Numerical study of the periodic Anderson model with a quarter-filled conduction band

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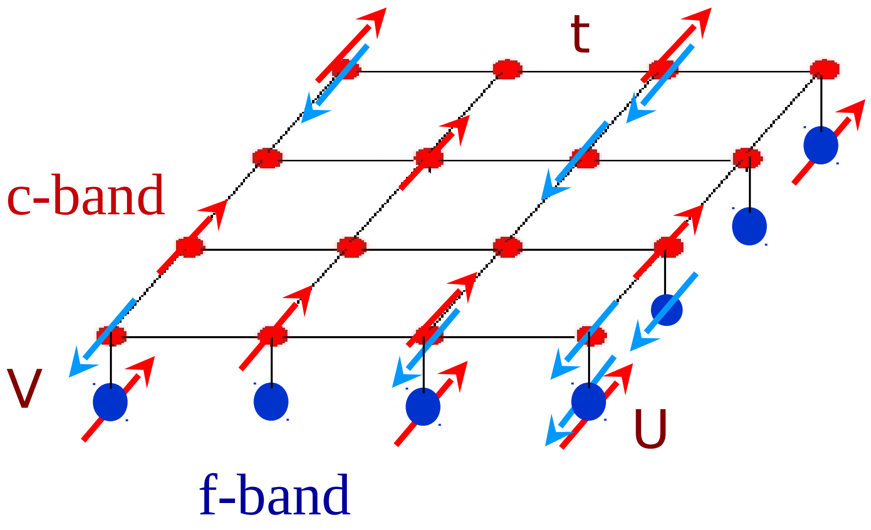
Outline

- Model
  - Periodic Anderson model
  - Relations with the Kondo lattice model and Hubbard model
- Numerical methods:
  - Dynamical mean-field theory (DMFT)
  - Dynamical cluster approximation (DCA)
  - Dual fermion method (DF)
- Numerical results for 2D and 3D lattice
  - Bench-mark DF with DMFT and DCA results
  - Phase-diagrams
  - Origin of the CDW ordering
- Conclusion

Model

- Periodic Anderson model:



$$\hat{H} = -t \sum_{<ij>,\sigma} (\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma}) + V \sum_{i\sigma} (\hat{c}^{\dagger}_{i\sigma}\hat{f}_{i\sigma} + \hat{f}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}) + \epsilon_f \sum_{i\sigma} \hat{f}^{\dagger}_{i\sigma}\hat{f}_{i\sigma} + U \sum_{i} \hat{n}_{f,i\uparrow}\hat{n}_{f,i\downarrow}$$

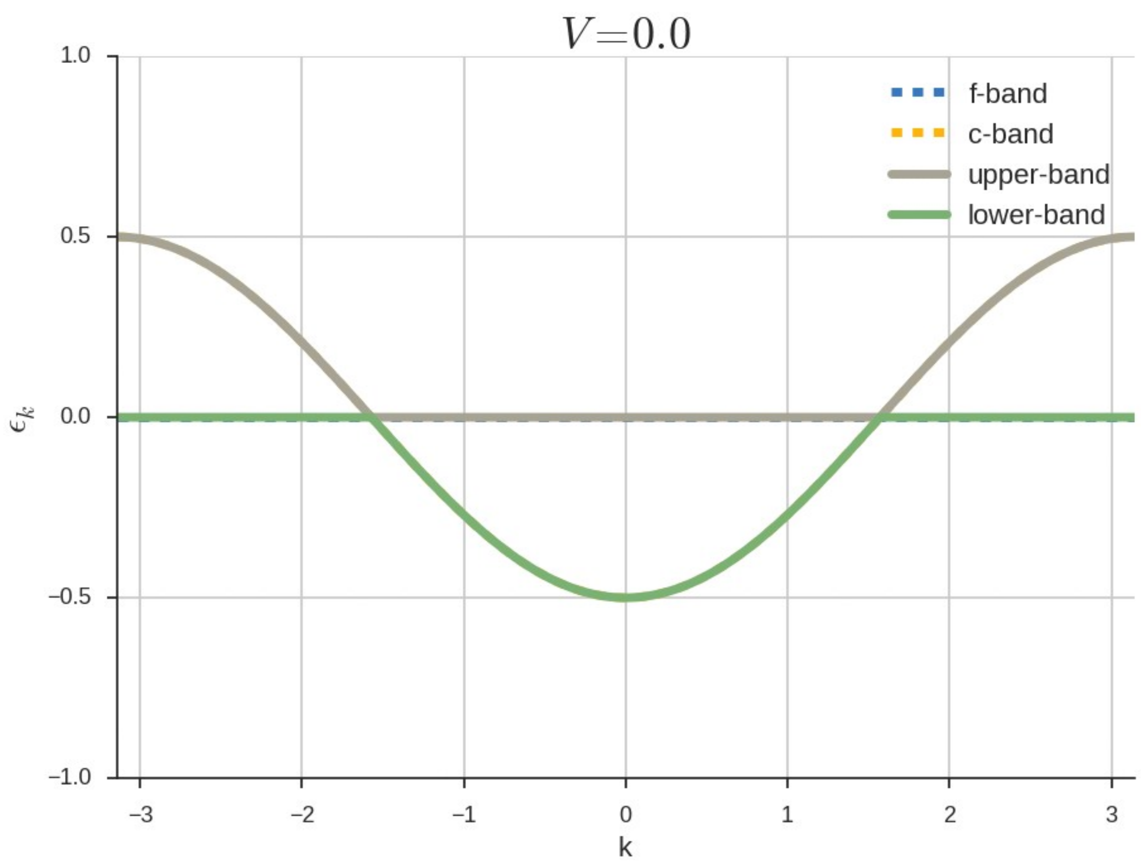
  - Two-band model
  - Conduction band: c-eletron can hop, no interaction
  - Localized band: f-electron cannot hop, Coulomb interaction
  - Hybrid through V term

Model

- U=0

$$\epsilon_{upper-band}(k) = \frac{\epsilon_k + \sqrt{\epsilon_k^2 + 4V^2}}{2}$$

$$\epsilon_{lower-band}(k) = \frac{\epsilon_k - \sqrt{\epsilon_k^2 + 4V^2}}{2}$$



Related to other models

- Kondo lattice model (freezing out f-electron charge fluctuations):

$$U \gg t, V \quad n_{f\uparrow} + n_{f\downarrow} = 1$$

$$\hat{H} = -t \sum_{<ij>,\sigma} (\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + h.c.) + J \sum_i \hat{\mathbf{s}}_i \cdot \hat{\mathbf{S}}_i$$

- Hubbard model (integrating out c-electron formally):

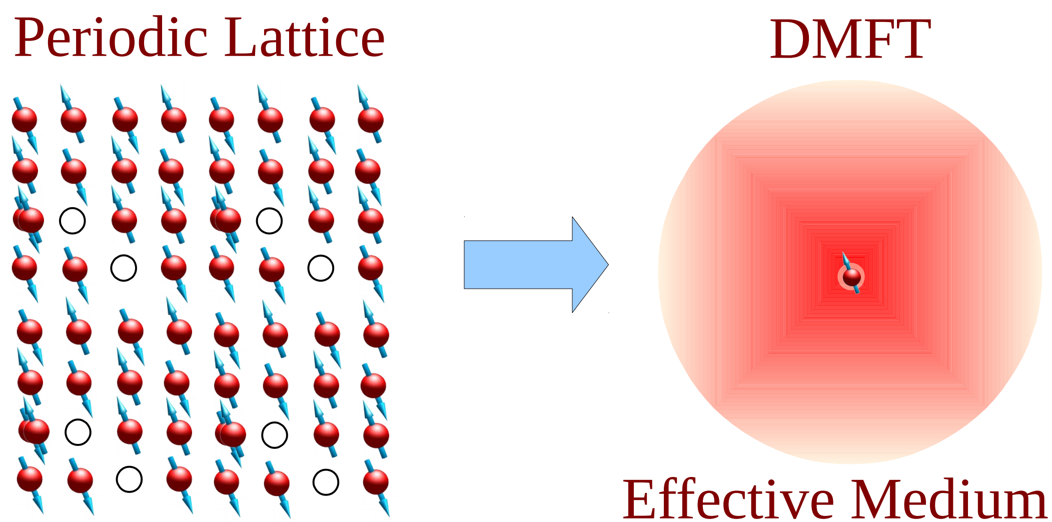
$$S[f^*, f] = -\sum_{k\omega\sigma} f^*_{\omega k\sigma} G_0(k, i\omega)^{-1} f_{\omega k\sigma} + U \sum_i \int_0^\beta d\tau \, n_{f,i\uparrow}(\tau) n_{f,i\downarrow}(\tau)$$

$$G_0(k, i\omega)^{-1} = i\omega + \mu - \epsilon_f - \sum_k \frac{V^2}{i\omega + \mu - \epsilon_k}$$

Adapting action-based codes from Hubbard model to PAM is easy!

