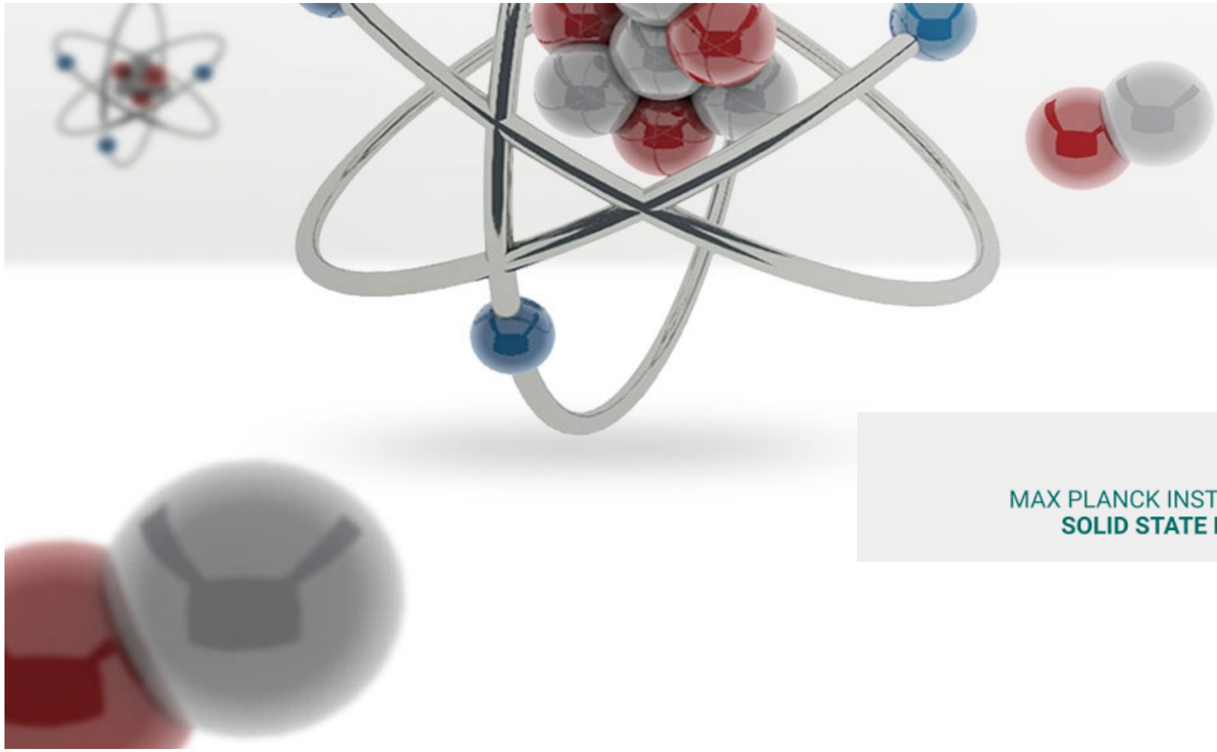


MAX PLANCK INSTITUTE FOR
SOLID STATE RESEARCH

Theory of strongly correlated
quantum matter (SCQM)

Multi-Method, Multi-Messenger Approaches to Models of Strong Correlations

Thomas Schäfer

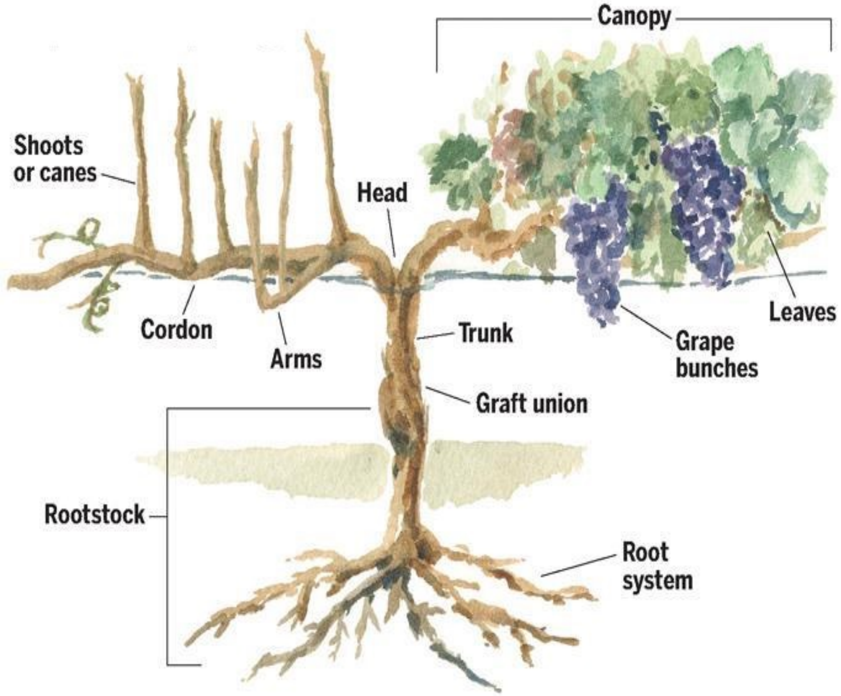
Head of Max Planck Research Group "Theory of strongly correlated quantum matter" (SCQM)

MPI for Solid State Research (MPI-FKF), Stuttgart

Strange metals: from the Hubbard model to AdS/CFT, Institute of Physics Belgrade (Online)

23rd May 2022

From roots to stems to harvest:
the application of multi-method, multi-messenger studies to…



…real materials

Magnetic correlations in infinite-layer nickelates: An experimental and theoretical multimethod study

R. A. Ortiz,[1,*] P. Puphal,[1,*] M. Klett,[1] F. Hotz,[2] R. K. Kremer,[1] H. Trepka,[1] M. Hemmida,[3] H.-A. Krug von Nidda,[3] M. Isobe,[1] R. Khasanov,[2] H. Luetkens,[2] P. Hansmann,[4] B. Keimer,[1] T. Schäfer,[1,†] and M. Hepting[1,‡]

Phys. Rev. Research **4**, *023093 (2022)*

…uncharted (model) territory

Mott Insulating States with Competing Orders in the Triangular Lattice Hubbard Model

Alexander Wietek,[1,*] Riccardo Rossi,[1,2] Fedor Šimkovic IV,[3,4] Marcel Klett,[5] Philipp Hansmann,[6] Michel Ferrero,[3,4] E. Miles Stoudenmire,[1] Thomas Schäfer,[5] and Antoine Georges[4,1,3,7]

Physical Review X **11**, *041013 (2021)*

…a simple (?) test case

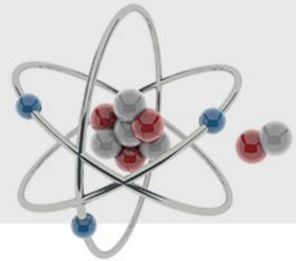
Tracking the Footprints of Spin Fluctuations: A MultiMethod, MultiMessenger Study of the Two-Dimensional Hubbard Model

Thomas Schäfer,[1,2,3,*] Nils Wentzell,[4] Fedor Šimkovic IV,[1,2] Yuan-Yao He,[4,5] Cornelia Hille,[6] Marcel Klett,[6,3] Christian J. Eckhardt,[7,8] Behnam Arzhang,[9] Viktor Harkov,[10,11] François-Marie Le Régent,[2] Alfred Kirsch,[2] Yan Wang,[12] Aaram J. Kim,[13] Evgeny Kozik,[13] Evgeny A. Stepanov,[10] Anna Kauch,[7] Sabine Andergassen,[6] Philipp Hansmann,[14,15] Daniel Rohe,[16] Yuri M. Vilk,[12] James P. F. LeBlanc,[9] Shiwei Zhang,[4,5] A.-M. S. Tremblay,[12] Michel Ferrero,[1,2] Olivier Parcollet,[4,17] and Antoine Georges[1,2,4,18]

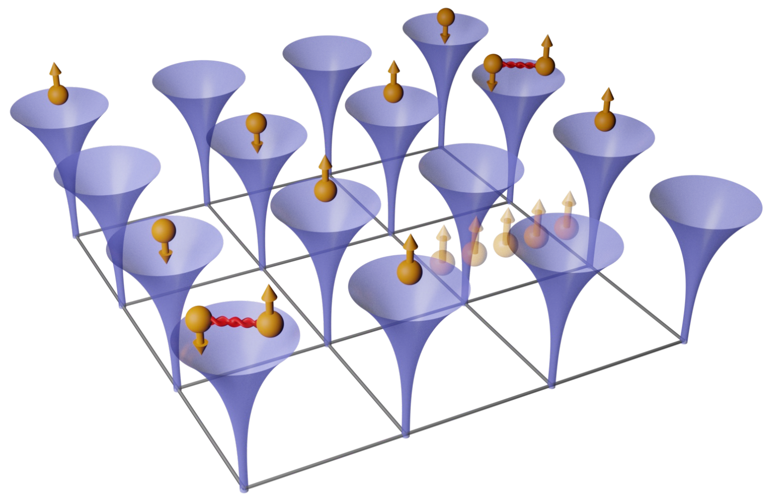
Physical Review X **11**, *011058 (2021)*

https://www.evineyardapp.com/blog/2017/05/30/overview-of-grapevine-structure-and-function/

Strongly correlated systems: fascinating physics - and a simple (?) modellization



Hubbard model



$$H = -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

-t : hopping

U: local Coulomb interaction

ANNUAL REVIEWS

Annual Review of Condensed Matter Physics

The Hubbard Model: A Computational Perspective

Mingpu Qin,[1] Thomas Schäfer,[2] Sabine Andergassen,[3] Philippe Corboz,[4] and Emanuel Gull[5]

[1] Key Laboratory of Artificial Structures and Quantum Control, School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai, China

[2] Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

[3] Institut für Theoretische Physik and Center for Quantum Science, Universität Tübingen, Germany

[4] Institute for Theoretical Physics and Delta Institute for Theoretical Physics, University of Amsterdam, Amsterdam, The Netherlands

[5] University of Michigan, Ann Arbor, Michigan, USA

Annu. Rev. Condens. Matter Phys. 2022. 13:275–302

The *Annual Review of Condensed Matter Physics* is online at conmatphys.annualreviews.org

https://doi.org/10.1146/annurev-conmatphys-090921-033948

Keywords

quantum many-body theory, model Hamiltonians, strongly correlated electron systems

Abstract

The Hubbard model is the simplest model of interacting fermions on a lattice and is of similar importance to correlated electron physics as the Ising model is to statistical mechanics or the fruit fly to biomedical science. Despite its simplicity, the model exhibits an incredible wealth of phases, phase transitions, and exotic correlation phenomena. Although analytical methods have provided a qualitative description of the model in certain limits, numerical tools have shown impressive progress in achieving quantitative accurate results over the past several years. This article gives an introduction to the model, motivates common questions, and illustrates the progress that has been achieved over recent years in revealing various aspects of the correlation physics of the model.

