The effect of the local moment on the metal-insulator transition in the Hubbard model

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in collaboration with: Silke Biermann and Evgeny Stepanov

30/05/2023

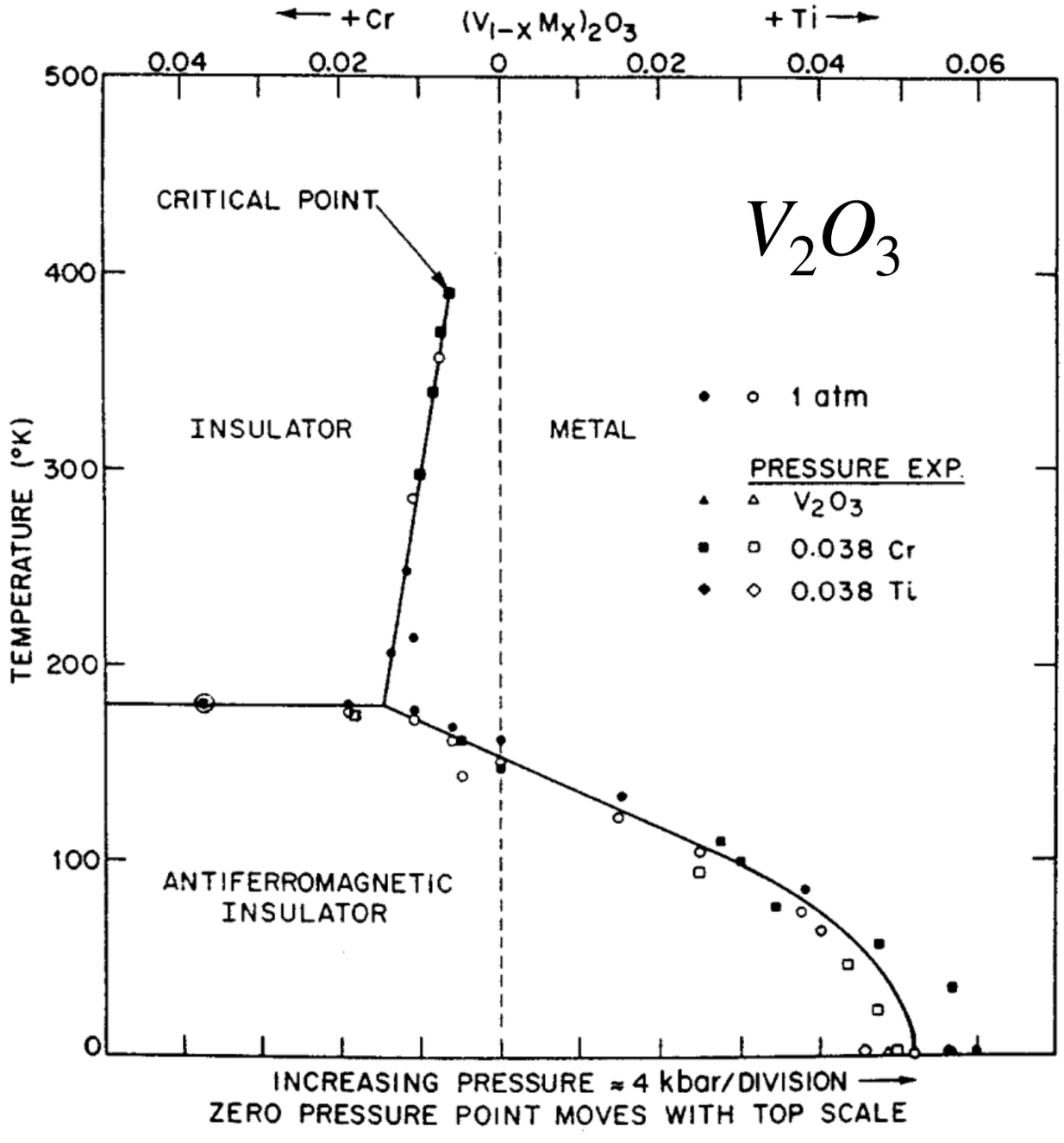
GDR MEETICC

Metal-insulator transition in correlated systems

Louis Néel

John C. Slater

Nevill F. Mott



D. B. McWhan et al. PRB **7**, 1920 (1973)

Metal-insulator transition in Hubbard model

Single-orbital Hubbard model: $\hat{H} = \sum_{jj'\sigma} t_{jj'} c^{\dagger}_{j\sigma} c_{j'\sigma} + U \sum_{j} n_{j\uparrow} n_{j\downarrow}$

Mechanisms for metal-insulator transition (MIT)

spatial fluctuations (Slater, Néel)

local correlations (Heisenberg, Mott)

$t_{jj'}$: hopping integral, $c^{(\dagger)}_{j\sigma}$: annihilation/creation operator,

U : Coulomb repulsion, $n_{j\sigma}$: density operator

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How do the two limits connect and how does the intermediate region evolve ?

