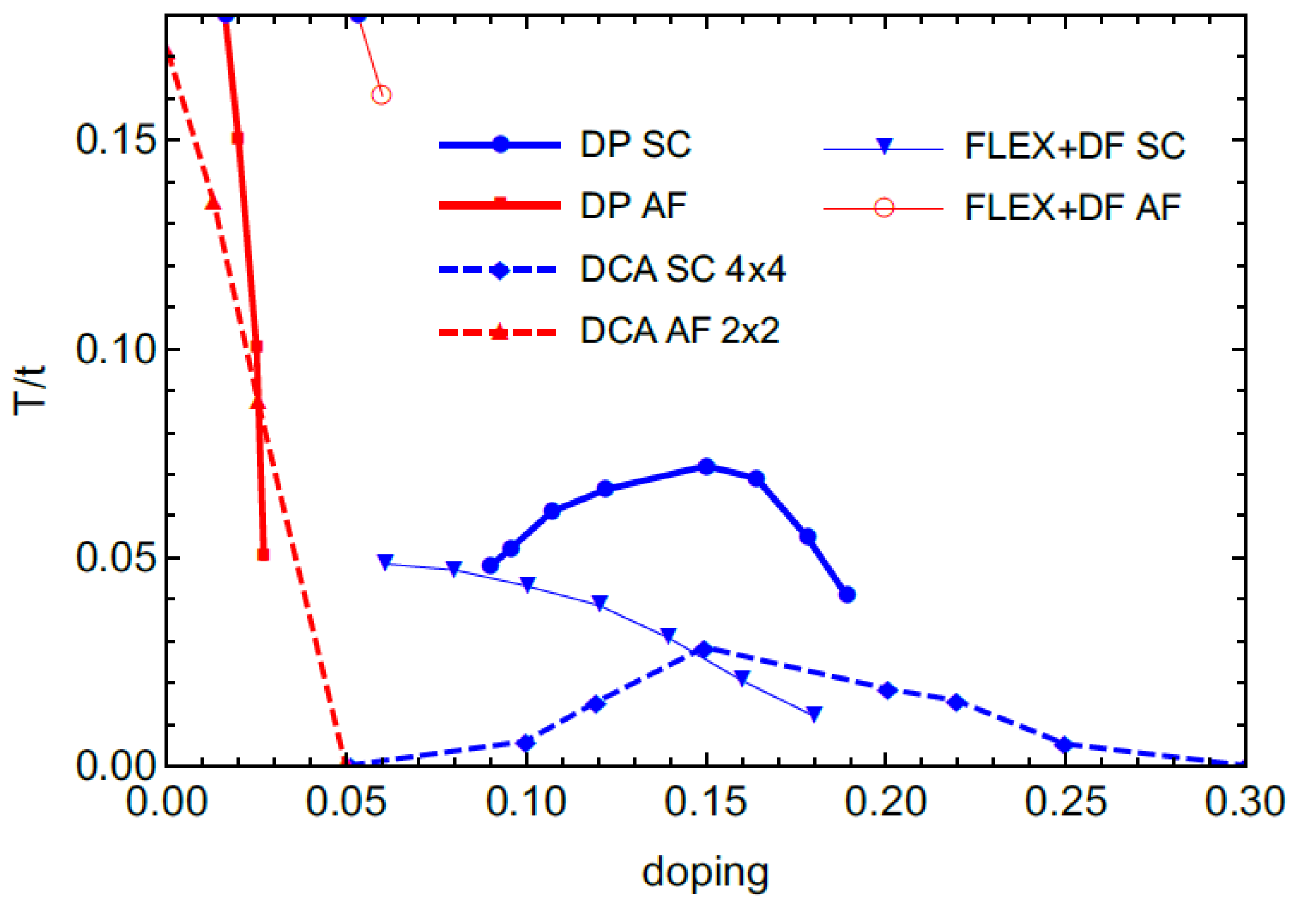
1p quantities: effective dispersion



“Pure Hubbard” – no superconductivity

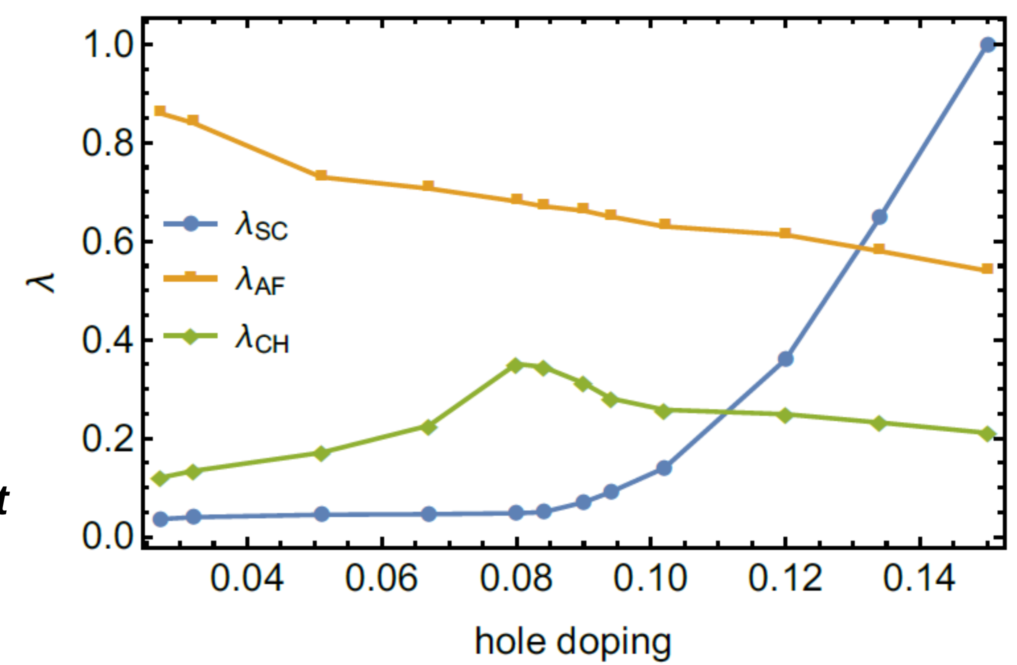


Phase diagram: comparison with others