275

J. Hubbard, Proc. Royal Soc. A, ***276****, 238– 257 (1963)*

M. Qin, TS, et al., „The Hubbard model – a computational perspective", Annual Review of Condensed Matter Physics ***13*** *(2022)*

Several ways to attack the Hubbard model

Numerically exact te
- **Lattice quantum**
- **Diagrammatic M**

ld theory
(MFT)
eld theory (DMFT)

Let us put these methods to the test…

$$H = -t \sum c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum n_{i\uparrow} n_{i\downarrow}$$

PHYSICAL REVIEW X **11**, 011058 (2021)

Tracking the Footprints of Spin Fluctuations: A MultiMethod, MultiMessenger Study of the Two-Dimensional Hubbard Model

Thomas Schäfer,[1,2,3,*] Nils Wentzell,[4] Fedor Šimkovic IV,[1,2] Yuan-Yao He,[4,5] Cornelia Hille,[6] Marcel Klett,[6,3] Christian J. Eckhardt,[7,8] Behnam Arzhang,[9] Viktor Harkov,[10,11] François-Marie Le Régent,[2] Alfred Kirsch,[2] Yan Wang,[12] Aaram J. Kim,[13] Evgeny Kozik,[13] Evgeny A. Stepanov,[10] Anna Kauch,[7] Sabine Andergassen,[6] Philipp Hansmann,[14,15] Daniel Rohe,[16] Yuri M. Vilk,[12] James P. F. LeBlanc,[9] Shiwei Zhang,[4,5] A.-M. S. Tremblay,[12] Michel Ferrero,[1,2] Olivier Parcollet,[4,17] and Antoine Georges[1,2,4,18]

Extensions
Cluste
- Dy
- cel

Diagrammatic extensions (all length scales)
- **Dynamical vertex approximation** (DΓA)
- **Dual fermion** (DF)
- **Dual boson** (DB)
- **Triply irreducible local expansion** (TRILEX)

chniques
stent approach
ation group (fRG)
- **Parquet approximation** (PA)
- [tensor networks: DMRG, METTS, etc.]

Putting all these methods to the test

PHYSICAL REVIEW X **11,** 011058 (2021)

Tracking the Footprints of Spin Fluctuations: A MultiMethod, MultiMessenger Study of the Two-Dimensional Hubbard Model

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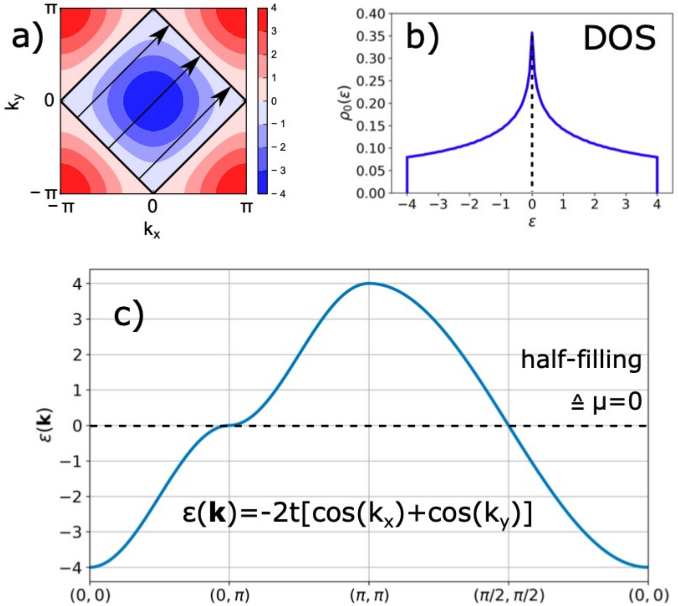


Test parameters

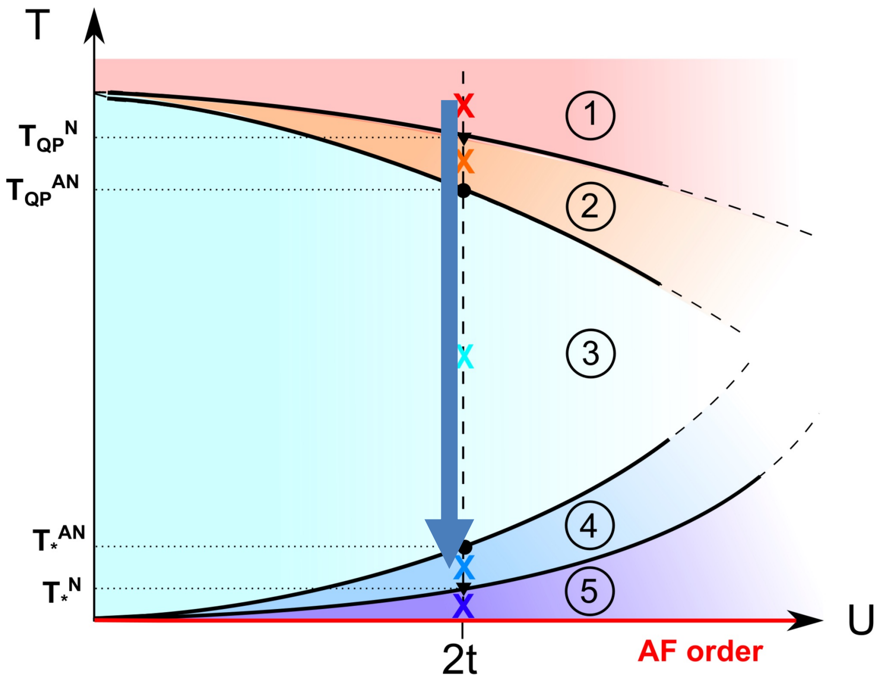
- 2d unfrustrated square lattice
- Half-filled
- U=2t

Observables (as function of T)

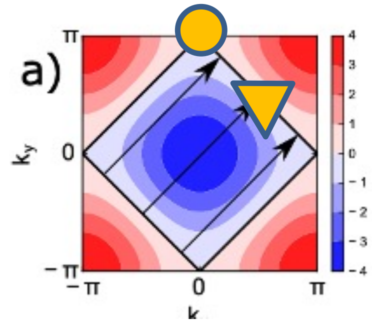
- Coherence temperature T_{QP}
- ”Pseudogap” temperature T_*
- Double occupancy D
- Magnetic susceptibility χ
- Magnetic correlation length ξ

T. Schäfer et al., Phys. Rev. X ***11,*** *011058 (2021)*

A tale of energy scales



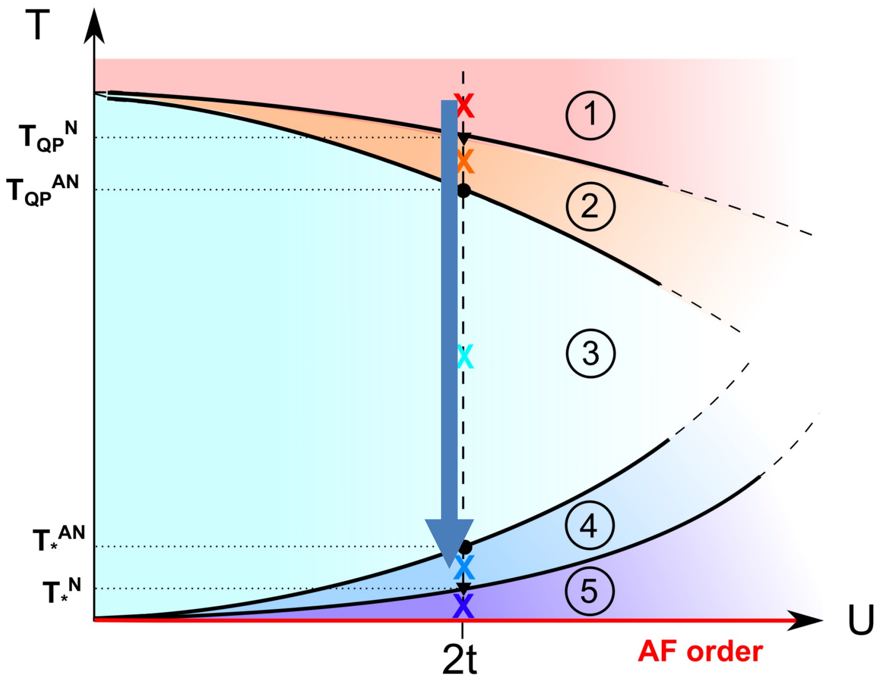
● AN = (π, 0)
▼ N = (π/2, π/2)

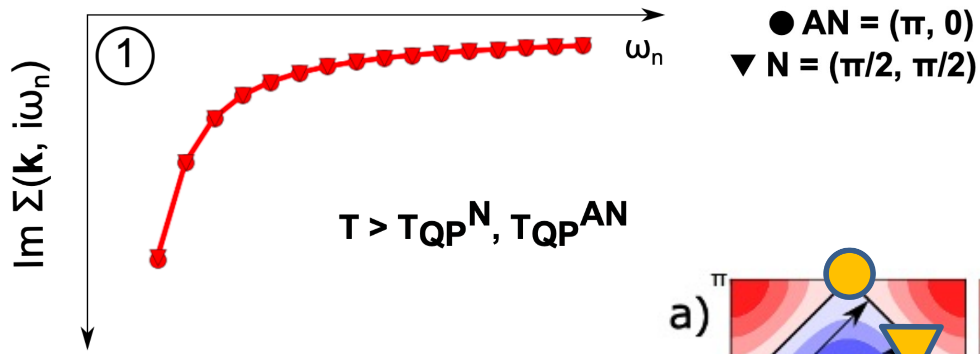


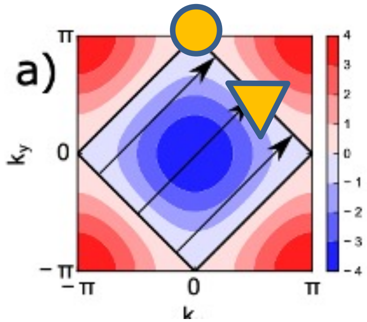
AF order only at **T=0** (Mermin-Wagner theorem)

T. Schäfer et al., Phys. Rev. X ***11,*** *011058 (2021)*
T. Schäfer et al., Phys. Rev. B ***91***, *125109 (2015)*
F. Šimkovic et al., Phys. Rev. Lett. ***124***, *017003 (2020), A. J. Kim, et al., Phys. Rev. Lett.* ***124***, *117602 (2020)*