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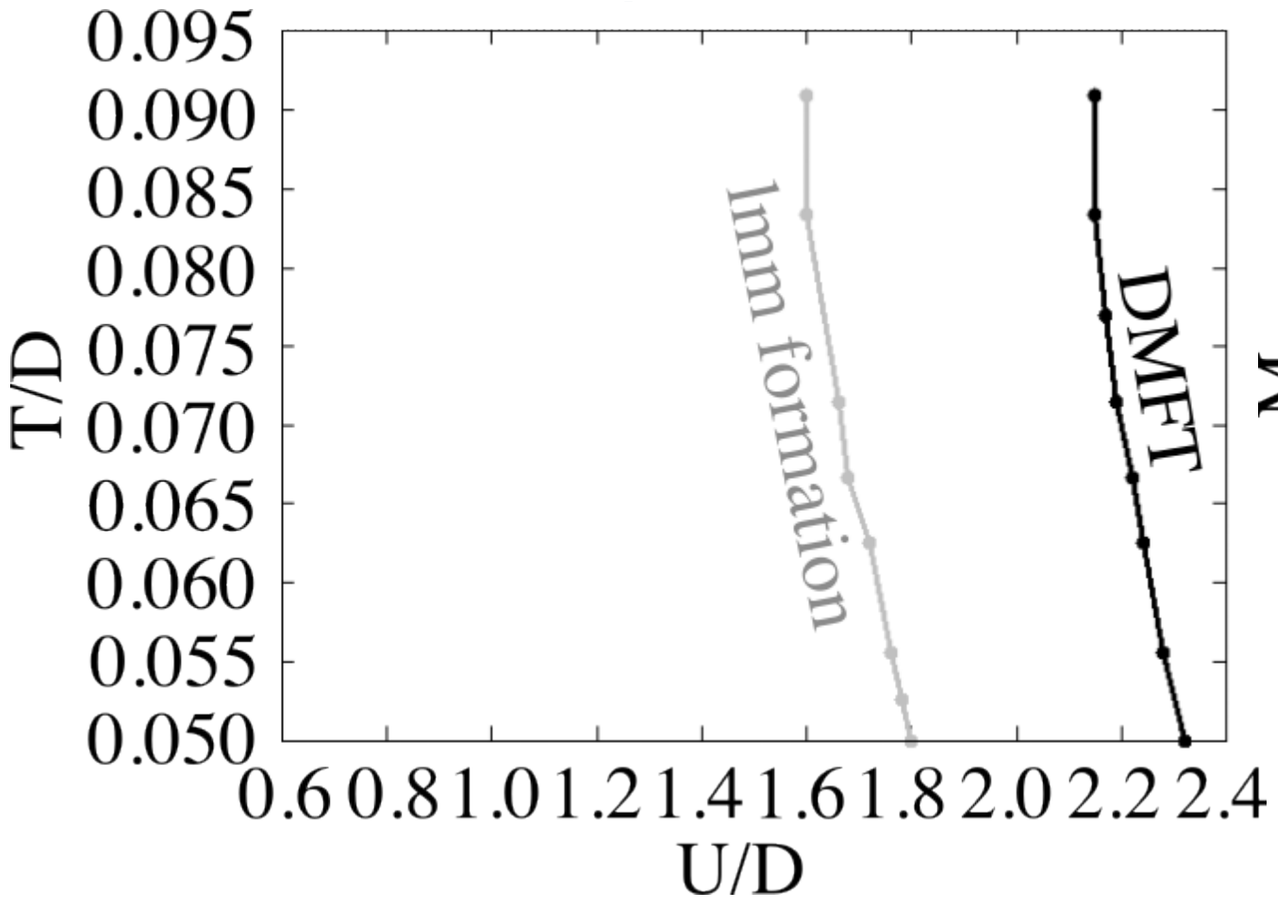
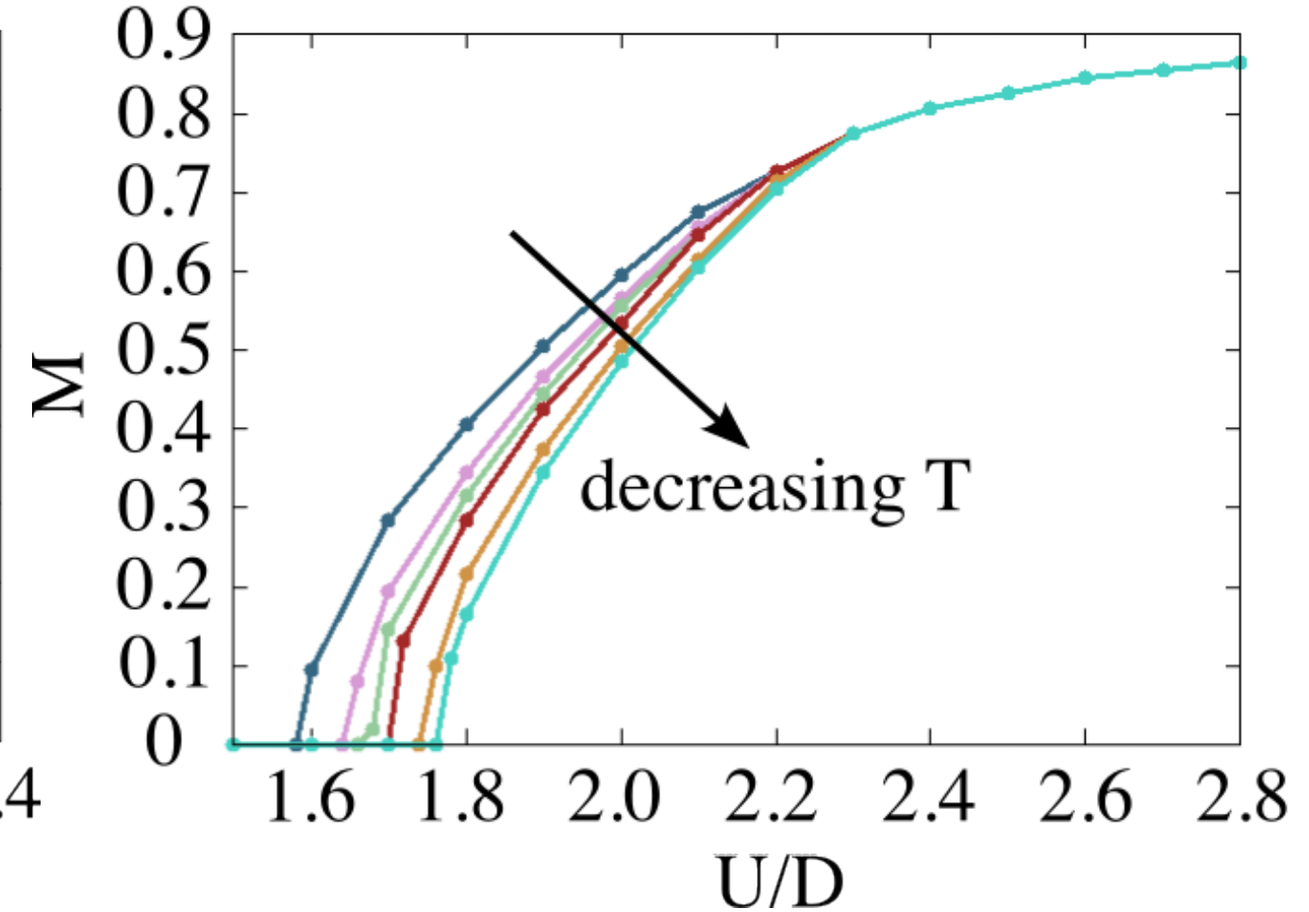
Methods for studying the MIT

Dynamical Mean-Field Theory (DMFT) [1] : treats the local interactions non-perturbatively and captures **only local** correlation effects

Pseudogap formation in the local spectral function



Local magnetic moment



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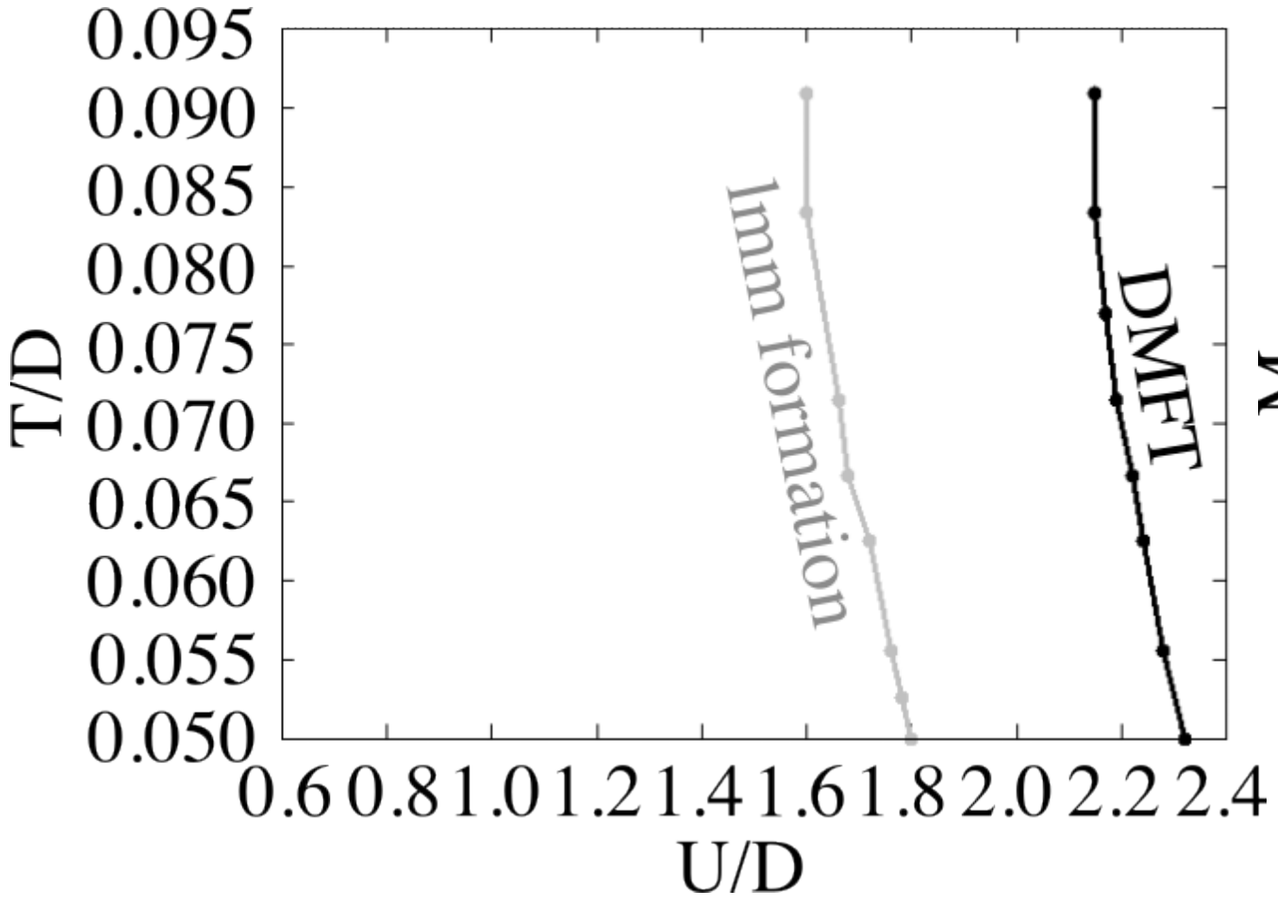