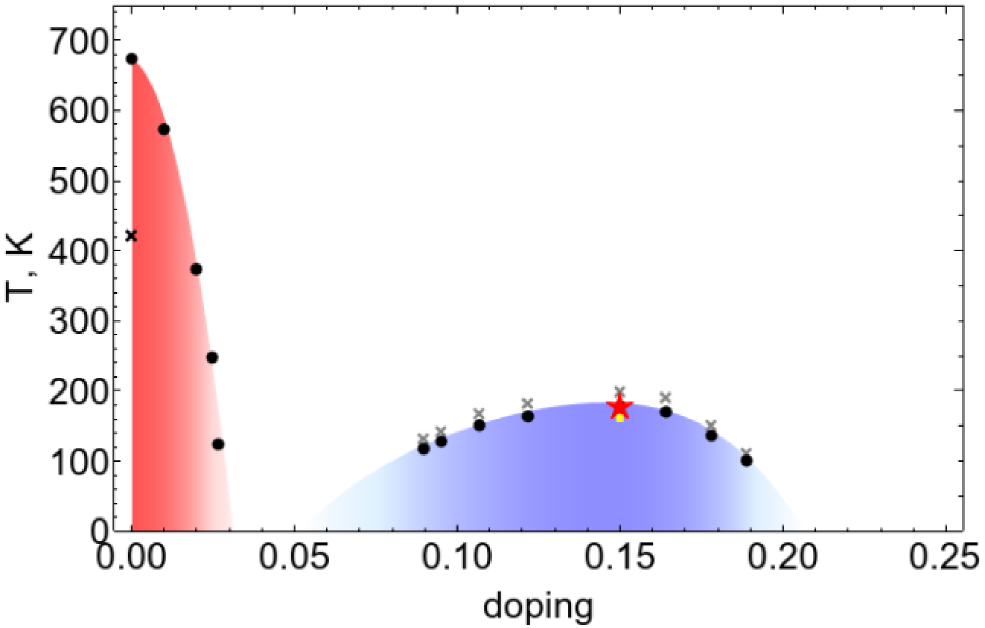
Phase diagram for different methods: dual-fermion parquet for $U = 8t$, $t' = -0.2t$, $t'' = 0.1t$, dual-fermion FLEX for $U = 8t$, $t' = t'' = 0$, DCA for $U = 6t$, $t' = -0.2t$, $t'' = 0$.