A tale of energy scales







① incoherent regime

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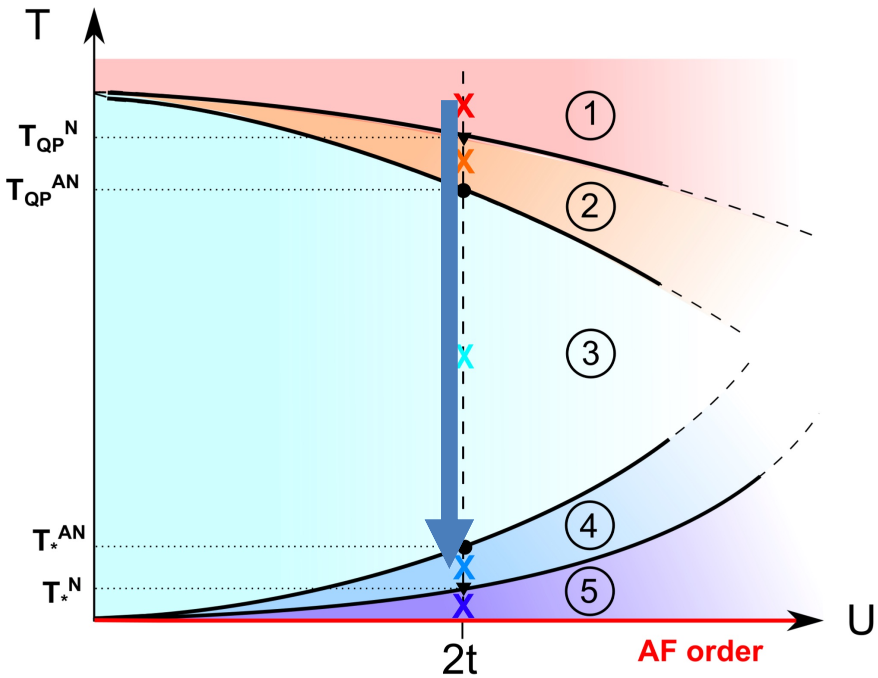
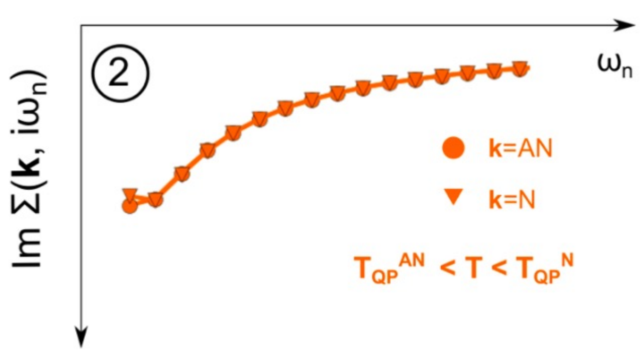
A tale of energy scales





● AN = (π, 0)
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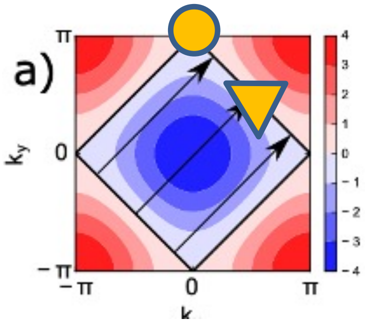

① incoherent regime
② quasiparticle coherence N

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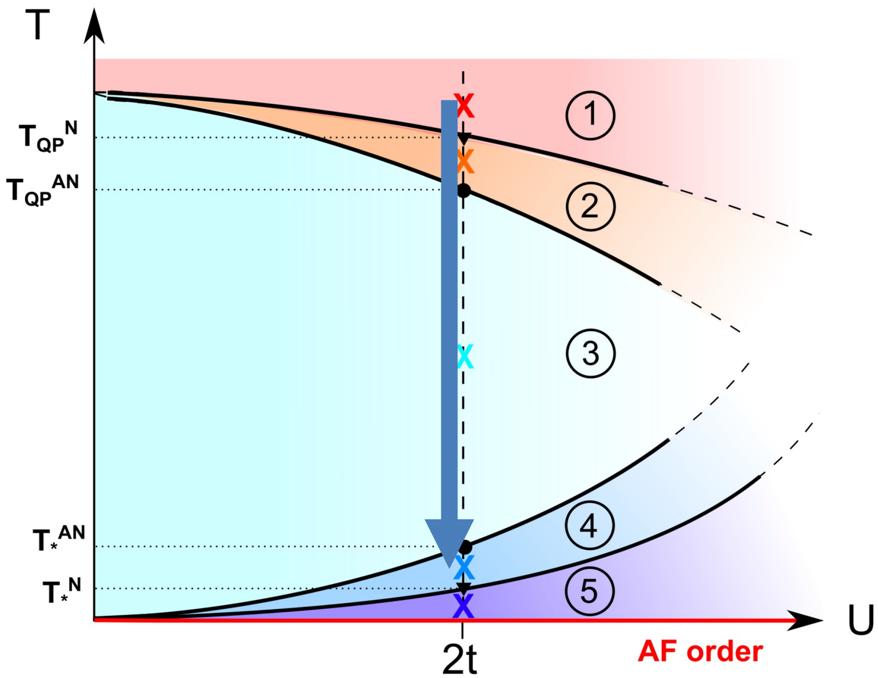
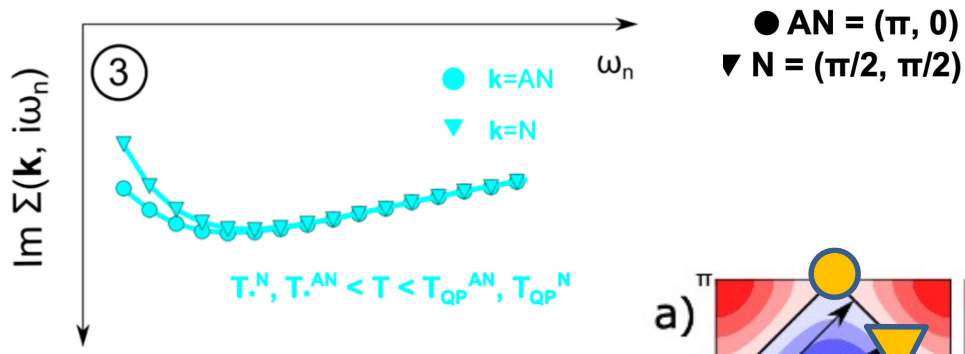
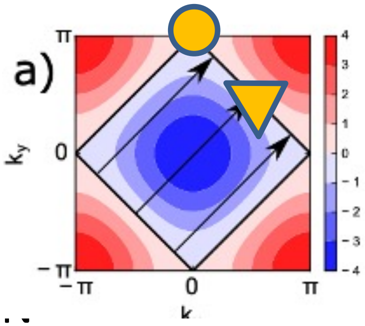
A tale of energy scales







① incoherent regime

② quasiparticle coherence at . .

③ QP coherence at both N/AN, metallic

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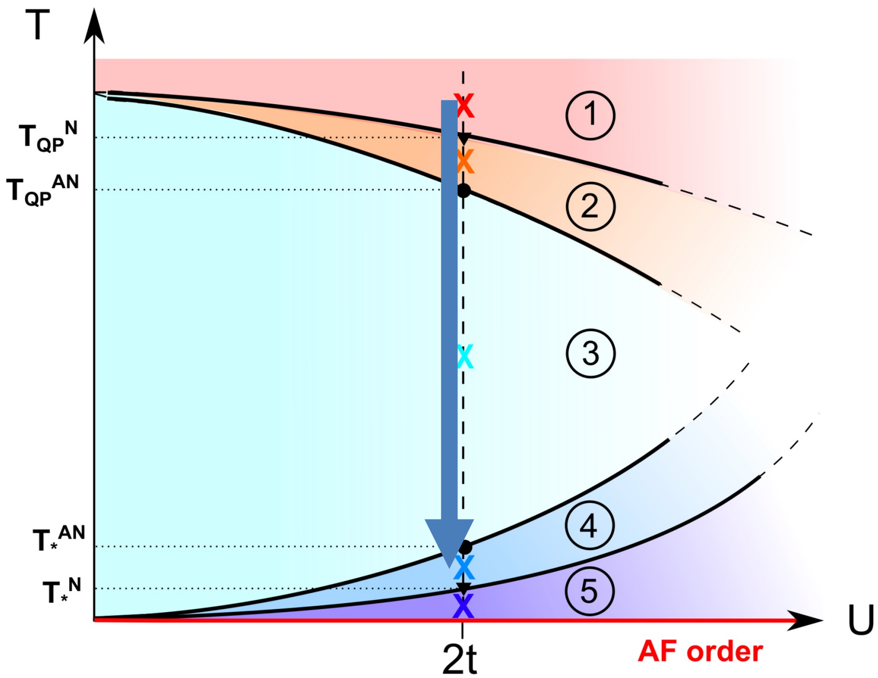
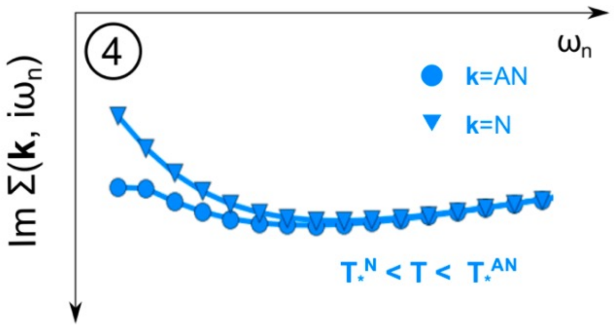
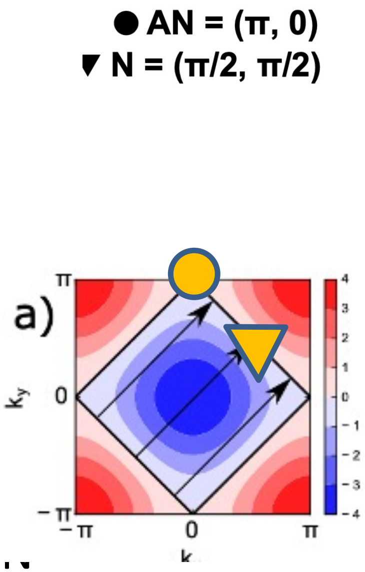
A tale of energy scales





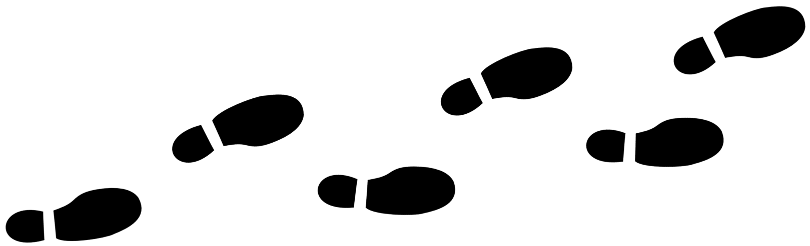


① incoherent regime

② quasiparticle coherence at ..