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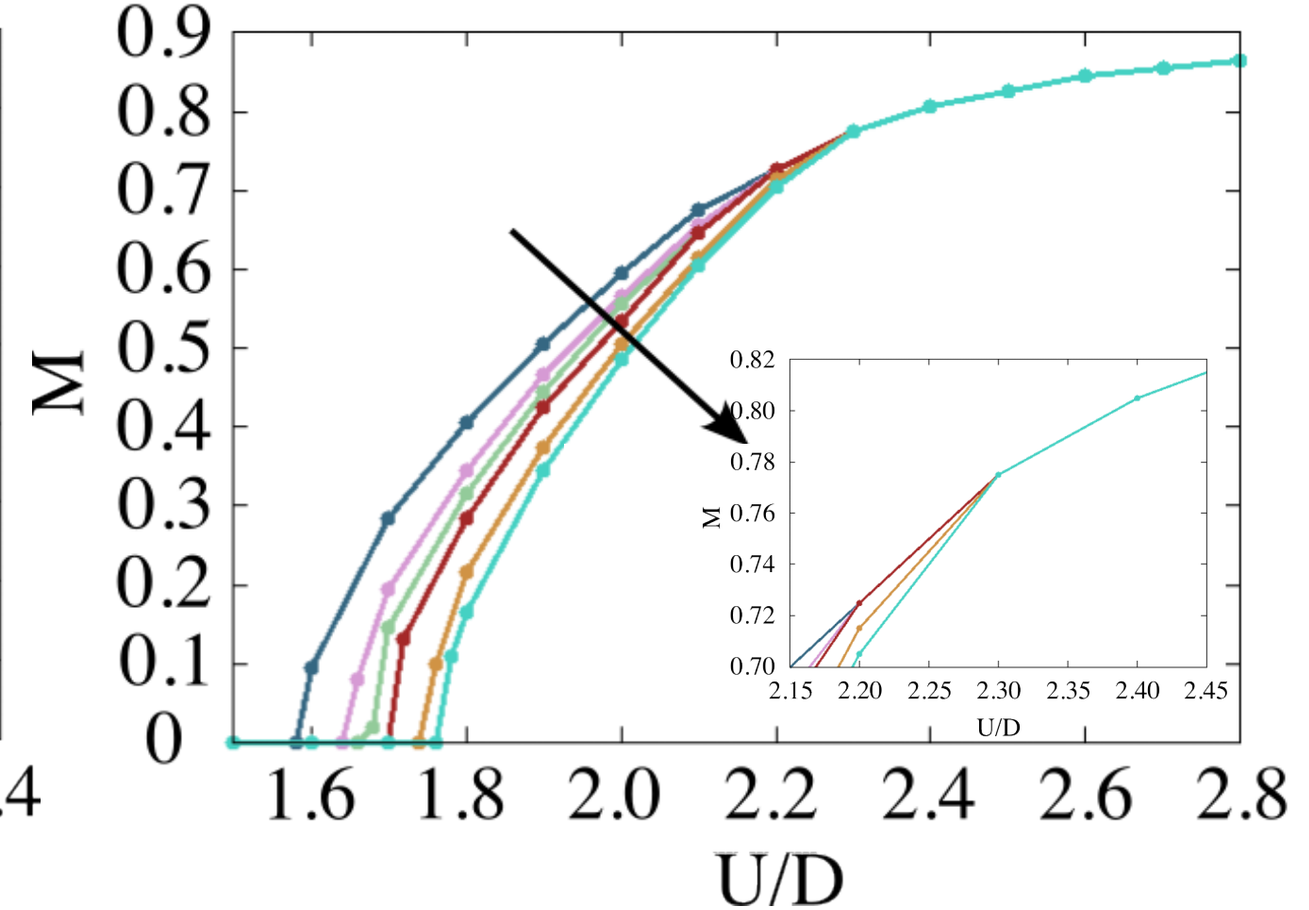

Methods for studying the MIT

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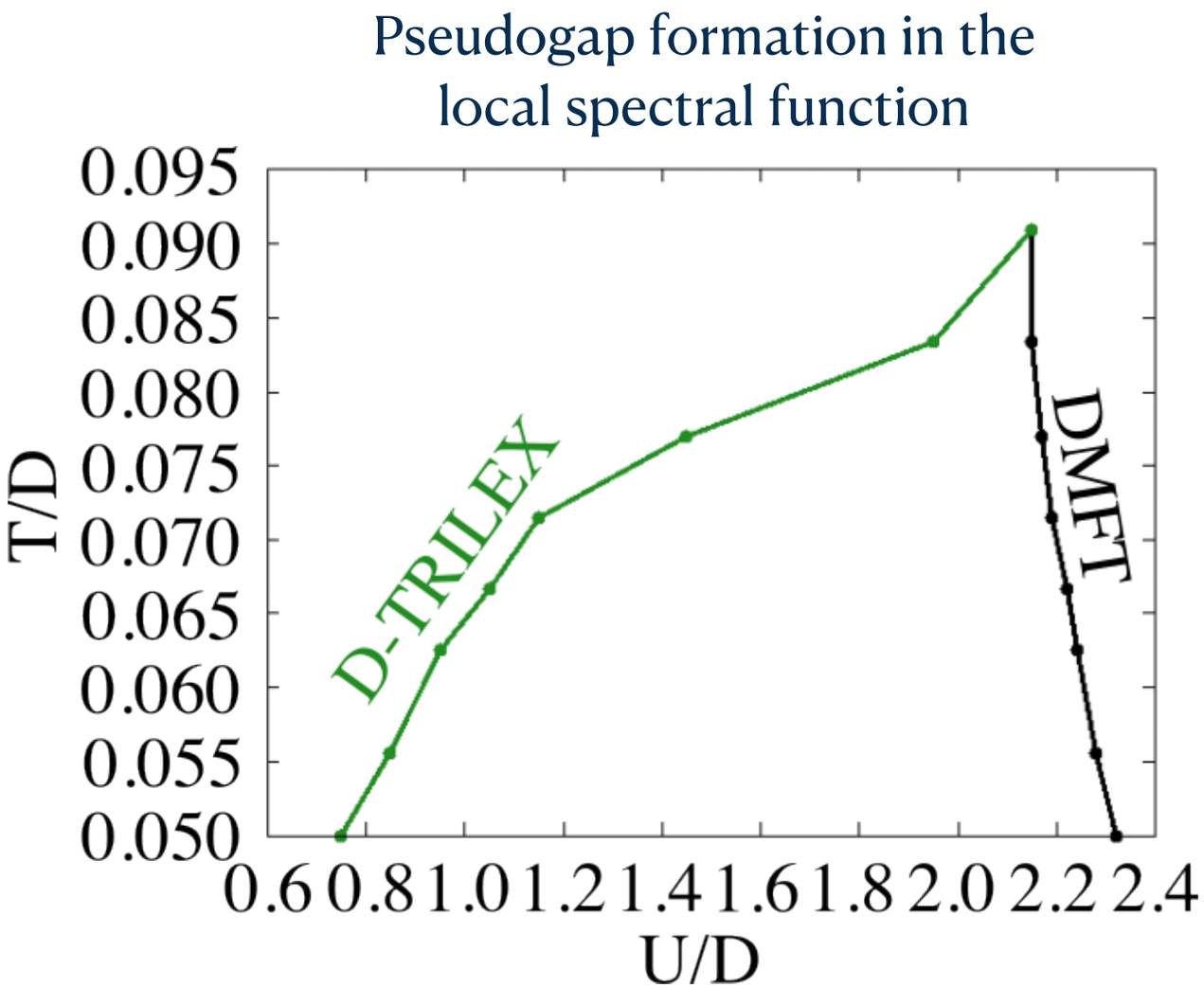
Extensions of DMFT [2] : incorporate **non-local** correlations beyond DMFT