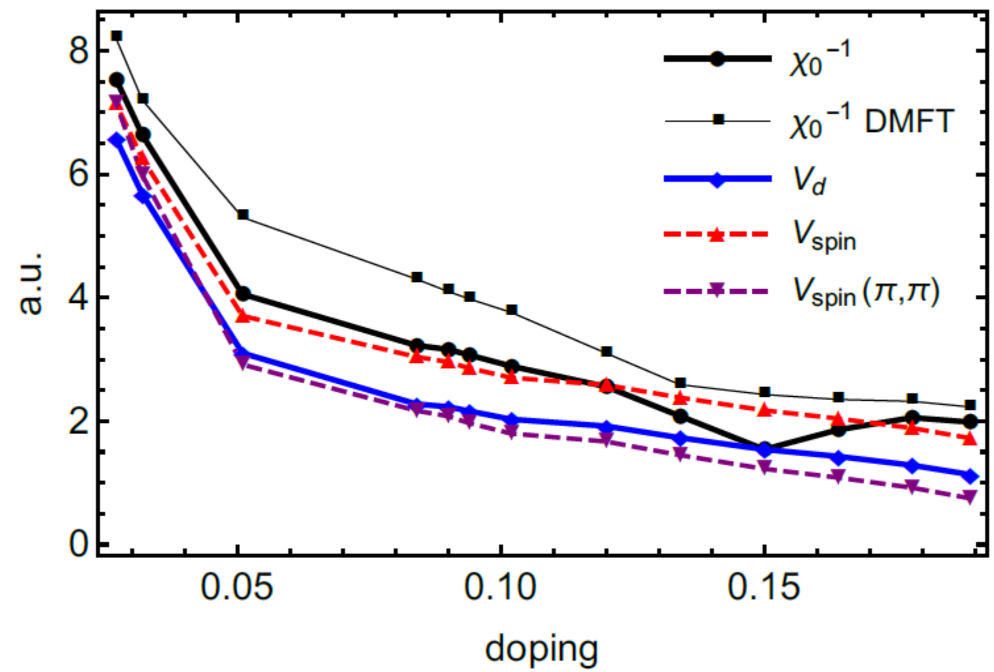
Take home results



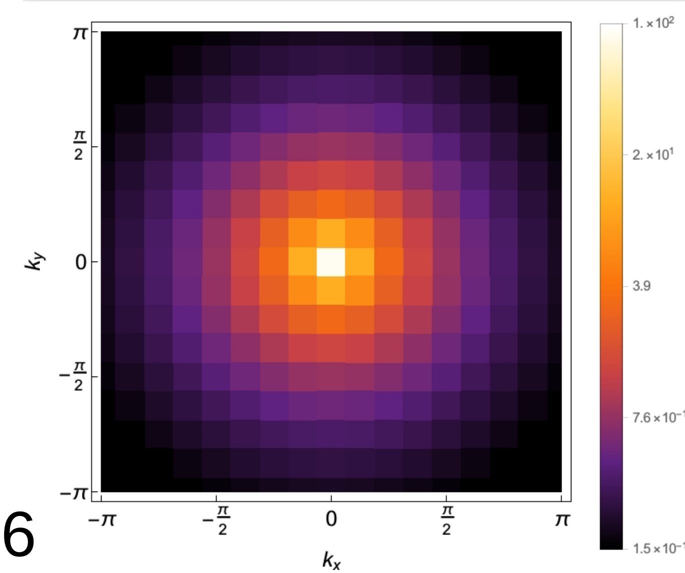
Ultra quantum:
wide energy and length ranges for correlations

Our prescription:
High-energy: local, threaten exactly
Low-energy: interacting collective modes, parquet