③ QP coherence at both N/AN, metallic

④ AN gaps out (weak-coupling “pseudogap”)



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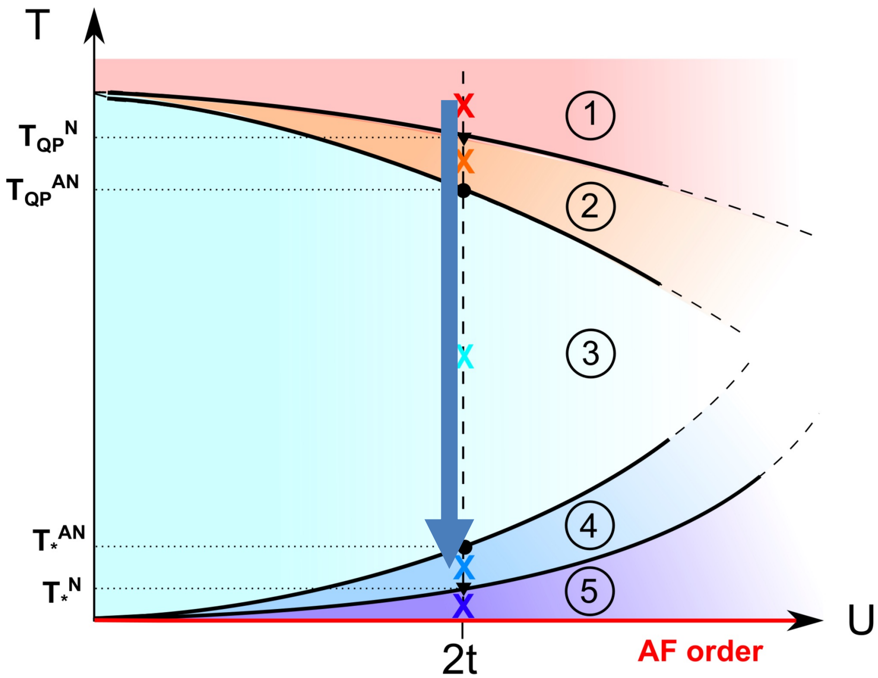
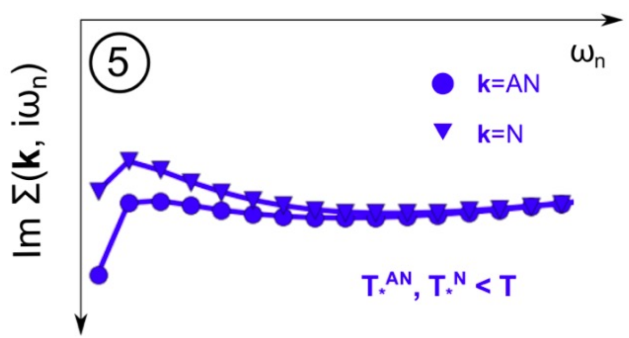
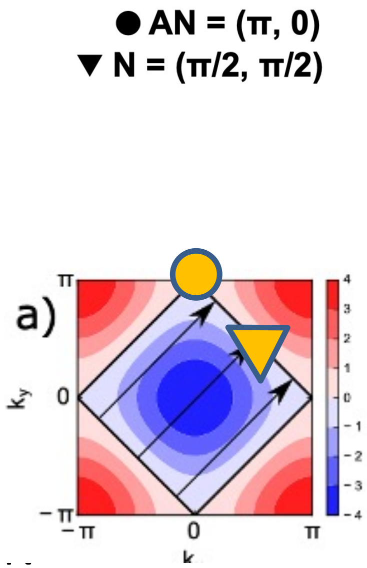
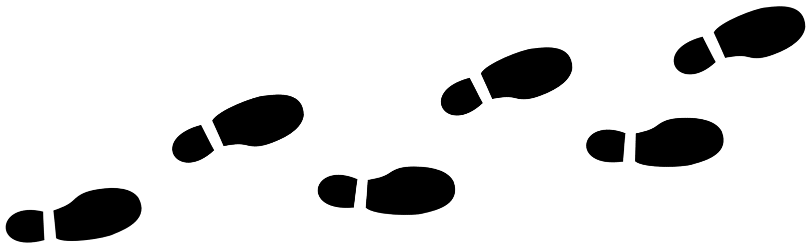
A tale of energy scales







1. incoherent regime
2. quasiparticle coherence at . .
3. QP coherence at both N/AN, metallic
4. AN gaps out (weak-coupling "pseudogap")
5. N gaps out, insulating regime



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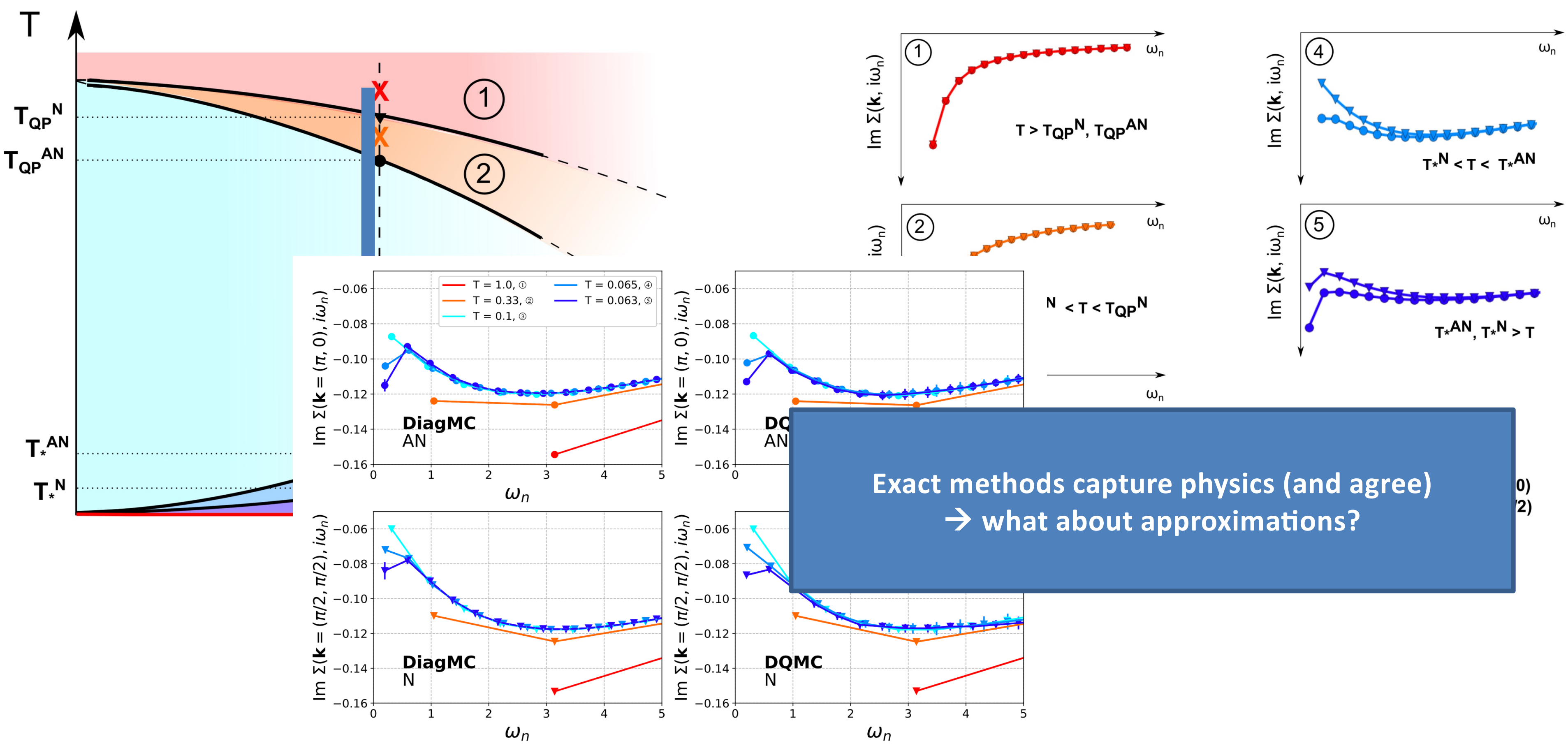
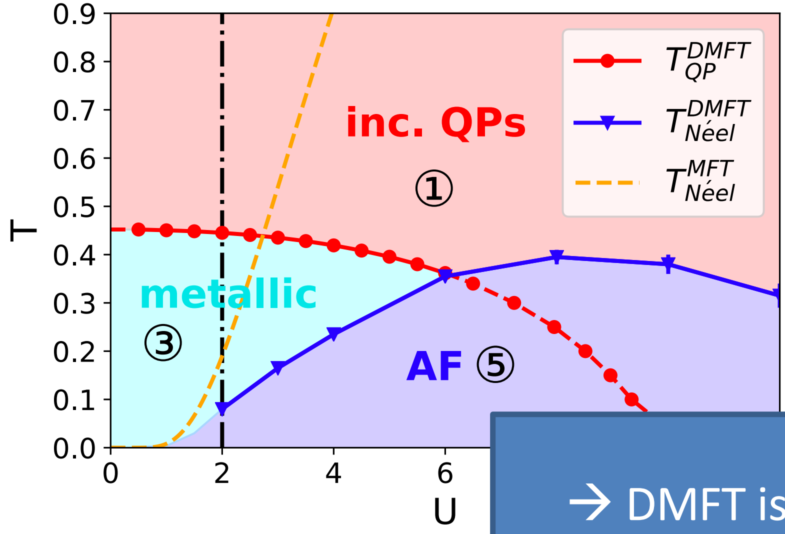
A tale of energy scales



Exact methods capture physics (and agree)
→ what about approximations?

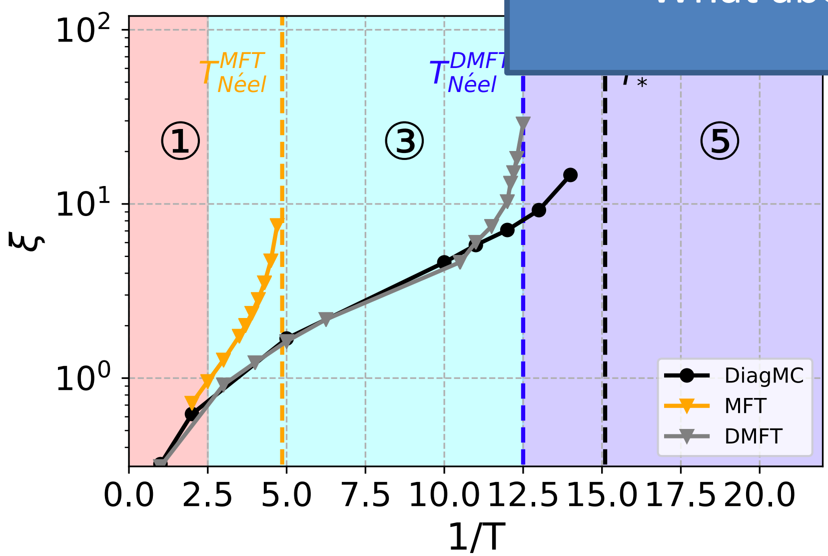
*T. Schäfer et al., Phys. Rev. X **11,** 011058 (2021)*

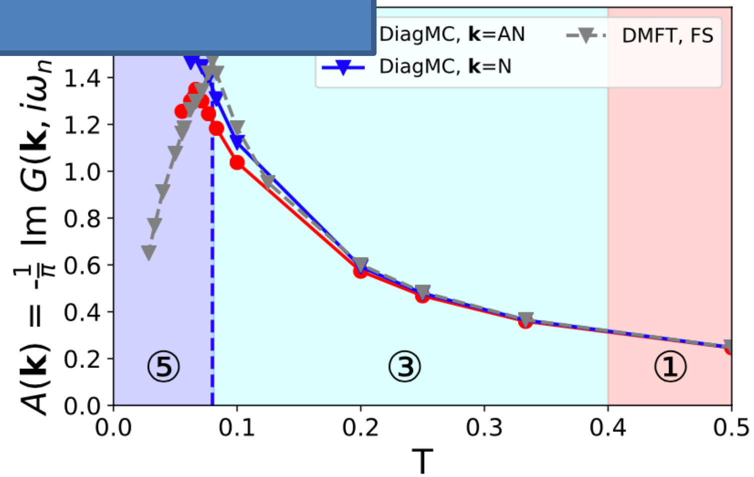
A tale of energy scales: the dynamical MF starting point



- DMFT: does not satisfy Mermin-Wagner (→ finite T_N)
- Captures the crossover from metallic to insulating via a **phase transition** (finite magnetization)
- …gnalled, when **correlation** …es large (→ fluctuations)

→ DMFT is a good starting point
What about fluctuations?