in this work

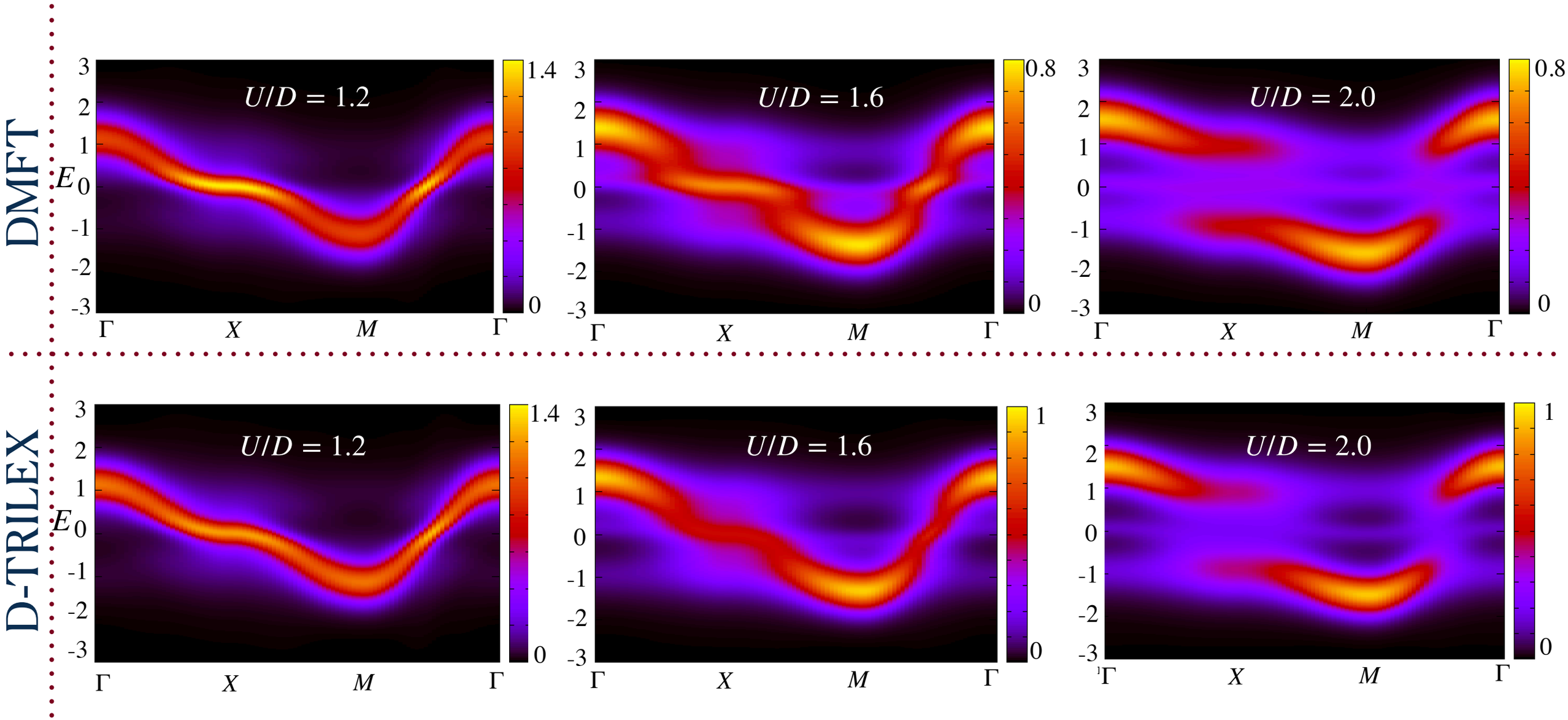
Dual TRILEX [3]

[1] A. Georges et al. Rev. Mod. Phys. **68**, 13 (1996)

[2] See, e.g., Refs.:
G. Rohringer et al. Rev. Mod. Phys. **90**, 025003 (2018)
T. Maier et al. Rev. Mod. Phys. **77**, 1027 (2005)

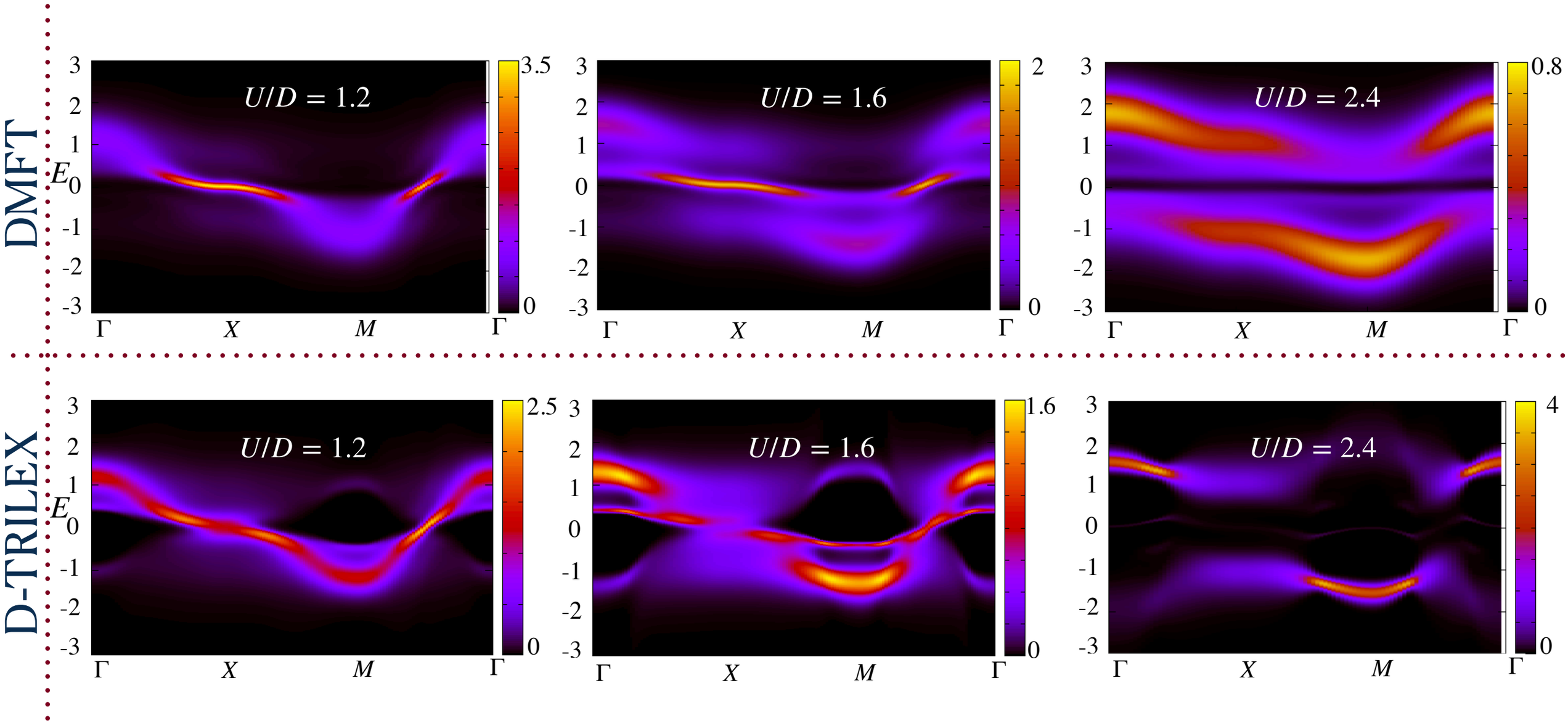
[3] E. A. Stepanov et al. Phys. Rev. B **100**, 205115 (2019)
V. Harkov et al. Phys. Rev. B **103**, 245123 (2021)
M. Vandelli et al. SciPost Phys. **13**, 036 (2022)

Non-local fluctuations at **high T**



At high T $(T/D = 0.14)$ far from $T_{Néel}$ non-local fluctuations are not important and DMFT describes accurately the Mott transition.