Numerical methods -- I

- Dynamical mean-field theory (DMFT)



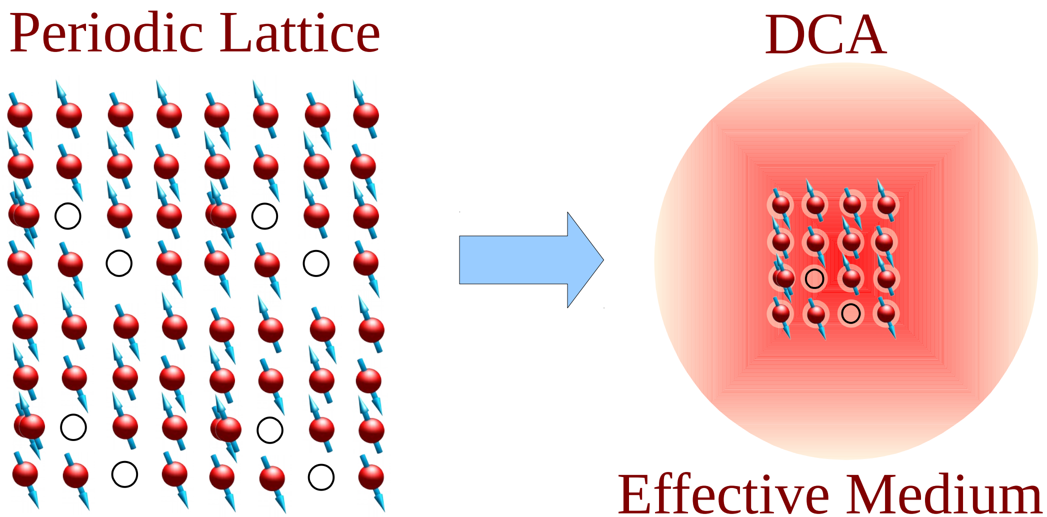
A. Georges, et.al., RMP 68, 13 (1996)

  - **Exact** in infinite dimension, **approximate** for finite dimensions
  - Local approximation
  - A great success. Best for the local physics, e.g. Mott physics
  - Missing non-local physics, e.g. pseudo-gap, d-wave superconductivity

  Many attempts to improve DMFT

Numerical methods -- II

- Dynamical cluster approximation (DCA)



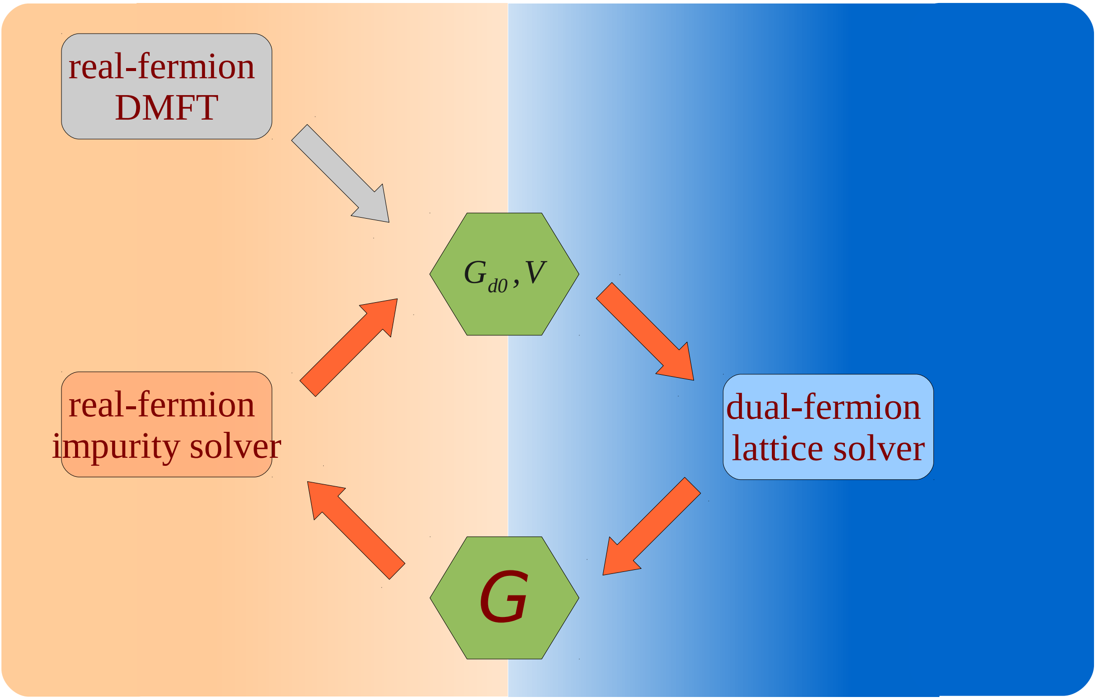
Th. Maier, et.al., RMP. 77, 1027 (2005)

  - One of the several proposals to go beyond single-site DMFT description
    similar proposal: cellular-DMFT
  - Short-ranged correlations included
  - Capture non-local physics, e.g. pseudo-gap, d-wave superconductivity

Numerical methods -- III

- Dual fermion method

A. N. Rubtsov et al., PRB 77, 33101 (2008)



DF mapping:

$$G_{d0} = G_{lat} - G_{imp}$$

$$V \approx F$$

CT-QMC **Real fermion** (strongly-correlated) ⟺ **Dual fermion** (weakly-correlated) Second-order perturbation

  - One of the several proposals to expand on DMFT solution
  - Similar to small cluster DCA results

Numerical methods -- IV

- DMFT
  - Fast and no minus-sign problem for PAM
  - Quick scan of the parameter space
- DCA
  - Expensive and has the minus problem
  - Check if short-ranged correlations change physics extracted from DMFT
  - Bench-mark DF results
- DF
  - No minus-sign, more expensive than DMFT, but less expensive than DCA
  - Used when sign problem in DCA is bad and thus DCA is too expensive