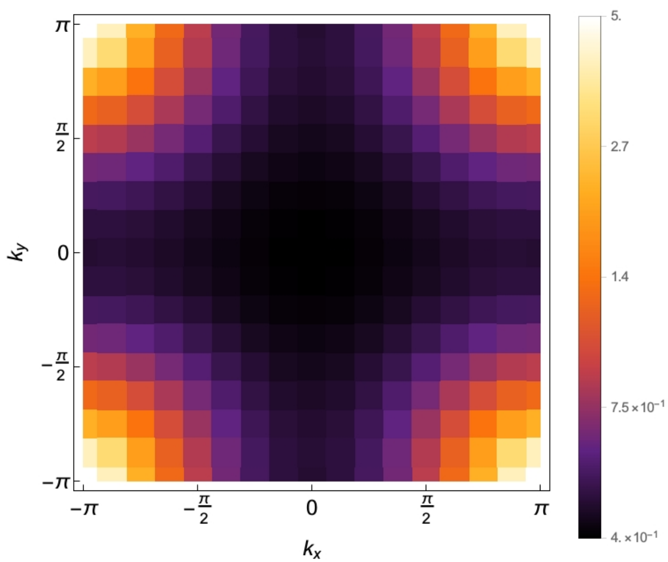


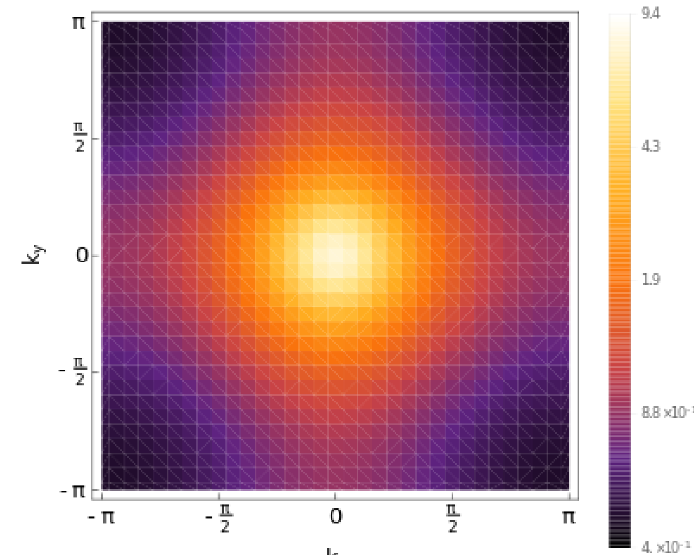


Finite size scaling, fixed T and doping

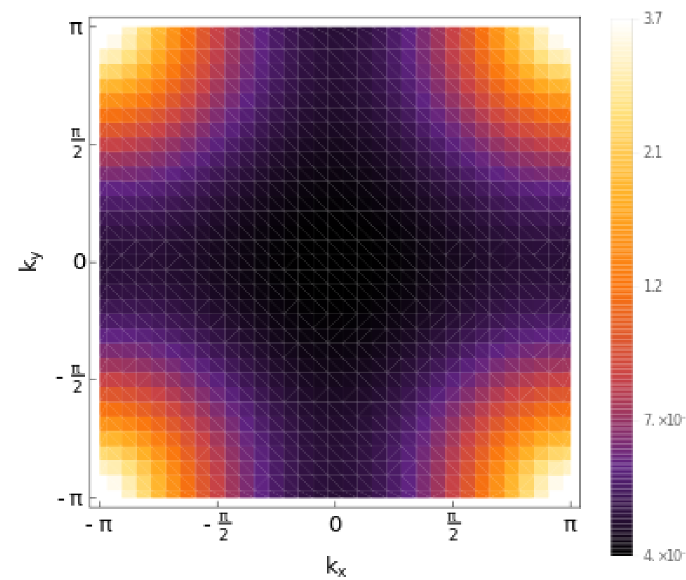


16 x 16





32 x 32



Analysis of approximations

BSCCO

↓

Hubbard

↓

Effective action

↓

L x L

↓

Parquet

- Neglect many-particle local vertices
- Control number of lowest Matsubaras (1, 2…)
- Second order perturbation theory for a renormalized interaction and a propagator

- 16x16 → 32x32 decreases critical temperature

- Self-consistent two-particle method