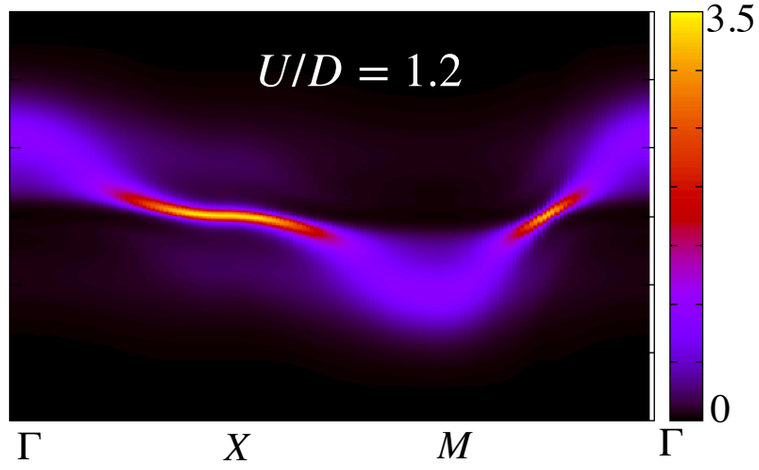
Non-local fluctuations at **low T**

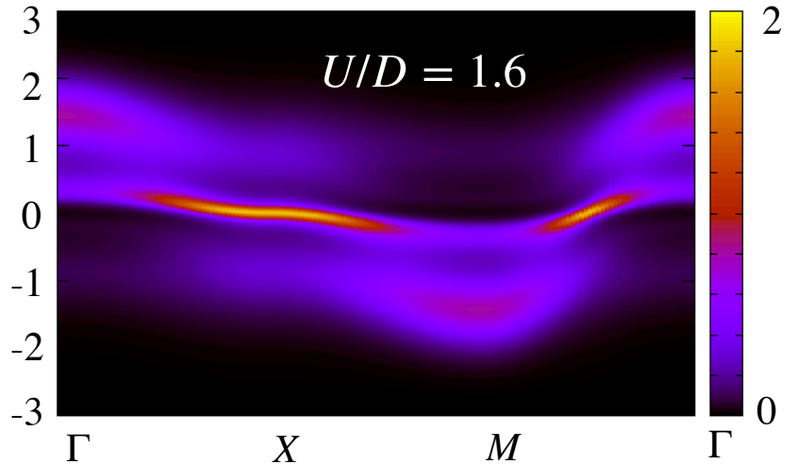


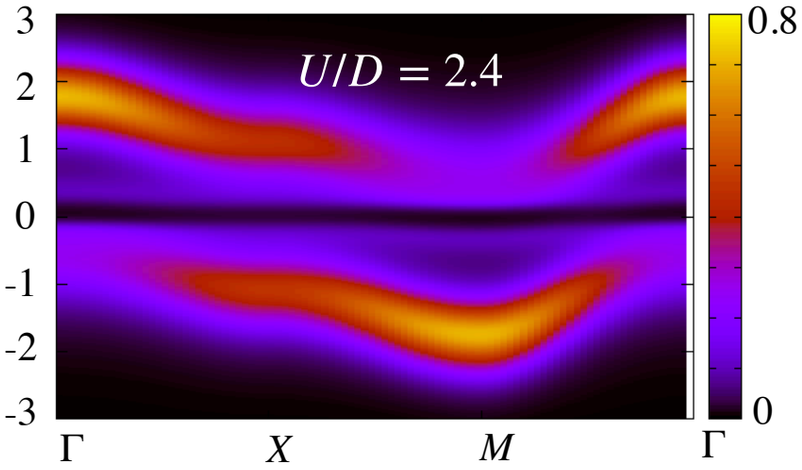
At low T ($T/D = 0.0625$) close to $T_{Néel}$ non-local fluctuations become important and their inclusion reveals the momentum-selective character of the pseudogap formation.

Non-local fluctuations at **low T**

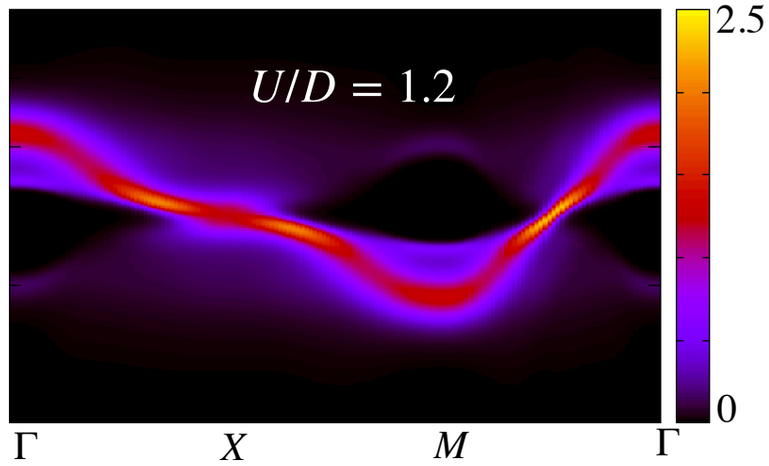
DMFT

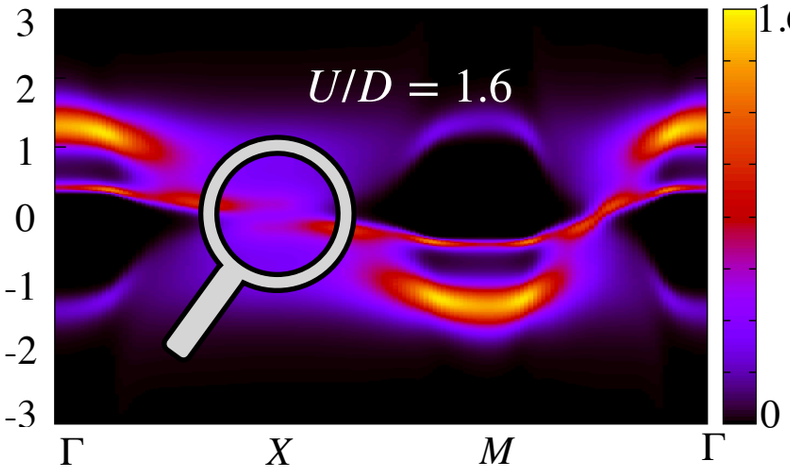


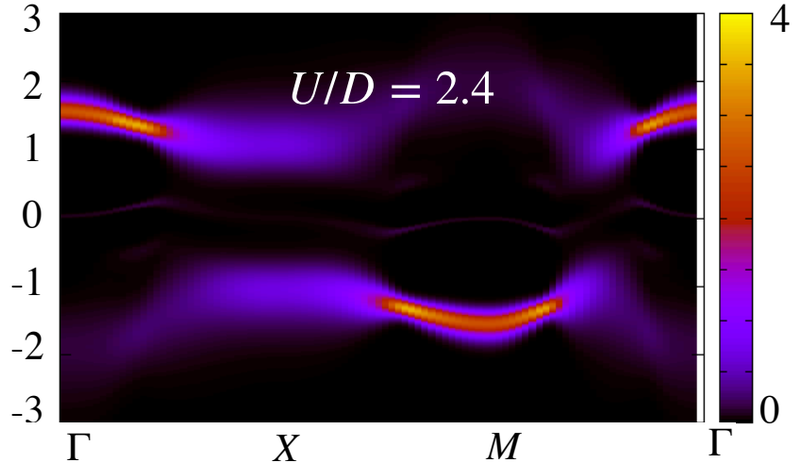




D-TRILEX







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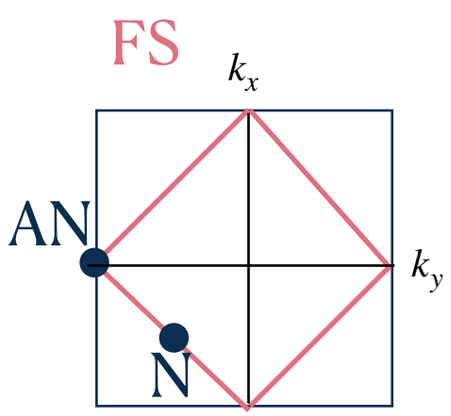
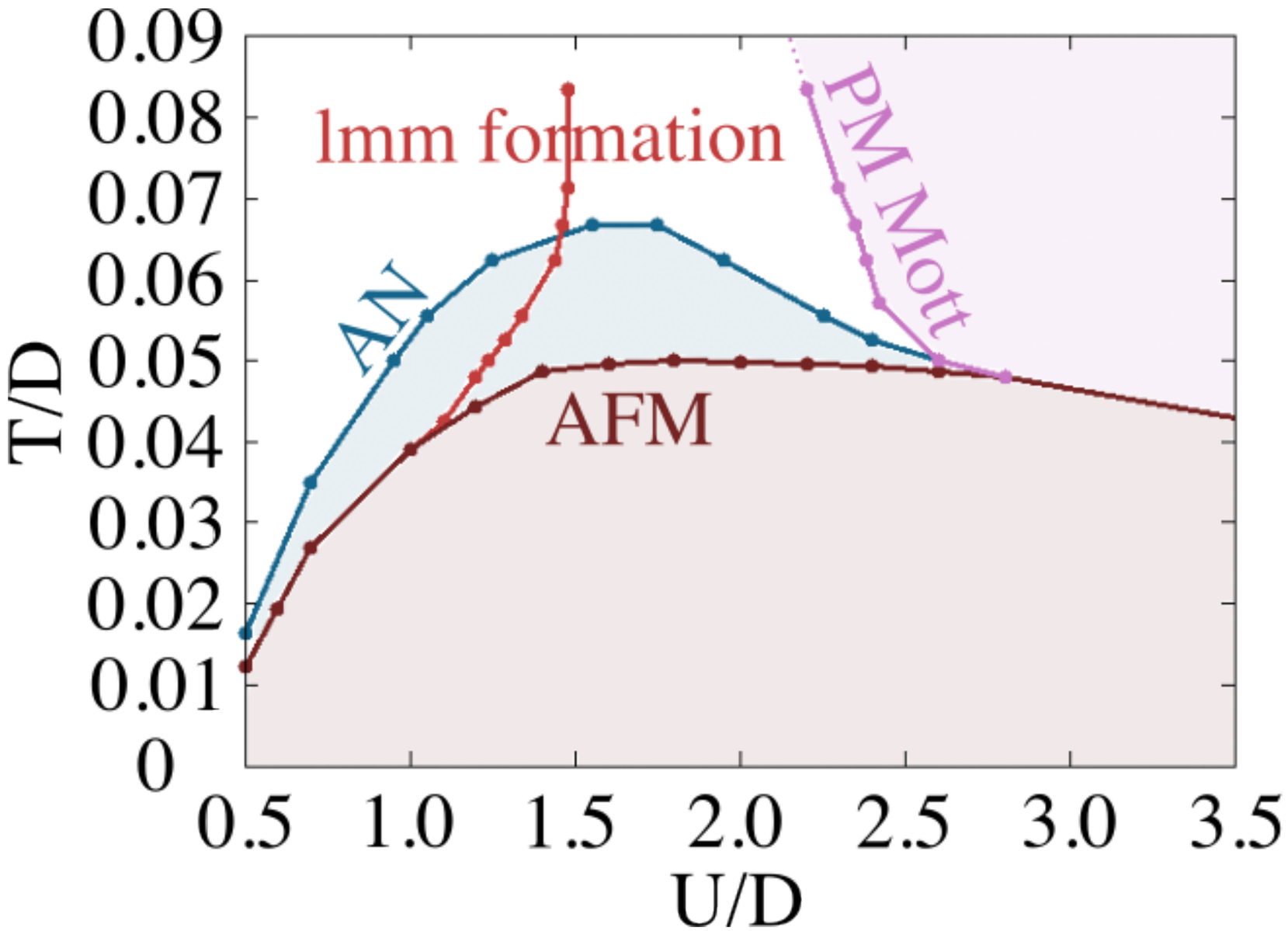
Momentum-selective opening of a pseudogap