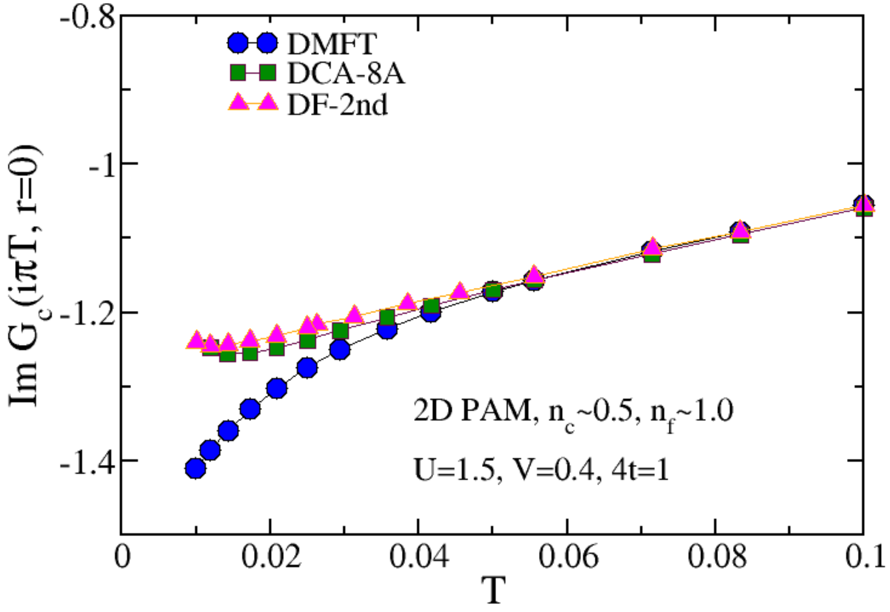
Results

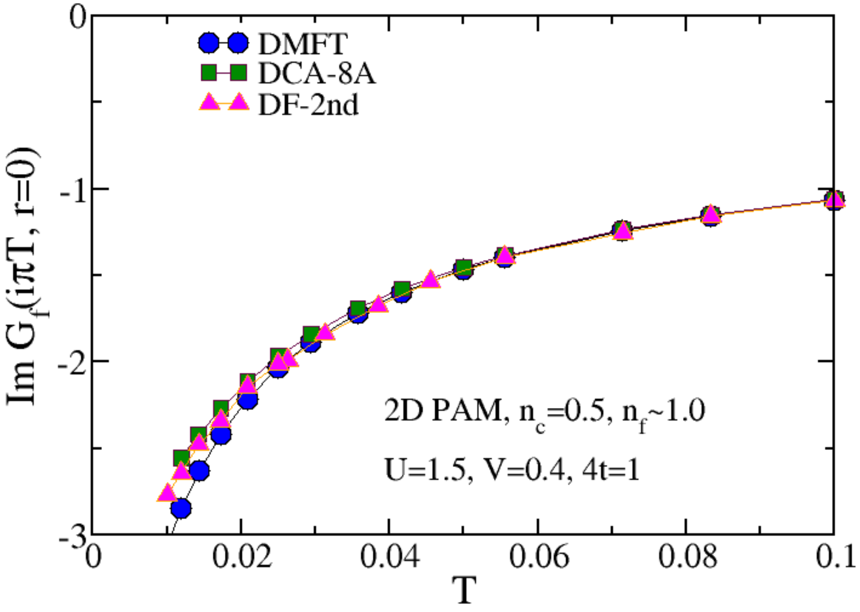
- Bench-mark
  - Compare DF results against DMFT and DF results
- Phase-diagram for 2D and 3D lattice

  Assume no symmetry broken in the system

  Divergence of the susceptibility signals phase-transition
- Origin of the CDW (q=(pi,pi)) ordering

Comparison of the DCA and DF results





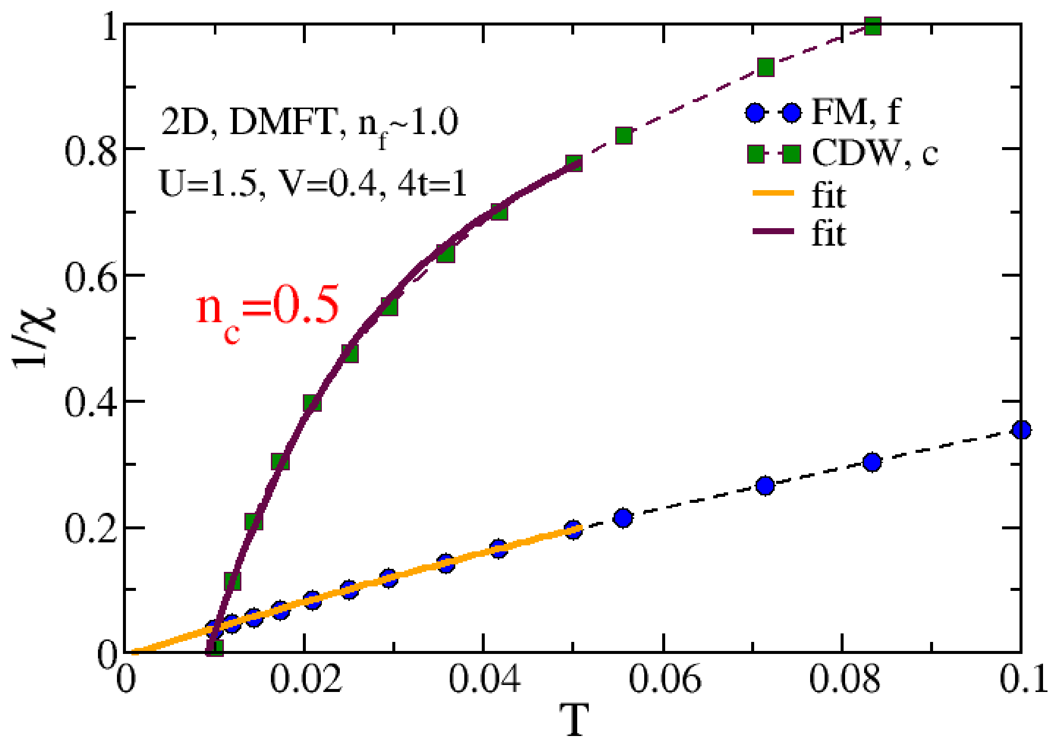
- For both c-band and f-band, DF can capture some essential short ranged correlations as the DCA calculation.

2D case

Assume no symmetry broken in the system

Divergence of the susceptibility signals phase-transition

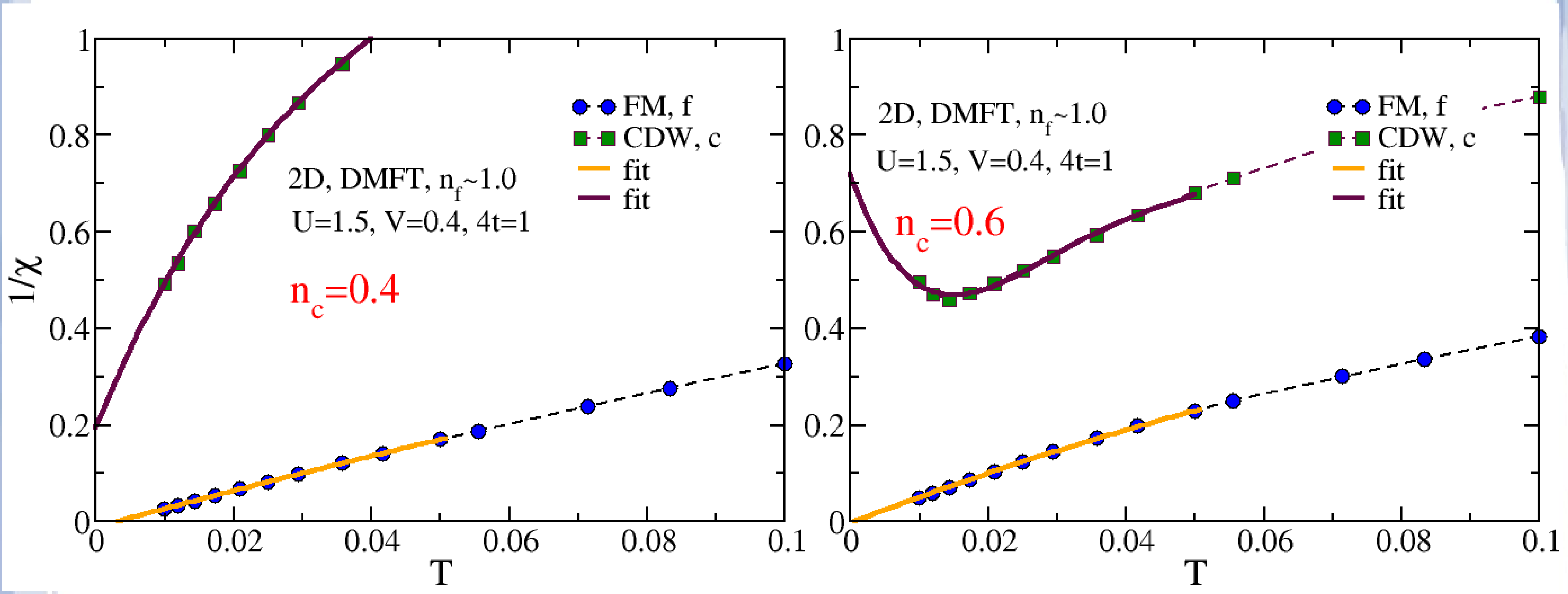
Quarter-filling



- Two phase-transitions, ferro-magnetic (FM) and charge-density-wave (CDW, q=(pi,pi))
- CDW Tc is higher than FM Tc