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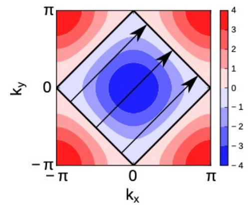
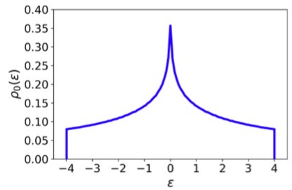
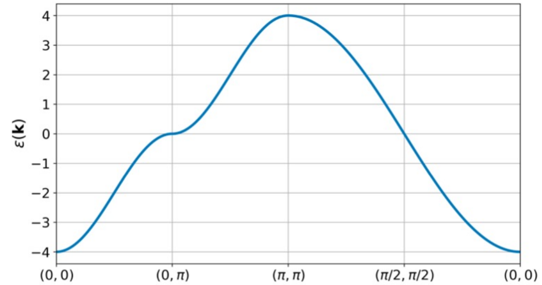
Measuring fluctuations: two-particle quantities



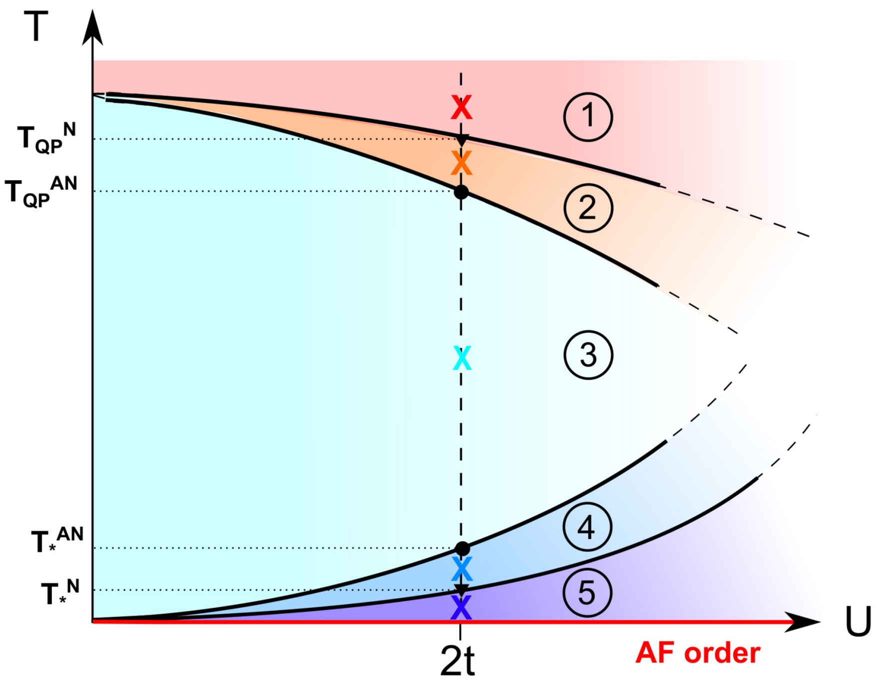




Static antiferromagnetic susceptibility

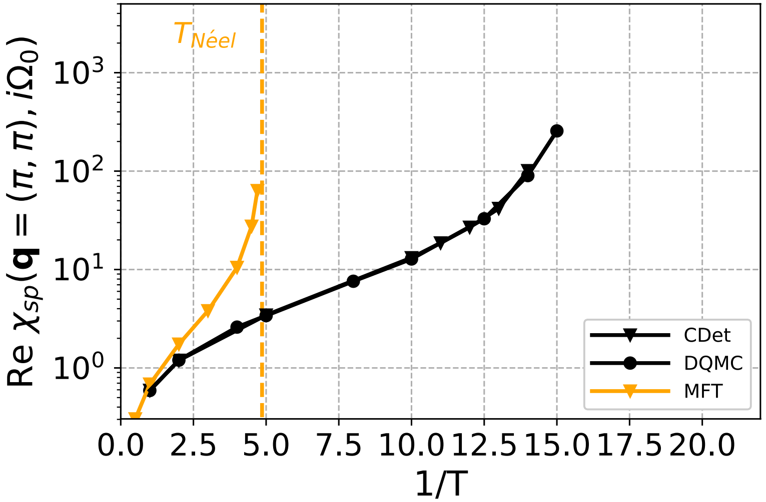
$$\chi_{\rm sp}(\mathbf{q}, i\Omega_n) = \int_0^\beta d\tau \sum_{\mathbf{r}} e^{i\tau\Omega_n} e^{-i\mathbf{q}\mathbf{r}} \langle S_z(\mathbf{r},\tau) S_z(0,0)\rangle$$

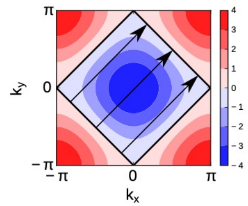
$$S_z(\mathbf{r},\tau) = n_\uparrow(\mathbf{r},\tau) - n_\downarrow(\mathbf{r},\tau)$$

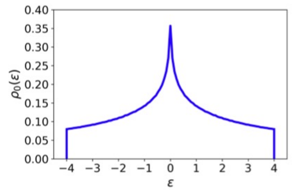


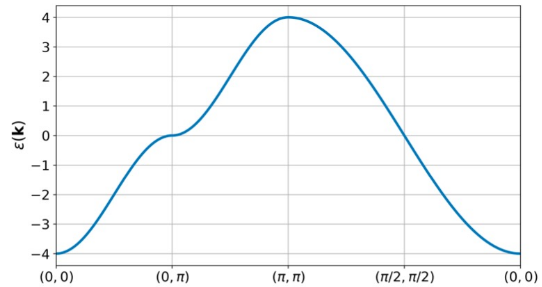
Measuring fluctuations: two-particle quantities