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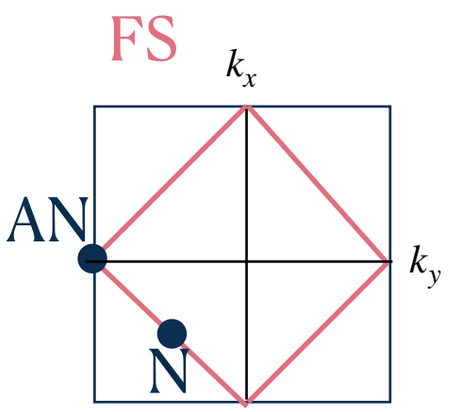
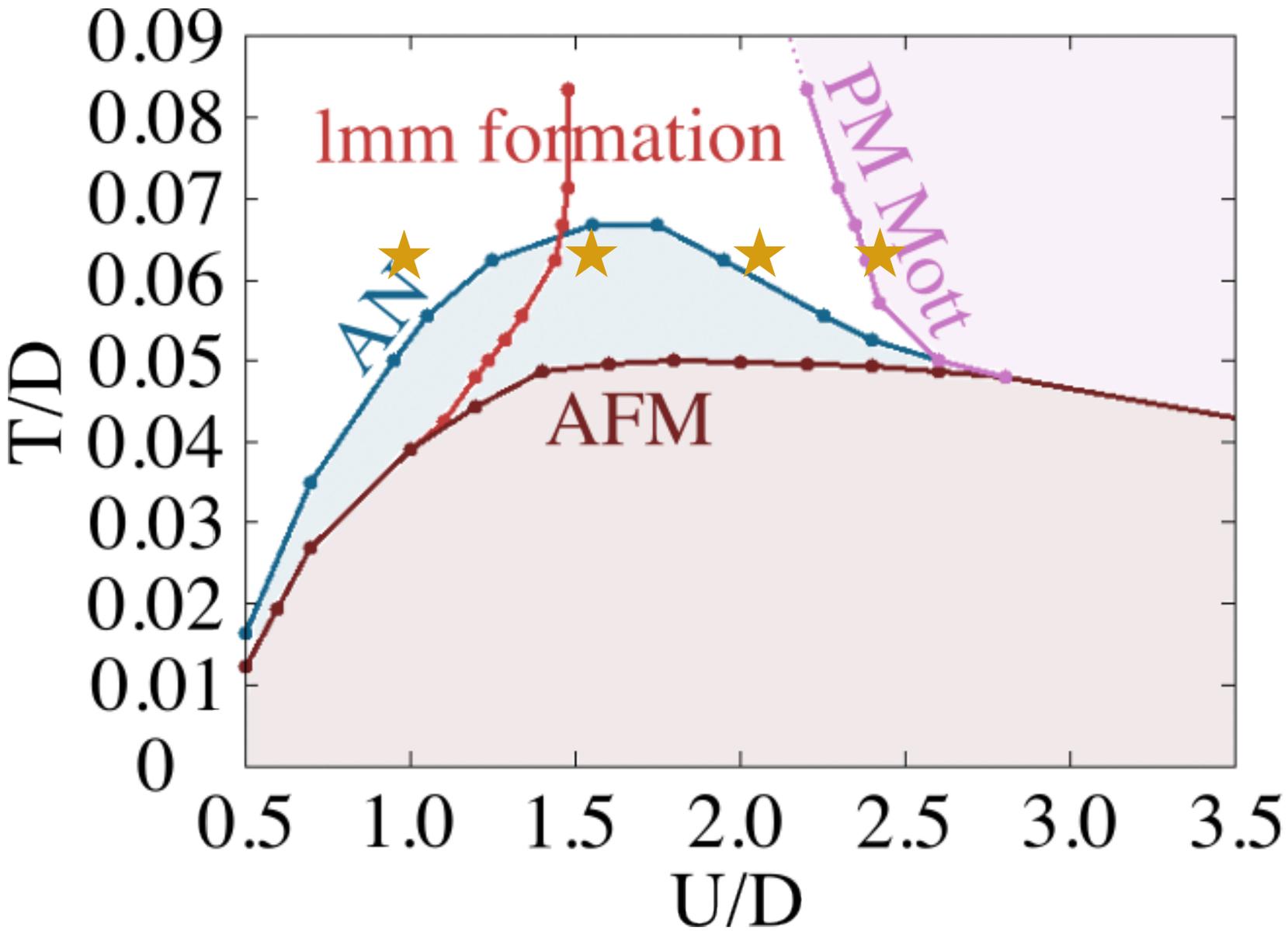
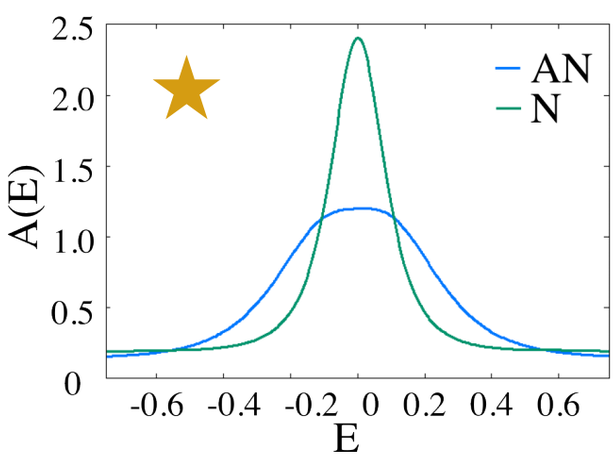
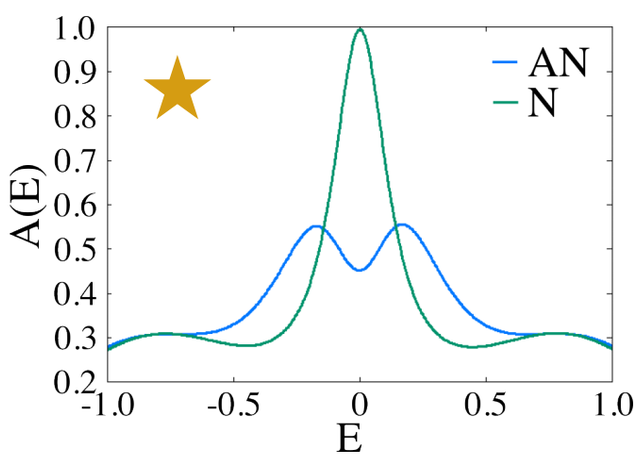
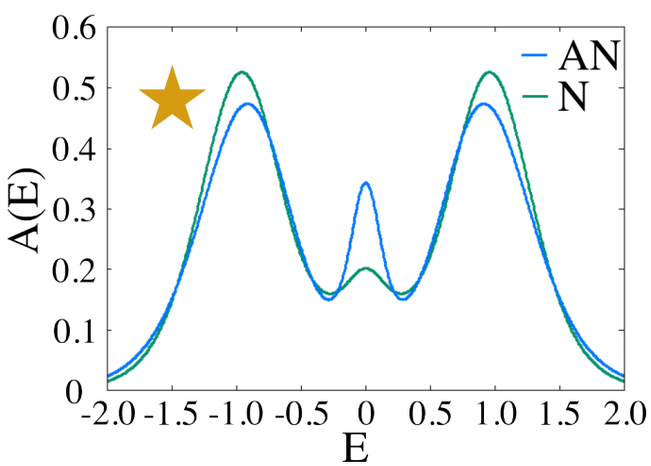
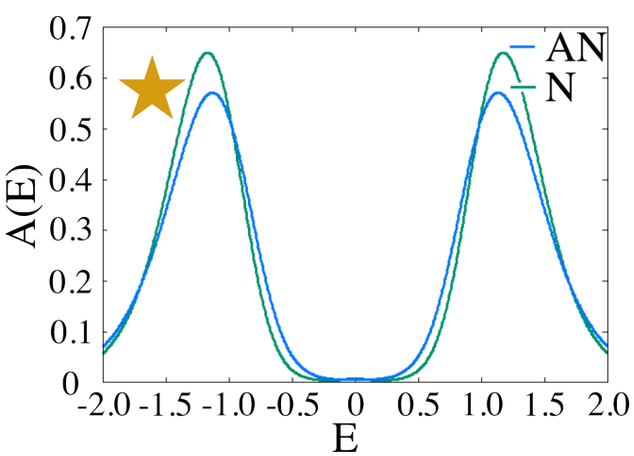