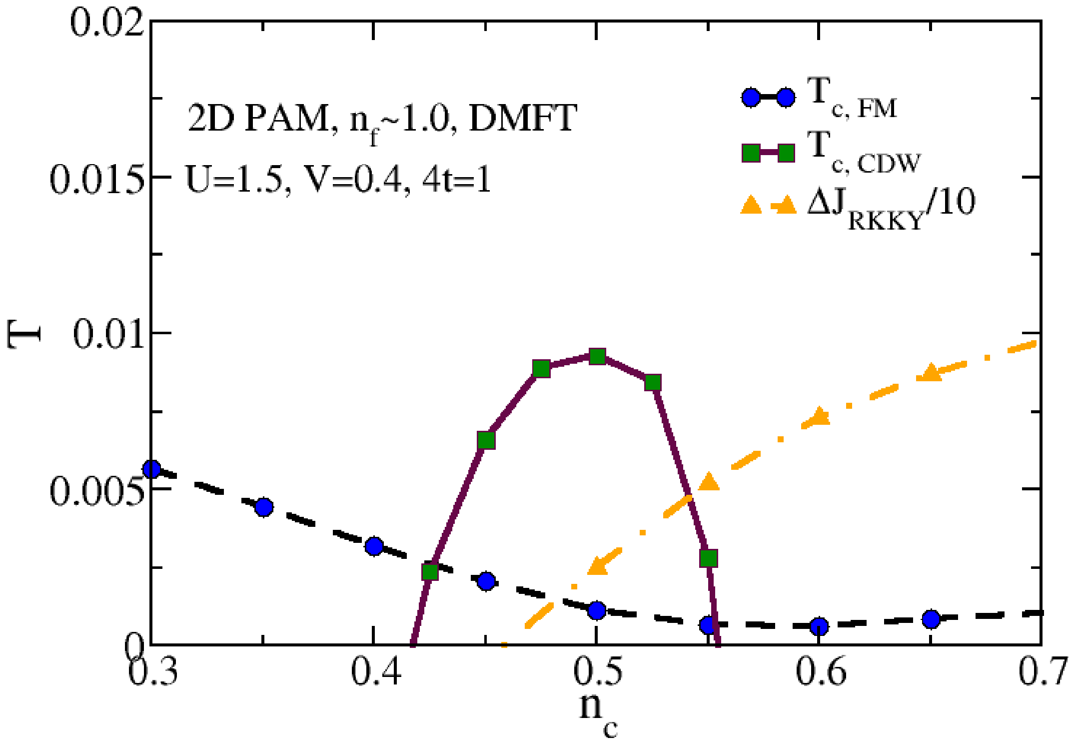
2D case

Off-quarter-filling



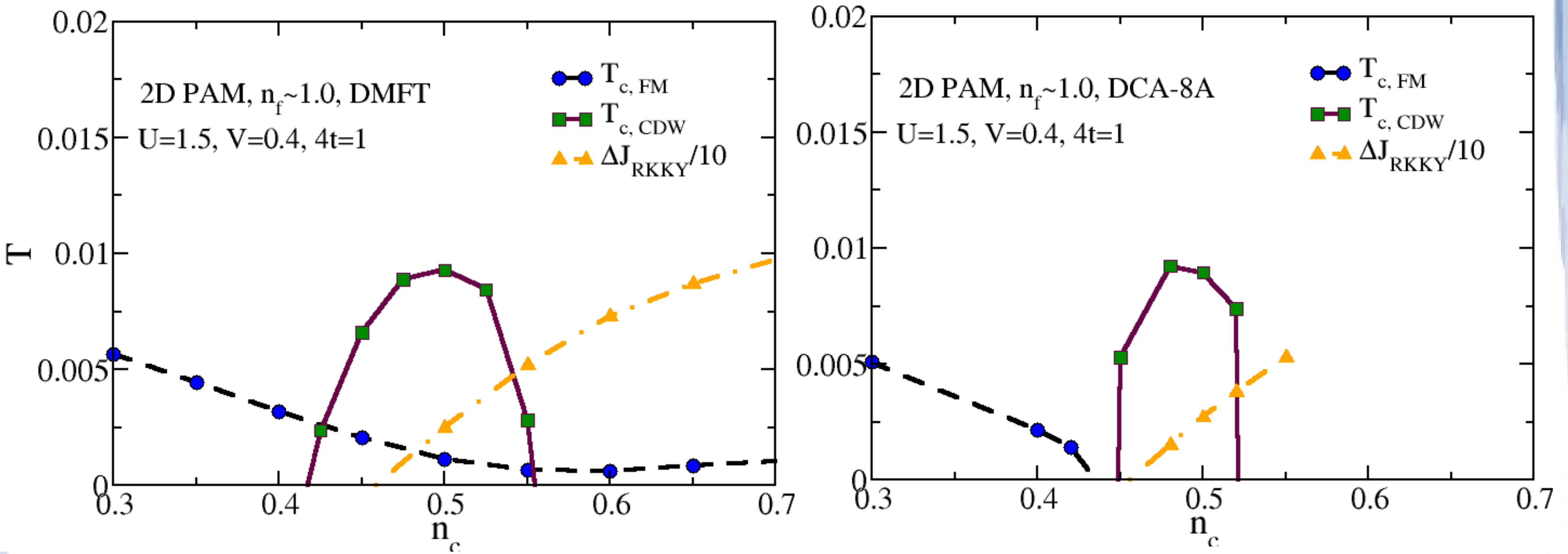
- Going either below or above quarter-filling, only FM diverges