Static antiferromagnetic susceptibility





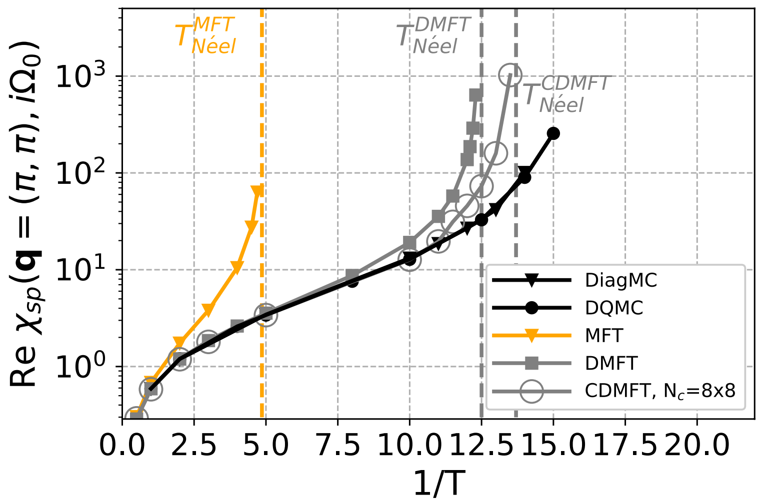


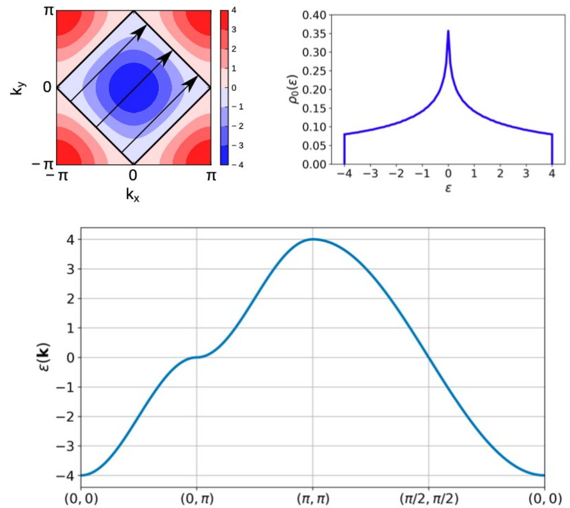


	DiagMC	DQMC
T_N	✓ 0	✓ 0
χ(T=0.1)	13.2	13.2

Measuring fluctuations: two-particle quantities

Static antiferromagnetic susceptibility

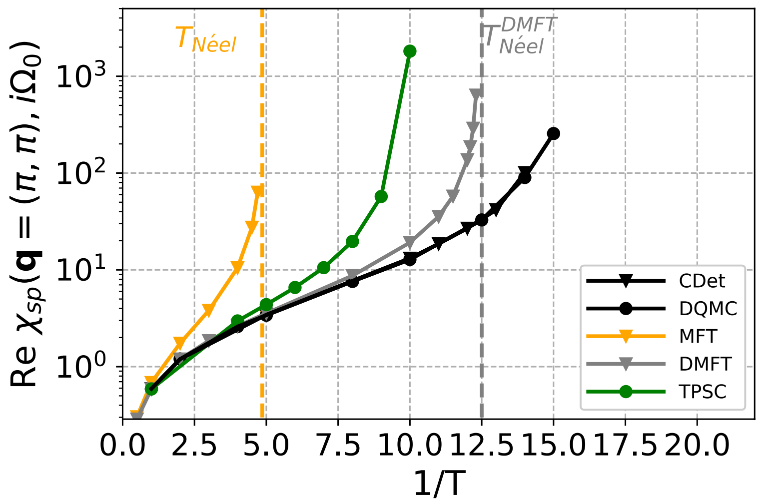


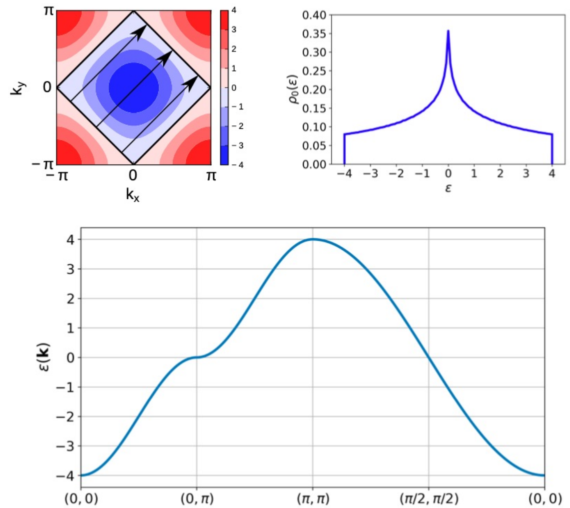


	DiagMC	DQMC	DMFT
T_N	✓ 0	✓ 0	✗ 0.08
χ(T=0.1)	13.2	13.2	19.2

Measuring fluctuations: two-particle quantities

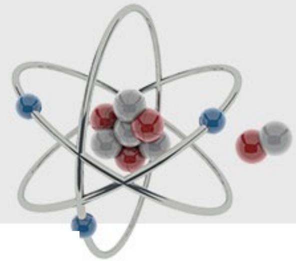
Static antiferromagnetic susceptibility



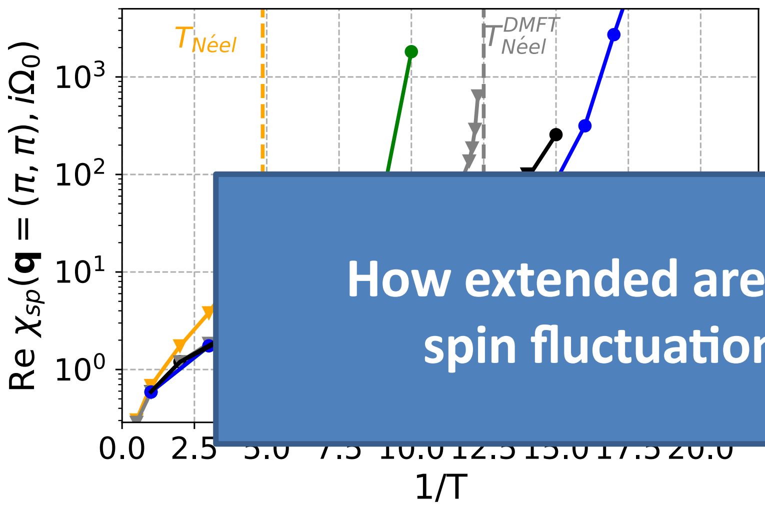


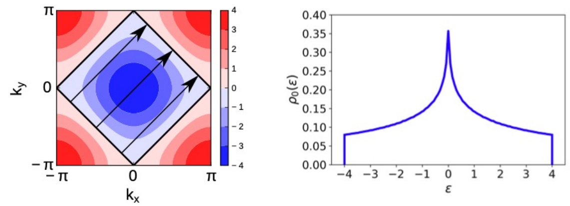
	DiagMC	DQMC	DMFT	TPSC
T_N	✓ 0	✓ 0	✗ 0.08	✓ 0
χ(T=0.1)	13.2	13.2	19.2	1816.5

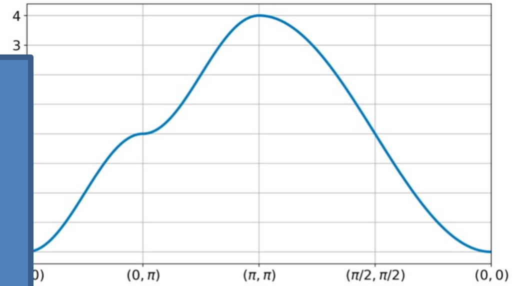
Measuring fluctuations: two-particle quantities



Static antiferromagnetic susceptibility



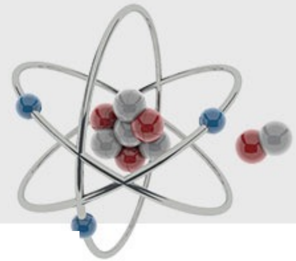




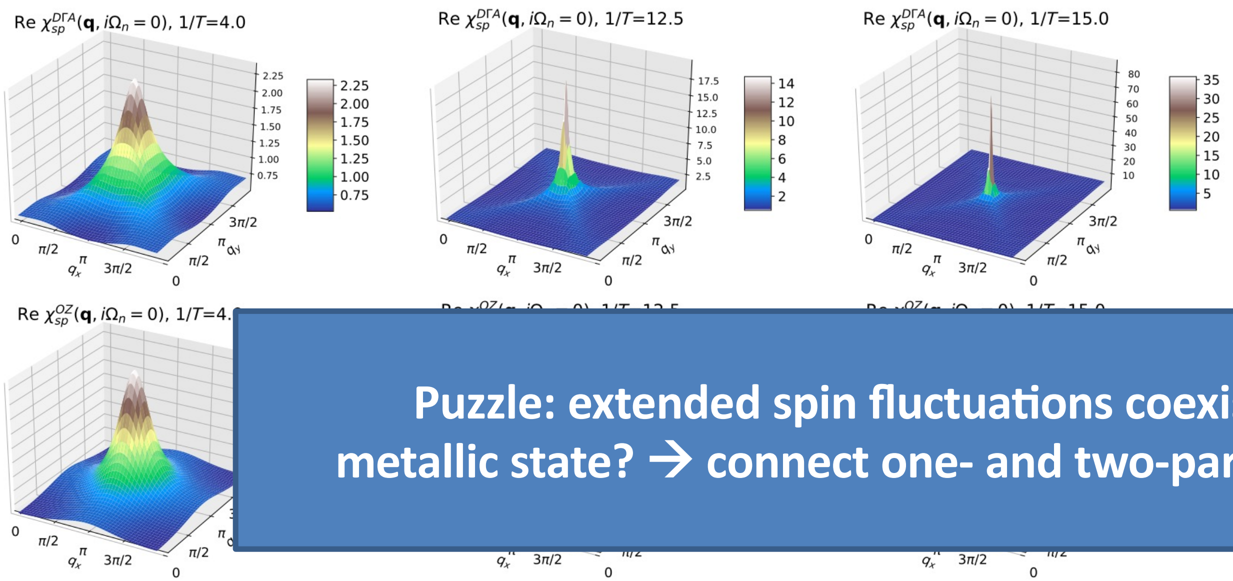
How extended are these spin fluctuations?

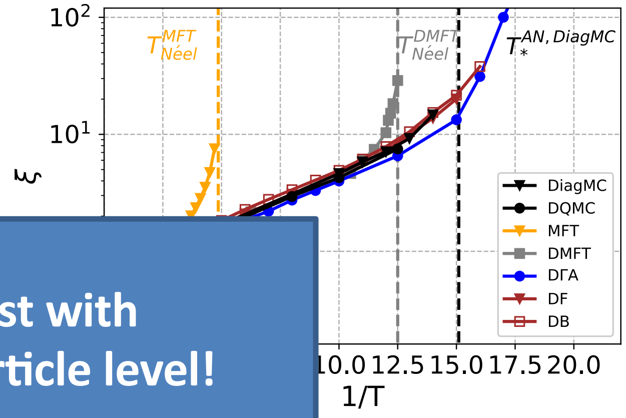
	DiagMC	DQMC	DMFT	TPSC	DΓA
T_N	✓ 0	✓ 0	✗ 0.08	✓ 0	✓ 0
χ(T=0.1)	13.2	13.2	19.2	1816.5	15.3

Measuring fluctuations: two-particle quantities



Magnetic correlation length via Ornstein-Zernike fits $\chi(\mathbf{q}, i\Omega_n) = \frac{A}{(\mathbf{q}-\mathbf{Q})^2 + \xi^{-2} + \frac{|\Omega_n|}{\gamma}}$





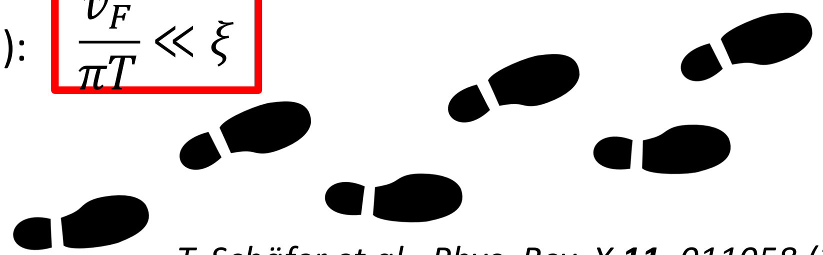
Puzzle: extended spin fluctuations coexist with metallic state? → connect one- and two-particle level!

Metallic, but ξ>5a!

Magnetic correlation length exponentially growing!

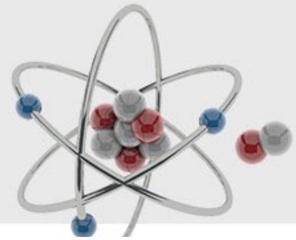
Condition for **pseudogap** at weak coupling (Vilk criterion): $\frac{v_F}{\pi T} \ll \xi$

→ Footprints of spin fluctuations in all observables (on the one- **and** two-particle level)



T. Schäfer et al., Phys. Rev. X ***11,*** *011058 (2021)*

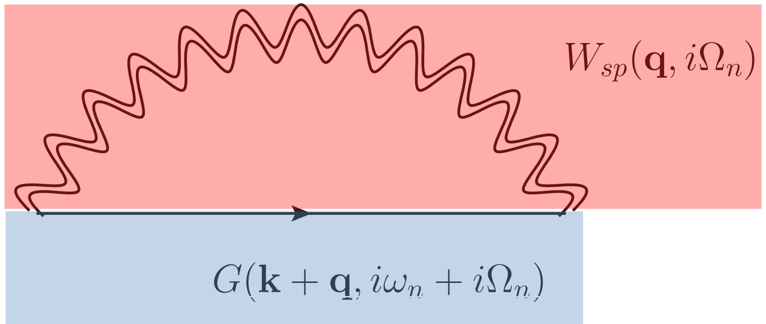
The (fairly "strange") metallic regime I:
Handshake with analytical spin fluctuation theory



$$\Sigma_{\mathrm{SF}}(\mathbf{k}, i\omega_n) = g^2 T \int \frac{d^2q}{(2\pi)^2} \sum_{\Omega_n} G(\mathbf{k}+\mathbf{q}, i\omega_n + i\Omega_n)\,\chi(\mathbf{q}, i\Omega_n)$$

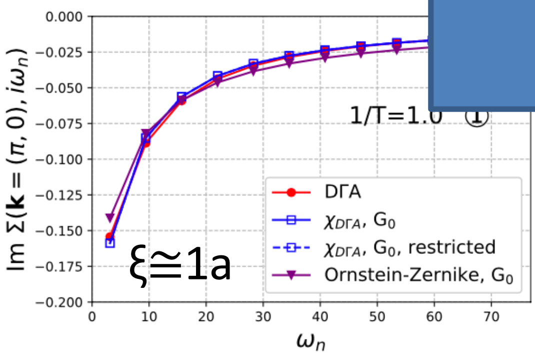
Non-interacting G_0

coupling of fermion to spin modes $\frac{3}{8}U^2$



Handshake with nume

How can extended spin fluctuations coexist with metallic behavior?