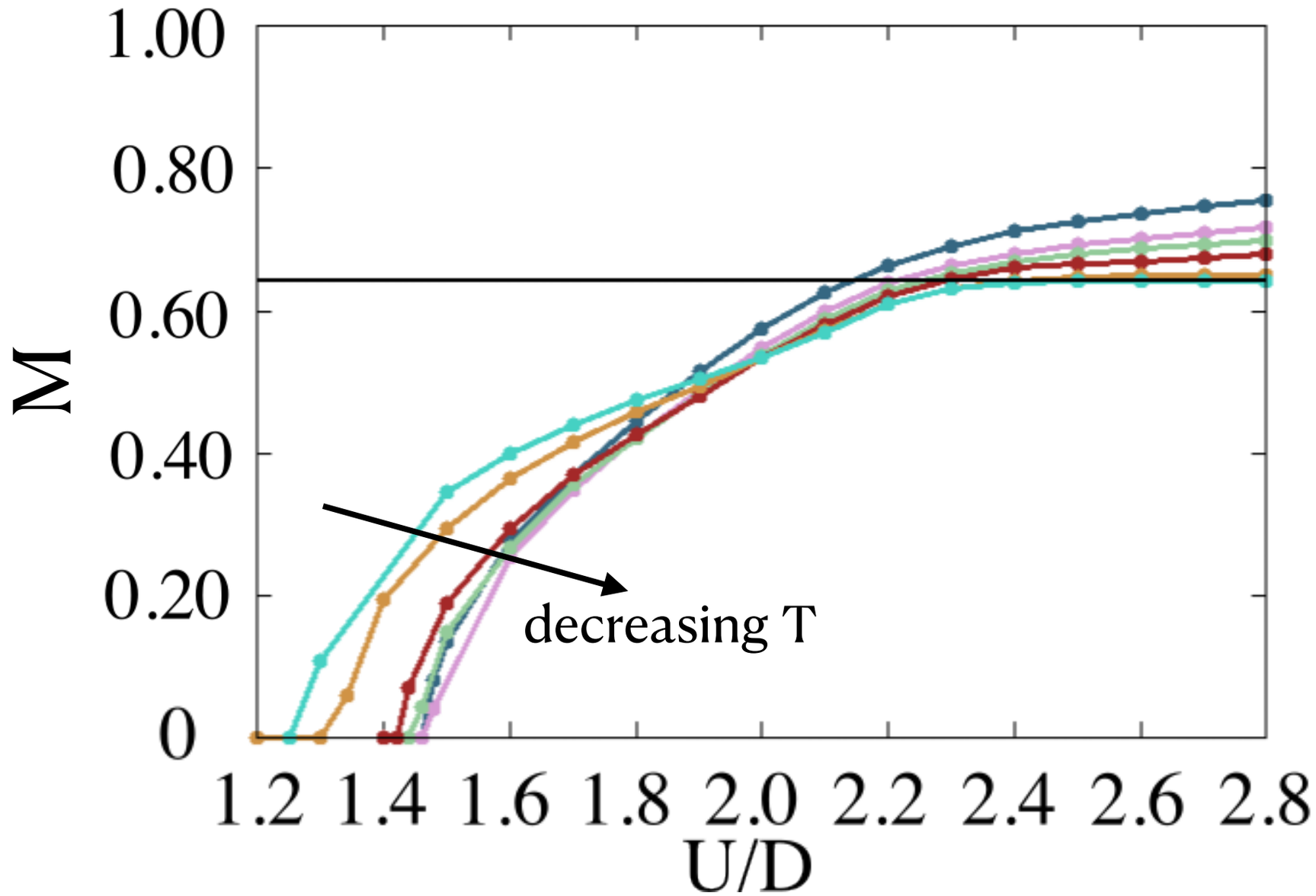








Local magnetic moment

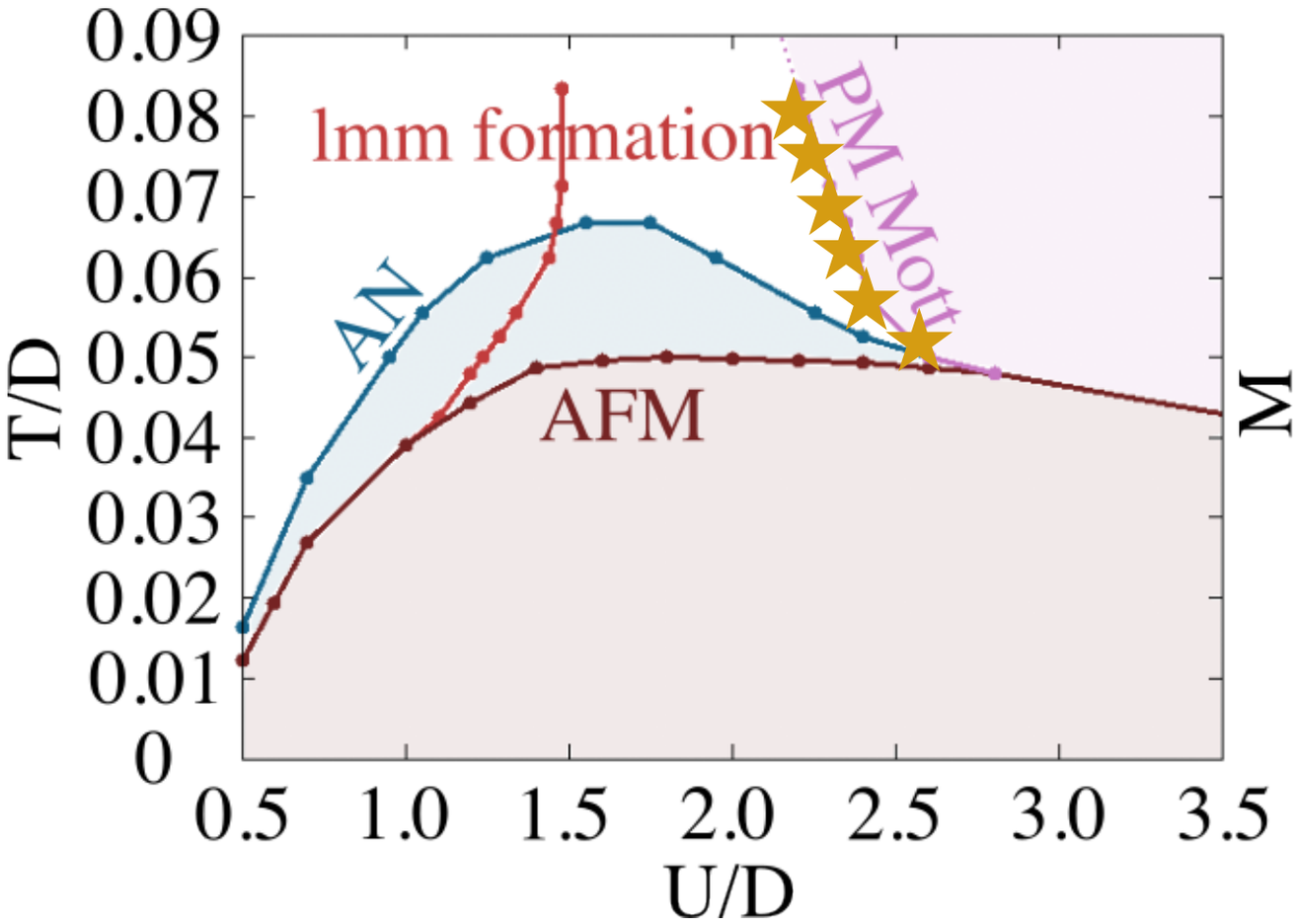


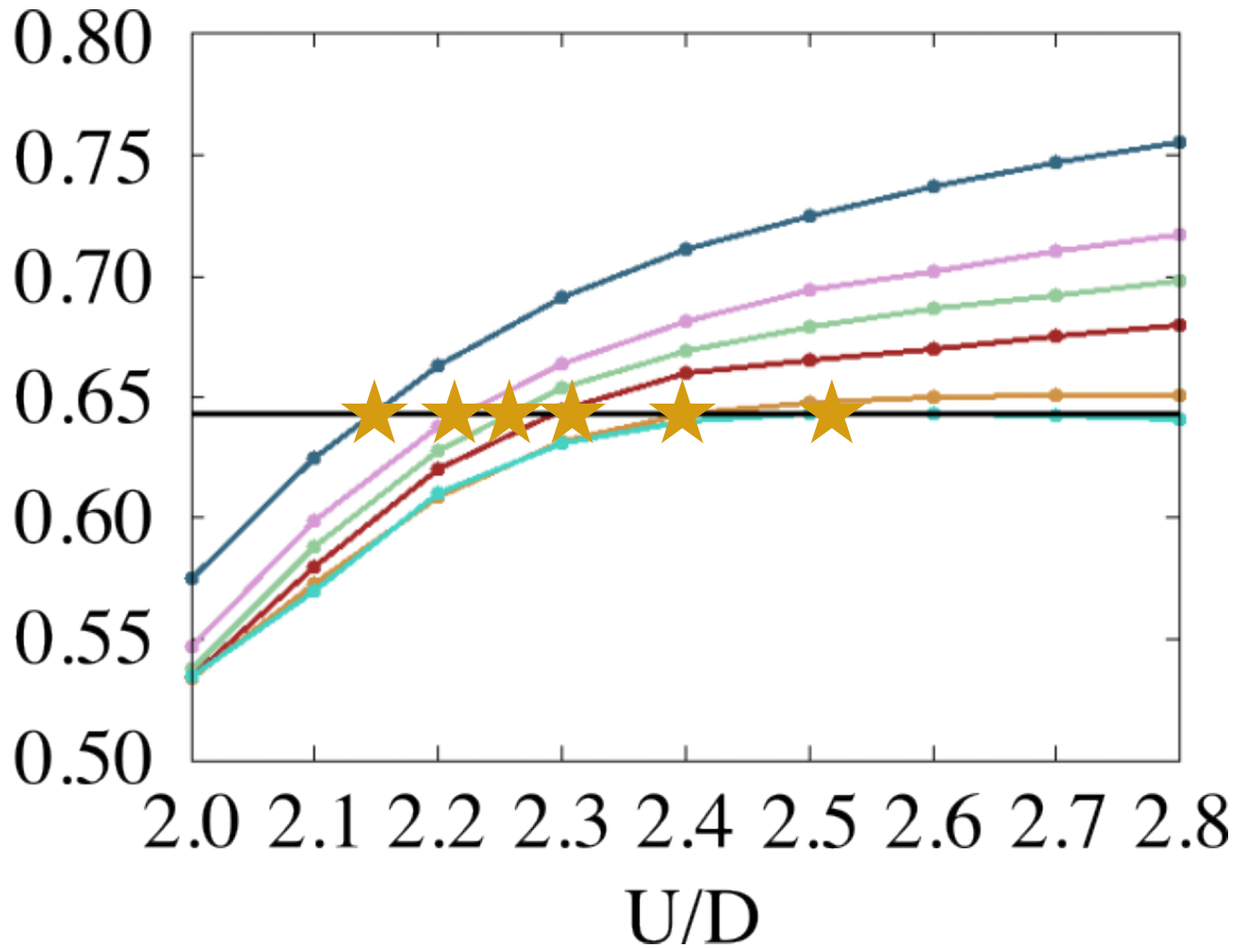
the local magnetic moment can fluctuate due to non-local correlations

↓

the lmm value is smaller compared to DMFT (even more for decreasing T)

Local magnetic moment

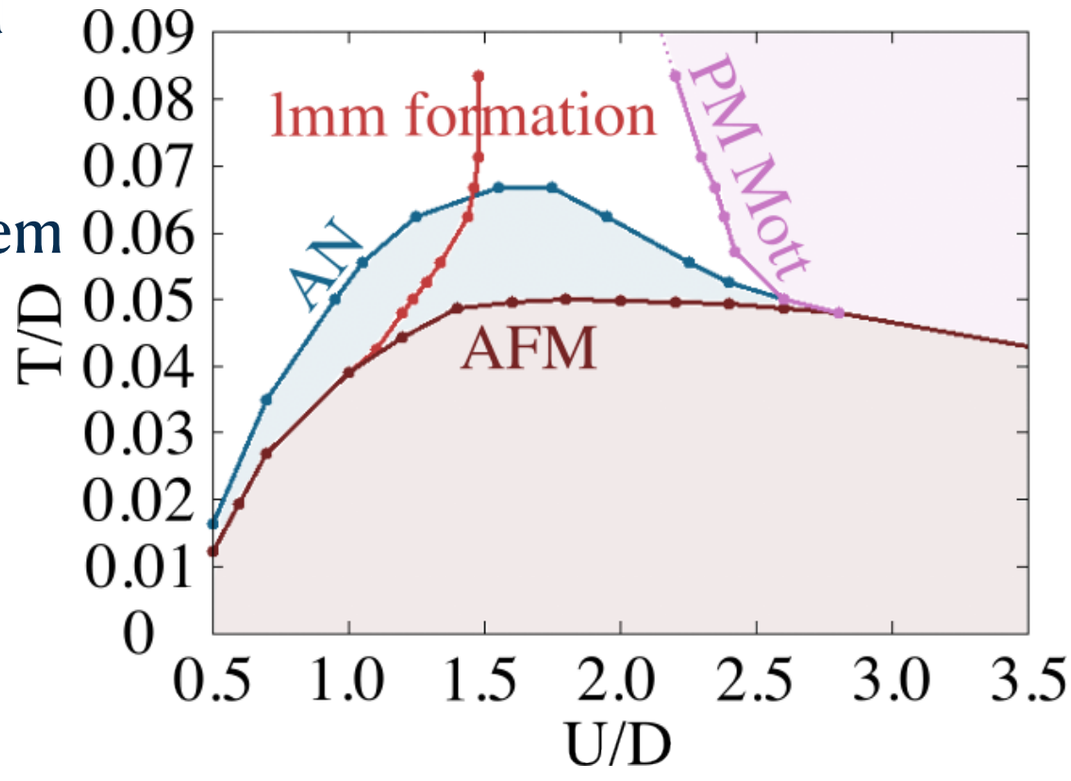




The value at which the local magnetic moment saturates for T just above the $T_{Néel}$, marks the paramagnetic MIT line.

Conclusions

- The local spectral function is not a reliable observable for the Mott transition in presence of non-local fluctuations.
- The MIT takes place when a pseudogap is opened everywhere across the Fermi surface.
- When there is no local magnetic moment the system is in the weak coupling - Slater regime.
- The lmm formation is a signature of entrance into the Mott physics region.
- Through the study of momentum-resolved observables and lmm we can disentangle the different mechanisms and identify the contribution of local and non-local effects.



Thank you for your attention !

Correlation length