2D phase-diagram



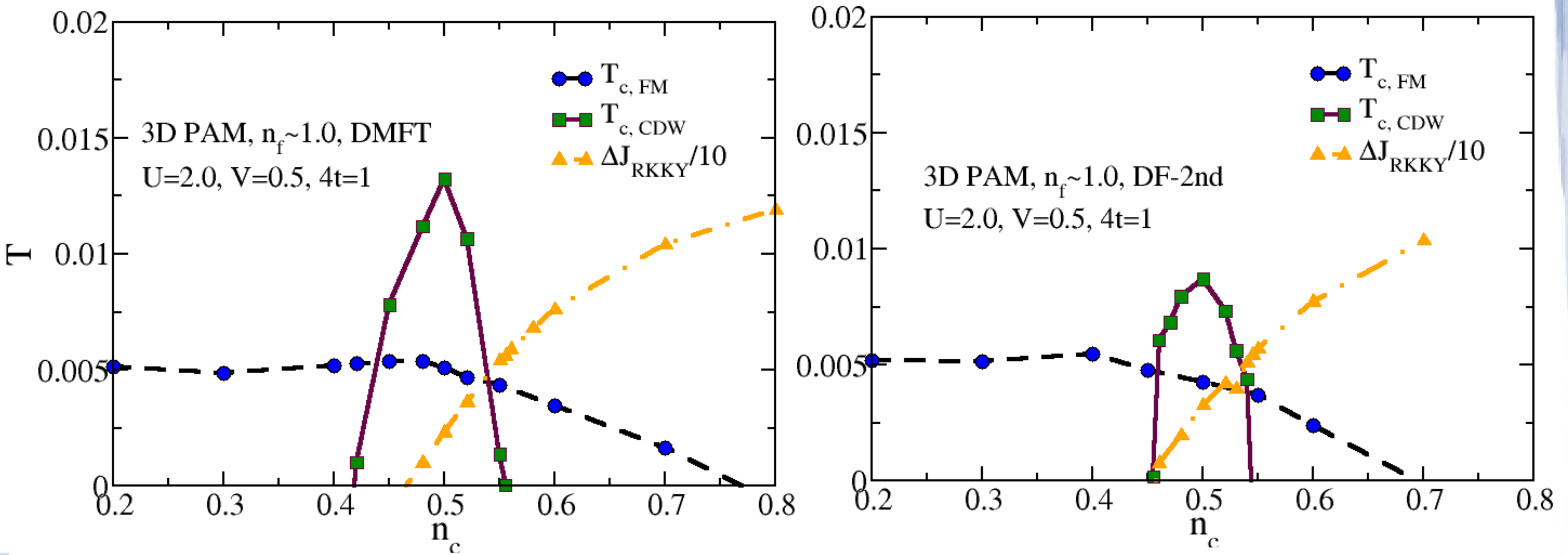
- FM Tc descreases when increasing c-electron filling
- CDW Tc has a dome shape around quarter-filling

2D phase-diagram



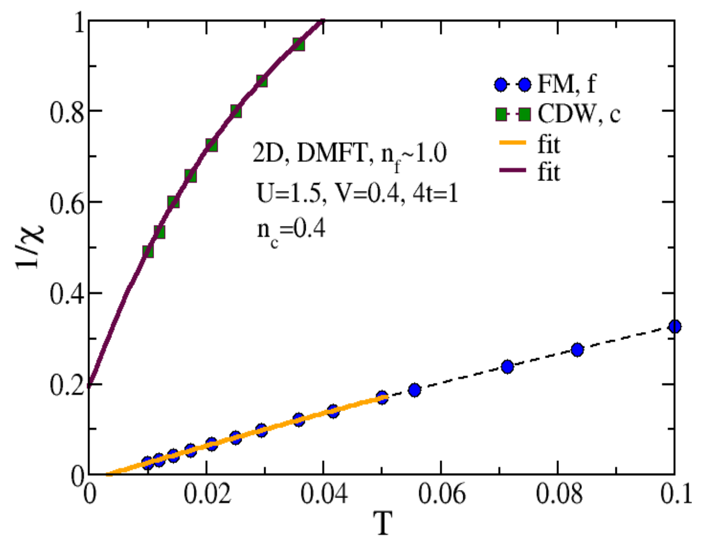
- FM ordering is reduced when short-range correlations are included
- CDW dome persists for DCA-8A results, but with reduced size

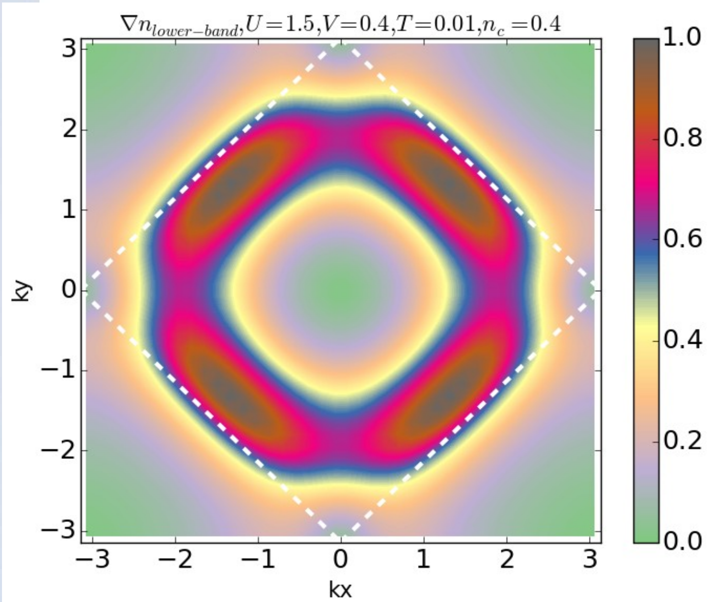
3D phase-diagram



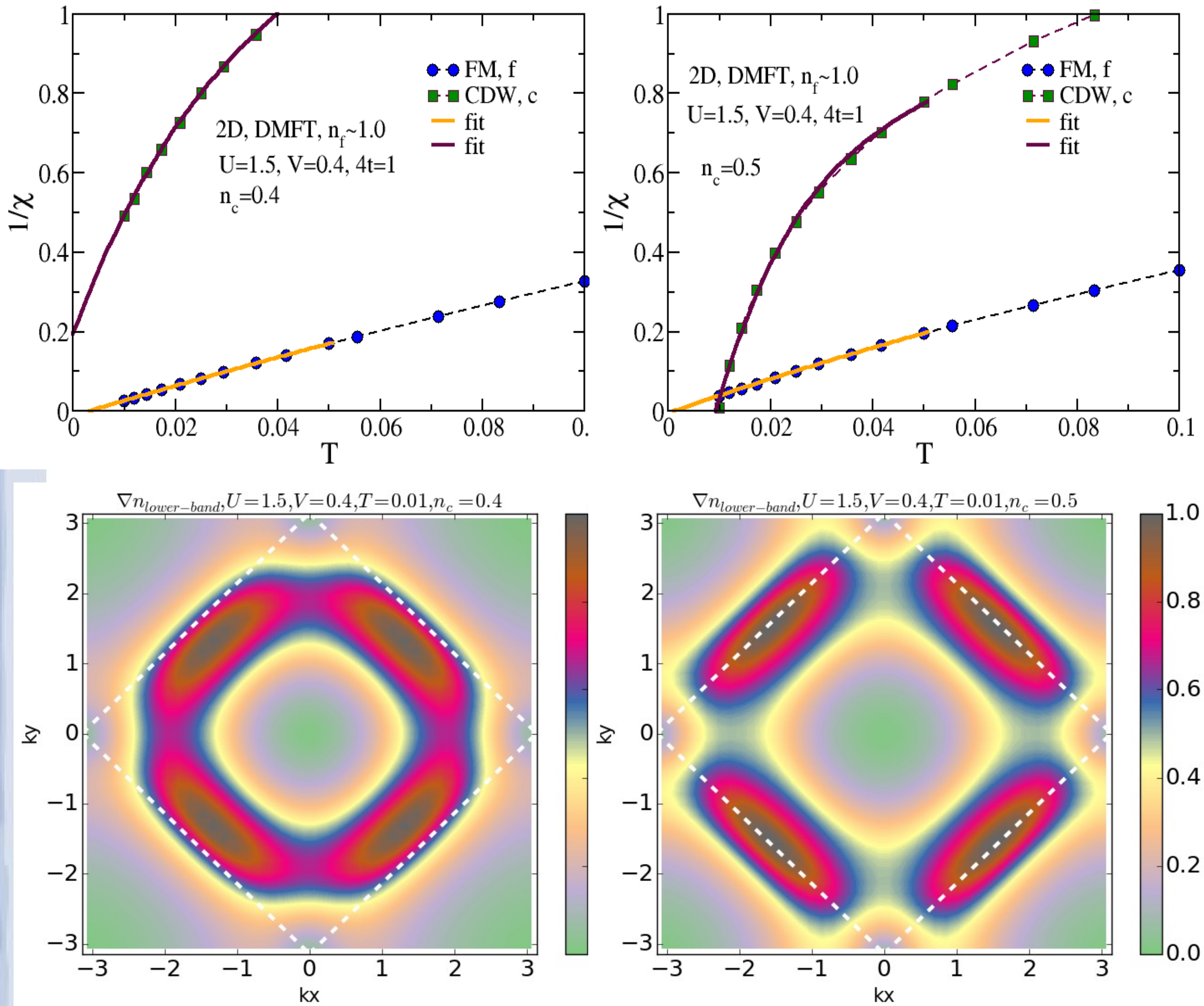
- 3D lattice shares similar phase-diagram as 2D
- Non-local correlations perserve CDW dome
- Origin??