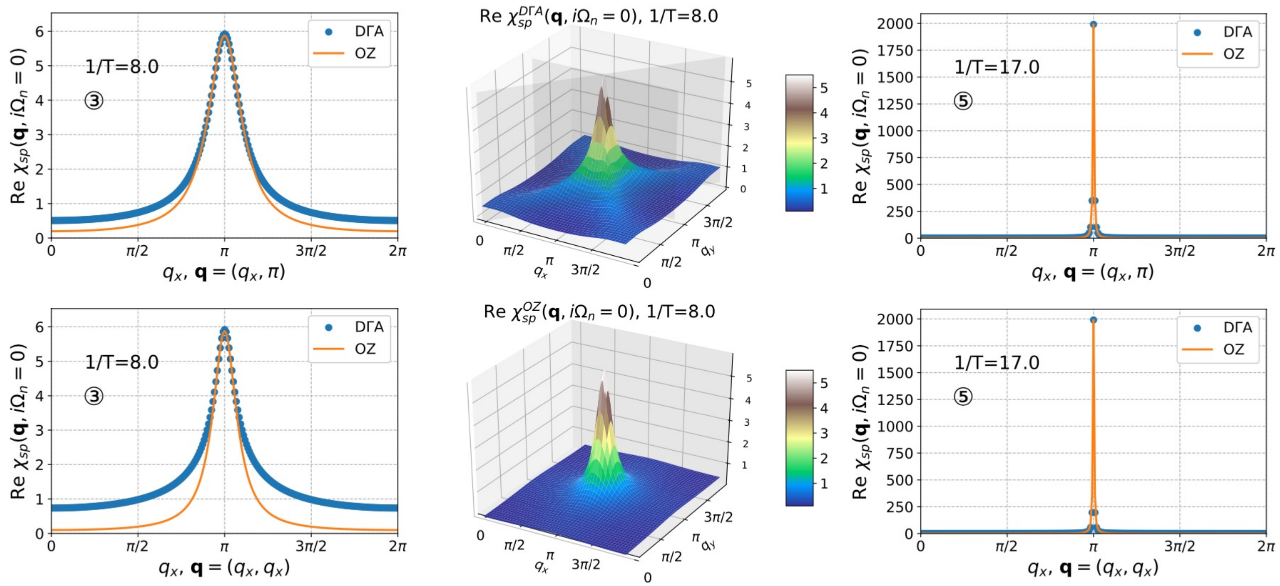
<u>Three choices for susceptibility</u>

- Full DΓA spin susceptibility
- DΓA spin susceptibility restricted to $|q_i - Q_i| < 2\xi^{-1}$ around AF peak
- Ornstein-Zernike fit

} Non-metallic self-energy in regime ③?!

The (fairly "strange") metallic regime I: **Handshake with analytical spin fluctuation theory**

$$\Sigma_{\rm SF}(\mathbf{k}, i\omega_n) = g^2 T \int \frac{d^2q}{(2\pi)^2} \sum_{\Omega_n} G(\mathbf{k}+\mathbf{q}, i\omega_n + i\Omega_n)\chi(\mathbf{q}, i\Omega_n)$$



→ Resolves dichotomy of sizeable correlation length and metallic state

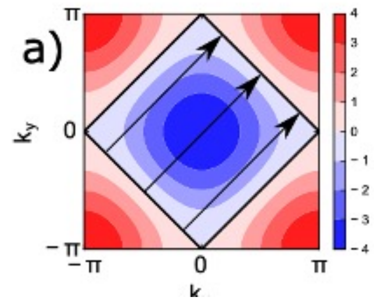
Many **q**-vectors contribute → metallic

q=(π, π) is dominant → insulating

T. Schäfer et al., Phys. Rev. X ***11,*** *011058 (2021)*

The (fairly "strange") metallic regime II:
Perfect nesting and **non-Fermi-liquid behavior**

How does perfect nesting influence the nature of the metal?

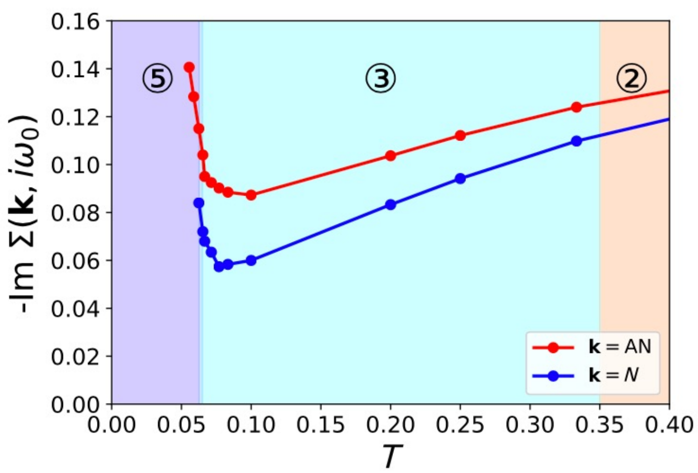


Fermi liquid self-energy on real frequencies:

$$-\mathrm{Im}\,\Sigma(\boldsymbol{k_F},\omega) \propto \underbrace{\omega^2 + (\pi T)^2}_{} + \cdots$$

$$-\omega_n^2 + (\pi T)^2$$ → vanishes for first Matsubara frequency

$$\Longrightarrow \mathrm{Im}\,\Sigma(\boldsymbol{k_F},\omega_0) \sim \left(1-\frac{1}{Z}\right)\omega_0 = \left(1-\frac{1}{Z}\right)\pi T$$ → Linear in T, "first Matsubara frequency rule"



Data from DiagMC indicates non-Fermi-liquid!
→ real-frequency data?

A. Virosztek and J. Ruvalds, Phys. Rev. B ***42****, 4064 (1990)*
A. V. Chubukov and D. L. Maslov, Phys. Rev. B ***86****, 155136 (2012)*
T. Schäfer et al., Phys. Rev. X ***11,*** *011058 (2021)*

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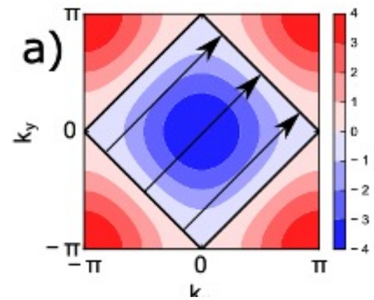

Fermi liquid self-energy on real frequencies:

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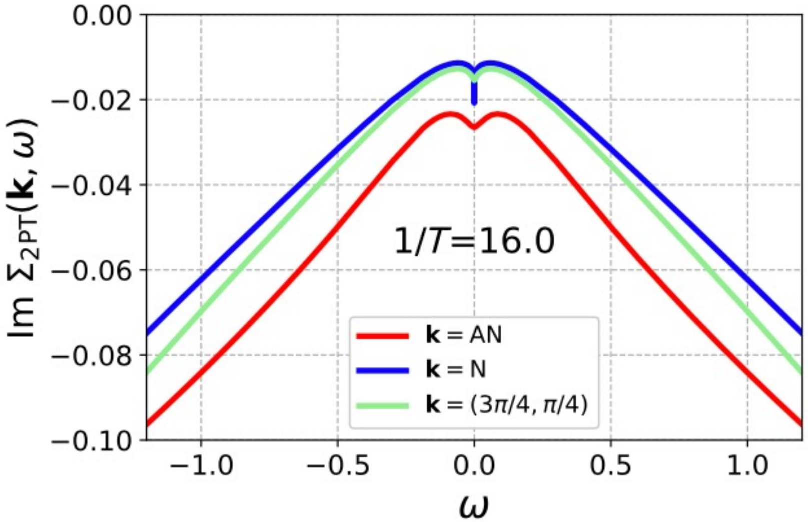
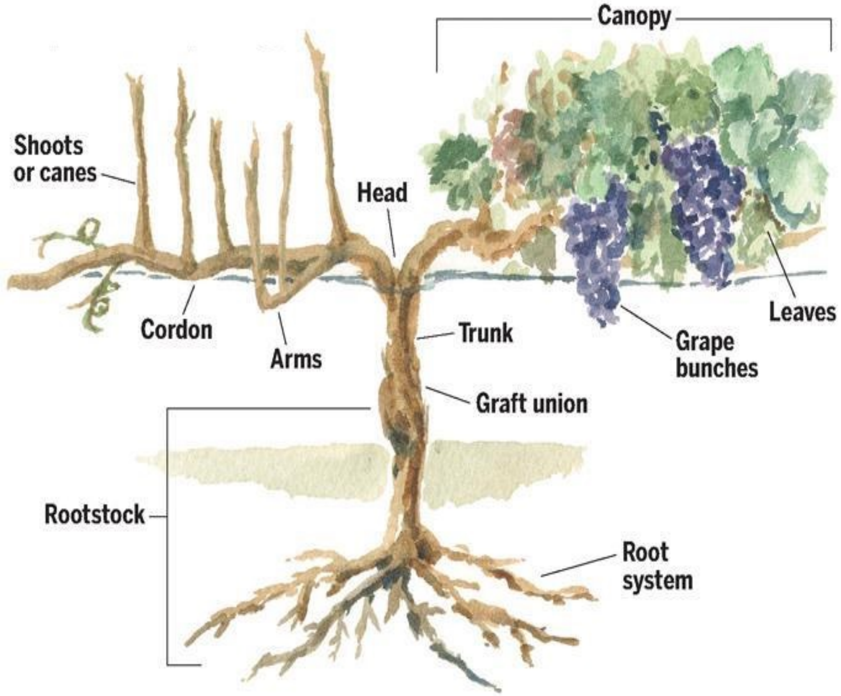


Real frequency data from **seconc**
→ wrong slope at |ω| < πT

Real frequency data highly desired!