Origin of CDW ordering

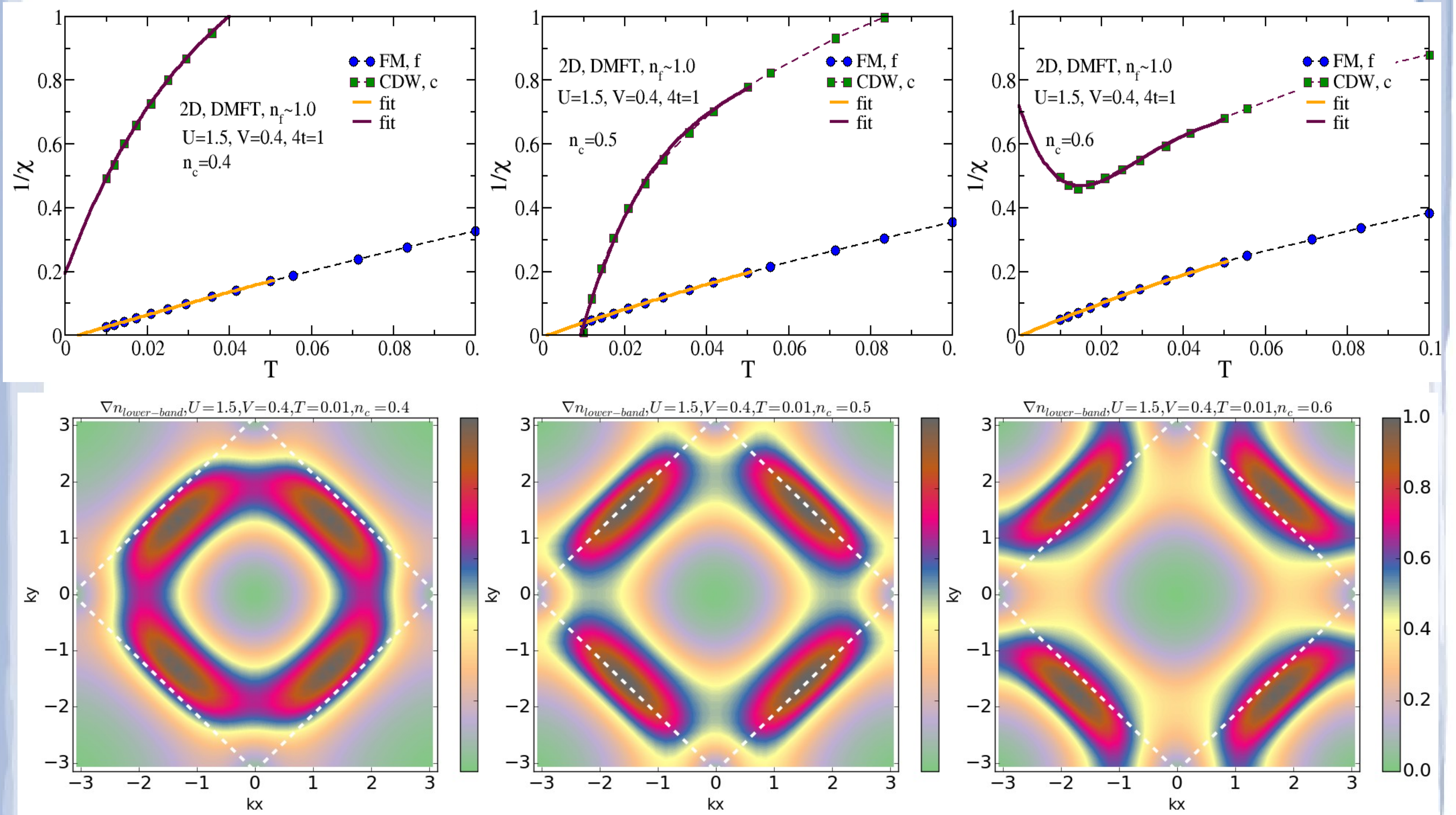




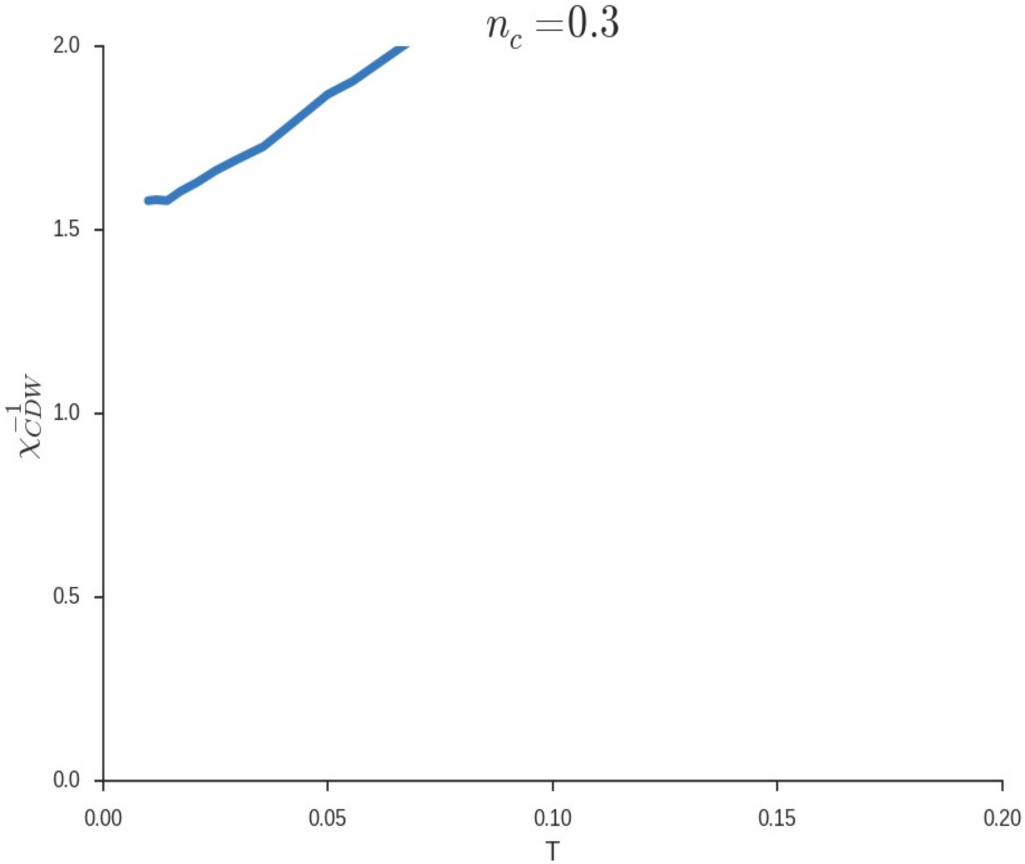
Origin of CDW ordering

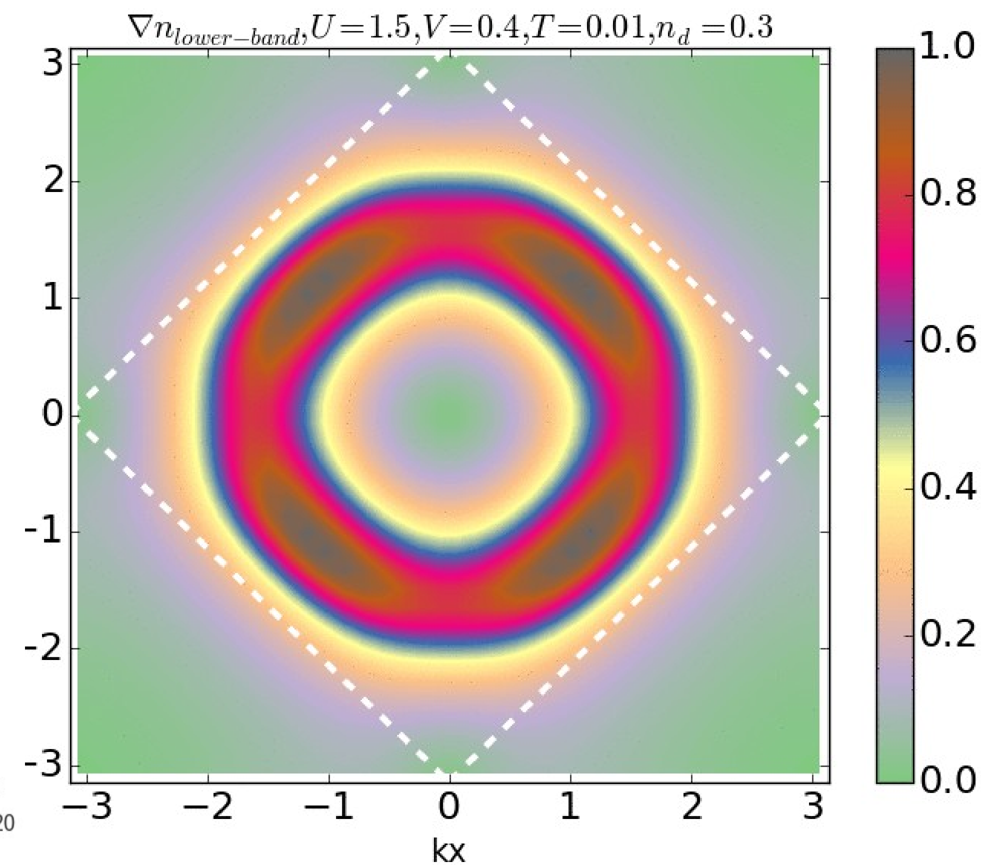


Origin of CDW ordering



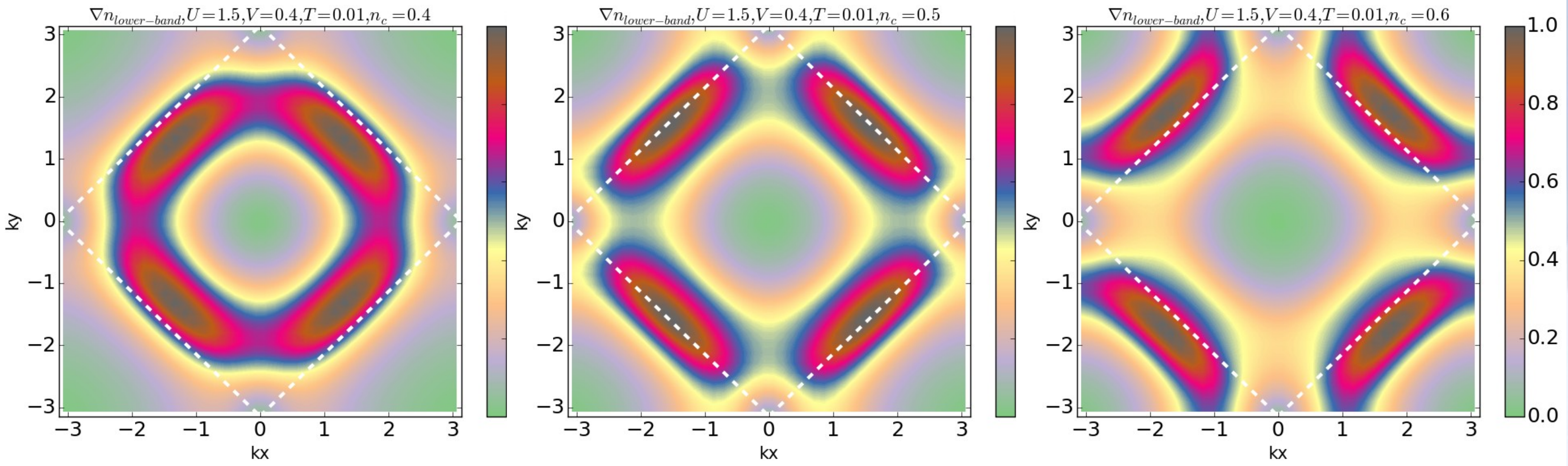
Origin of CDW ordering





- Divergence of susceptibility happens when the Fermi surface touchs on the magnetic zone boundary: perfect nesting
- Scattering is enhanced at q=(pi,pi) due to perfect nesting

Origin of CDW ordering



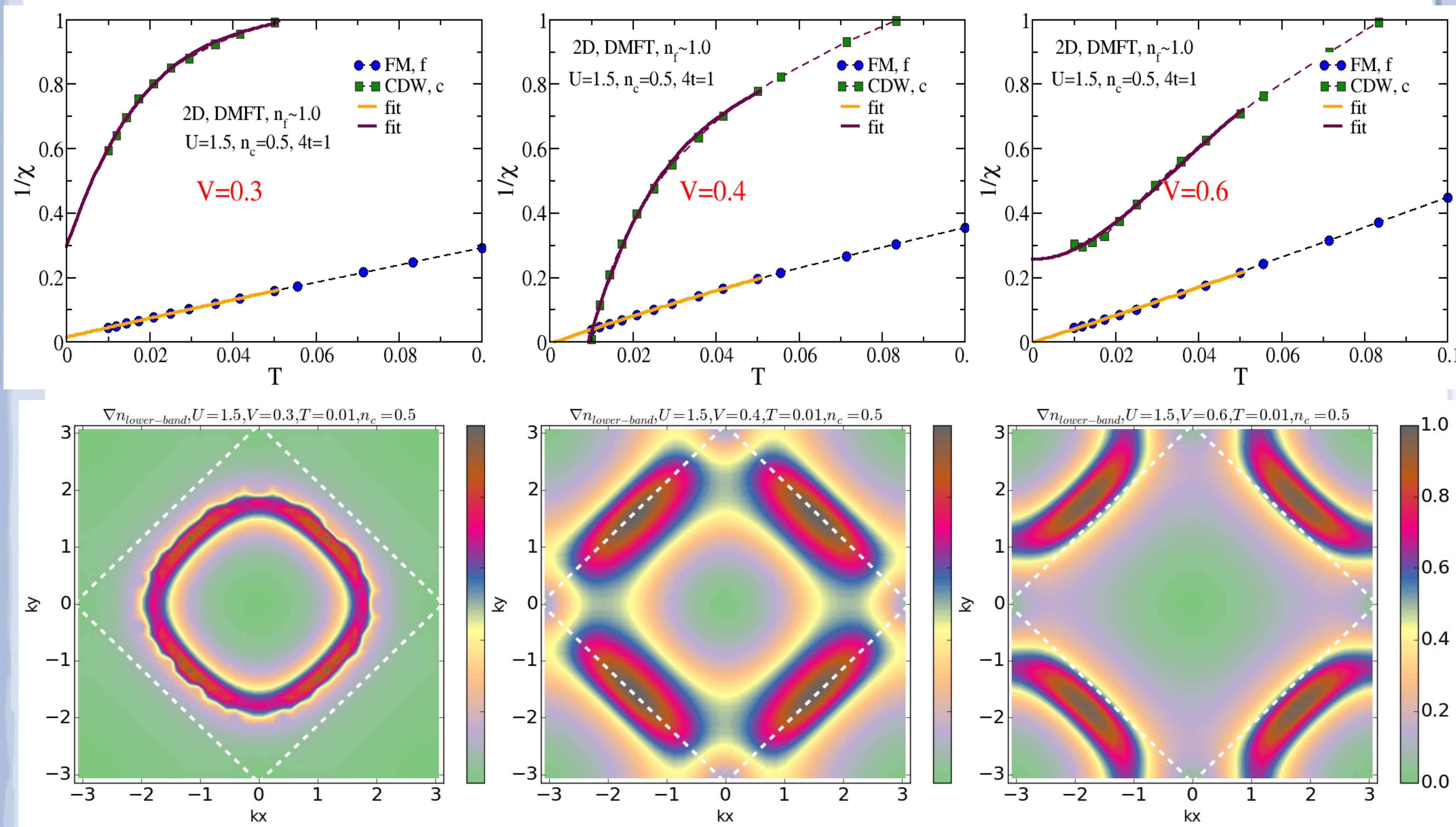
Particle-like

Perfect nesting!!

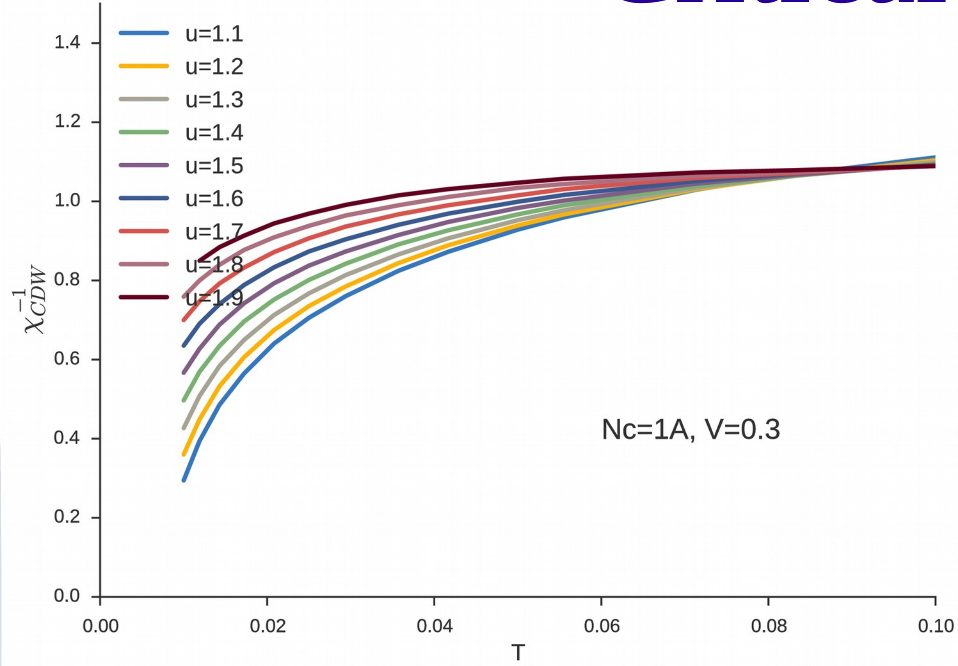
Hole-like

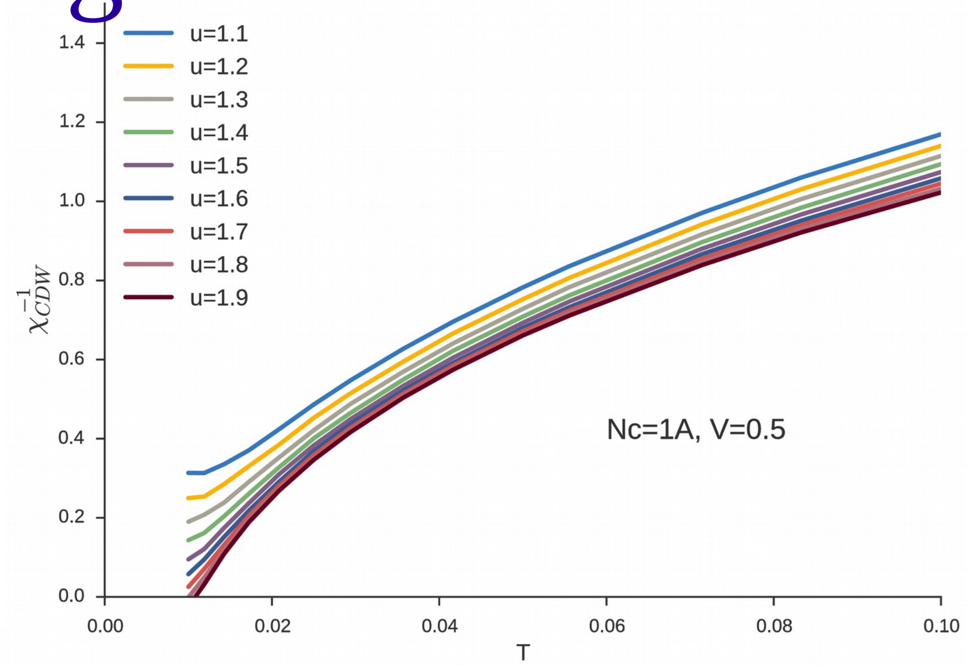
- The Fermi surface changes its topology from particle-like to hole-like at the transition and thus is a **Lifshitz transition**.
- Here the control parameter is the c-band filling

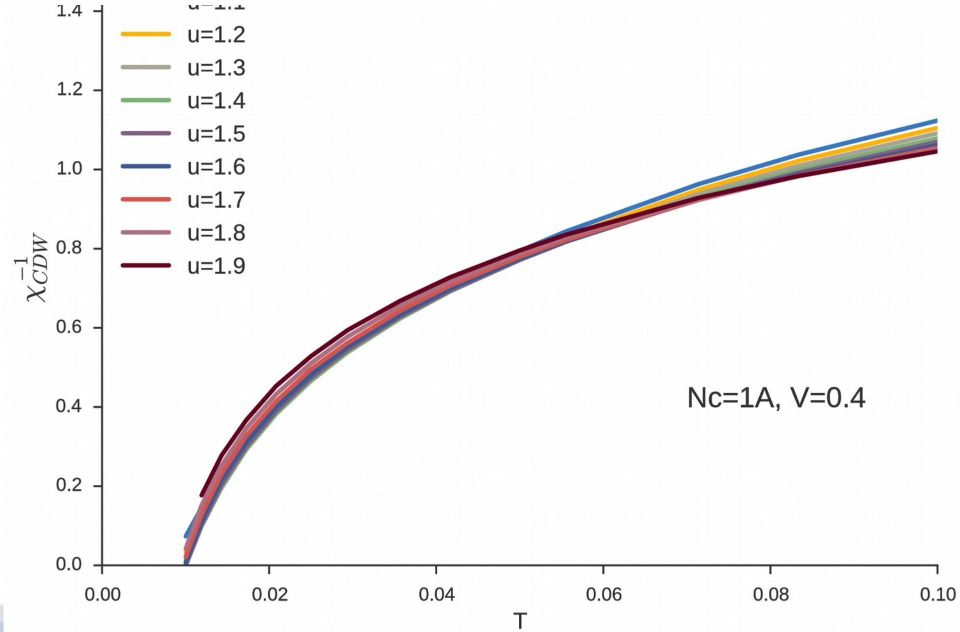
Hybridization as the control parameter



Critical region?







Conclusion

- Using DMFT, DCA and DF, we have determined the phase-diagram of periodic Anderson model with f-band at half-filling and c-band around quarter-filling for both 2D and 3D lattices.
- A dome-shape CDW phase surounding quarter-filling is found and persists when non-local correlations are incuded through DCA and DF.
- The CDW ordering is explained by the perfect nesting of the Fermi-surface of the renormalized lower-band.
- The Fermi surface changes its topology from particle-like to hole-like at the transition and thus is a Lifshitz transition.
- A critical V is found where CDW susceptibility lines collapse on a single curve.

Thank you!