F. Lemay, Ph.D. thesis (2000)
*T. Schäfer et al., Phys. Rev. X **11,** 011058 (2021)*

From roots to stems to harvest:
the application of multi-method, multi-messenger studies to…



…real materials

Magnetic correlations in infinite-layer nickelates: An experimental and theoretical multimethod study

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Phys. Rev. Research **4**, *023093 (2022)*

…uncharted (model) territory

Mott Insulating States with Competing Orders in the Triangular Lattice Hubbard Model

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Physical Review X **11**, *041013 (2021)*

…a simple (?) test case

Tracking the Footprints of Spin Fluctuations: A MultiMethod, MultiMessenger Study of the Two-Dimensional Hubbard Model

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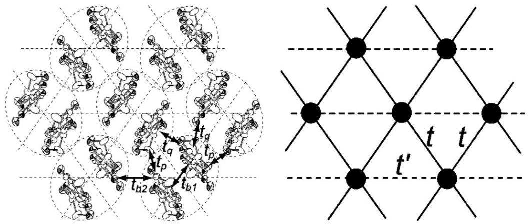
Physical Review X **11**, *011058 (2021)*

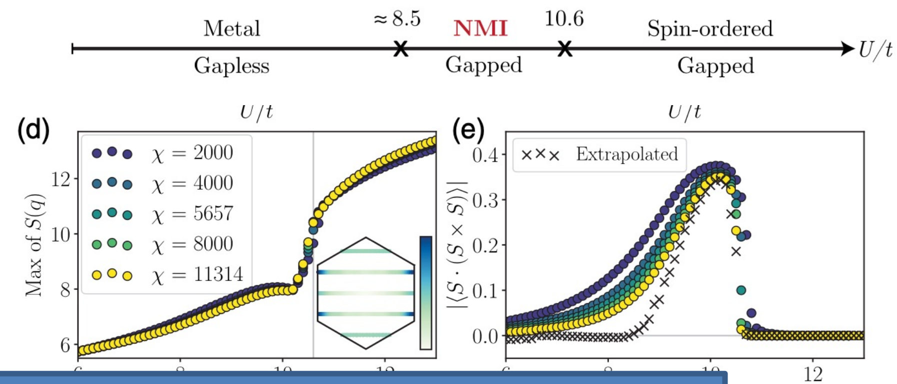
https://www.evineyardapp.com/blog/2017/05/30/overview-of-grapevine-structure-and-function/

A multimethod, multimessenger study in uncharted territory: The Hubbard model on the triangular lattice

Potential spin-liquid candidate: organic crystal κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$



Hubbard model on triangular lattice

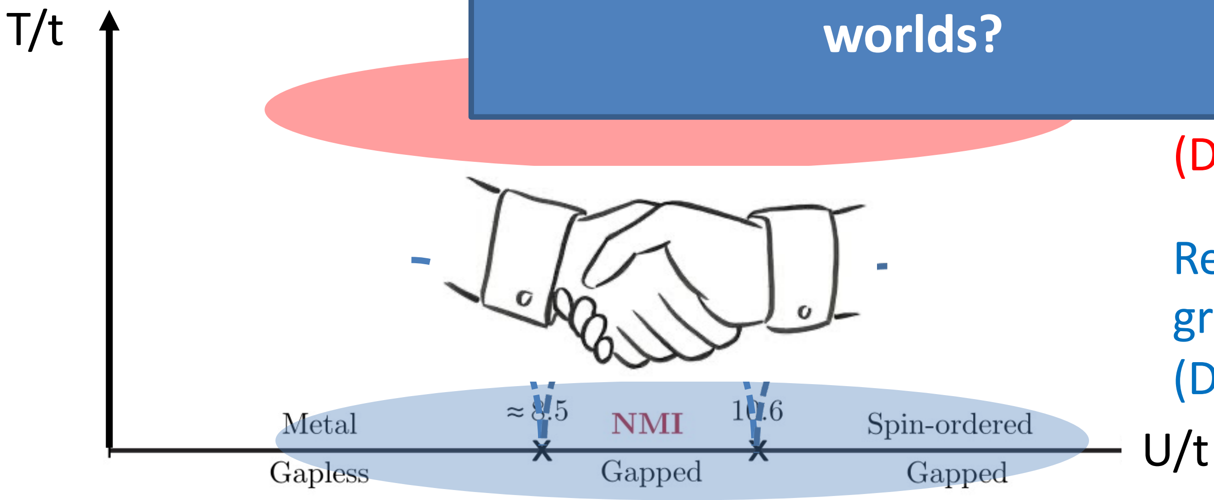


iDMRG calculations

Can we marry these two worlds?

Green function /
ng methods
(DMFT and extensions, DiagMC)

Realm of wave function / ground state methods (DMRG, METTS)



*Y. Shimizu et al., PRL **91**, 107001 (2003)*
*A. Szasz, et al., PRX **10**, 021042 (2020)*

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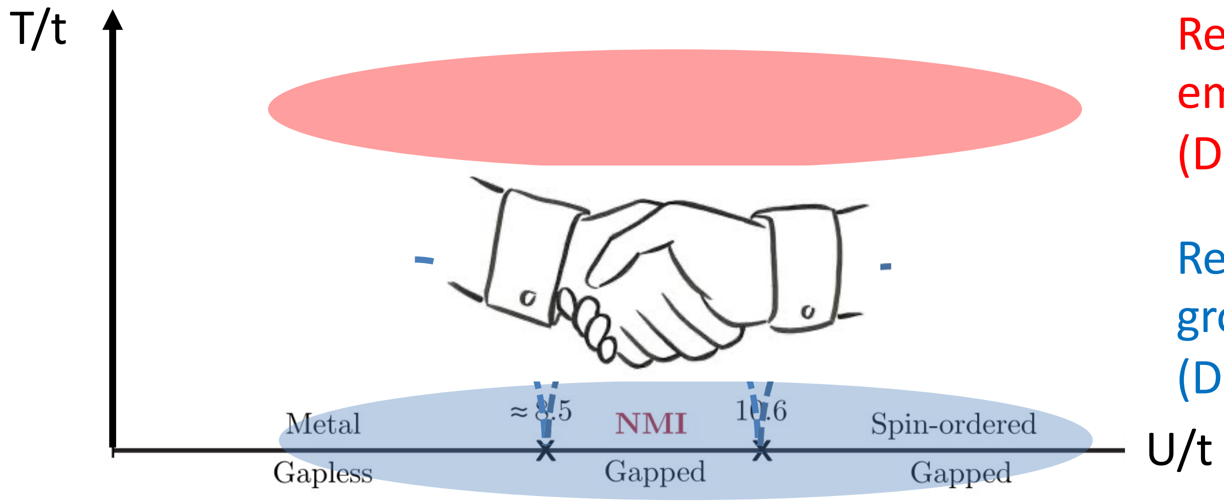
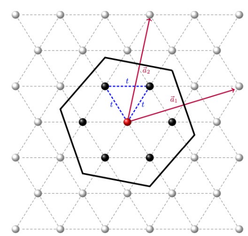


Realm of Green function / embedding methods (DMFT and extensions, DiagMC)

Realm of wave function / ground state methods (DMRG, METTS)



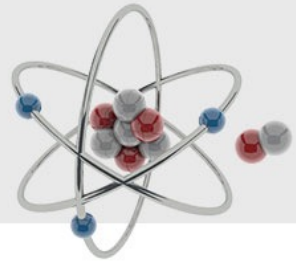
Methods used in this study:

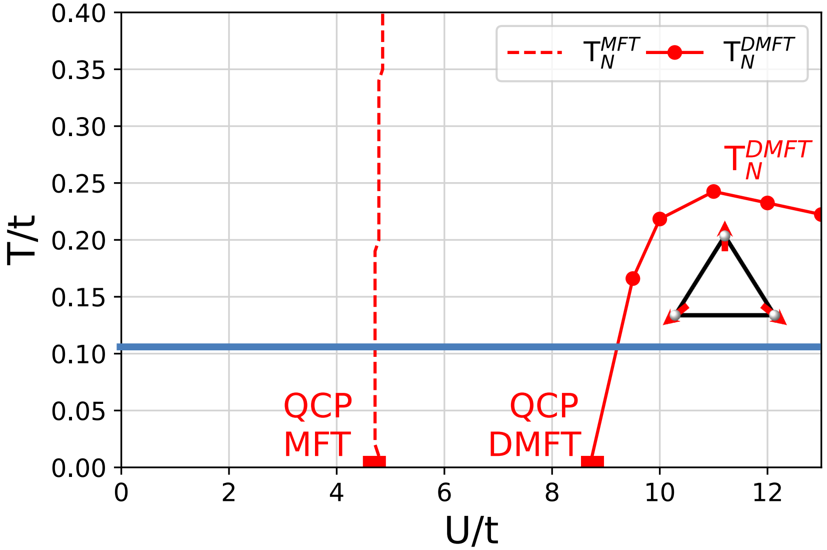
- Diagrammatic Monte Carlo (DiagMC): benchmark, however limited U/T-range
- Dynamical mean-field theory (both PM and symmetry-broken)
- Cellular dynamical mean-field theory (CDMFT, N_c=7), center-focused

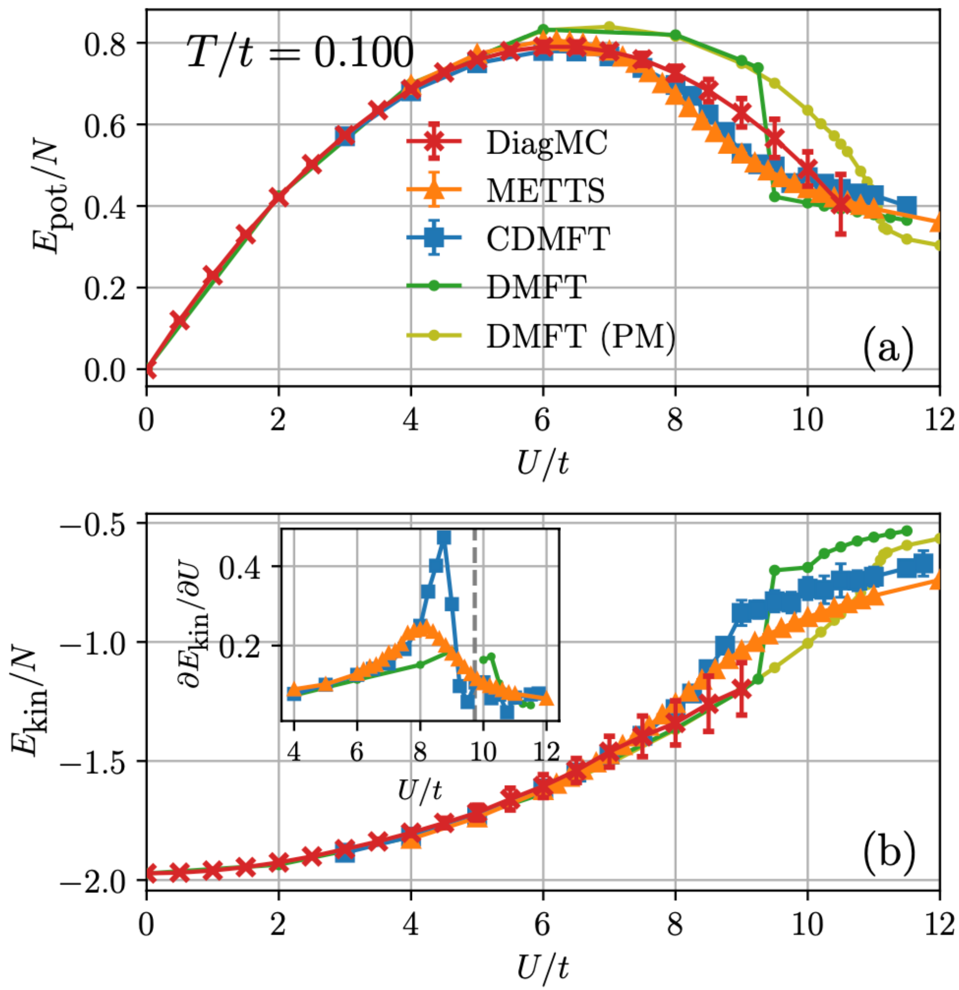
- Minimally entangled thermal typical states (METTS) on 16x4 finite-size cylinders [*S. R. White, Phys. Rev. Lett.* ***102****, 190601 (2009)*]

A. Wietek, …, TS and A. Georges, Phys. Rev. X ***11****, 041013 (2021)*

Establishing common grounds: from the mean-field phase diagram to energetics



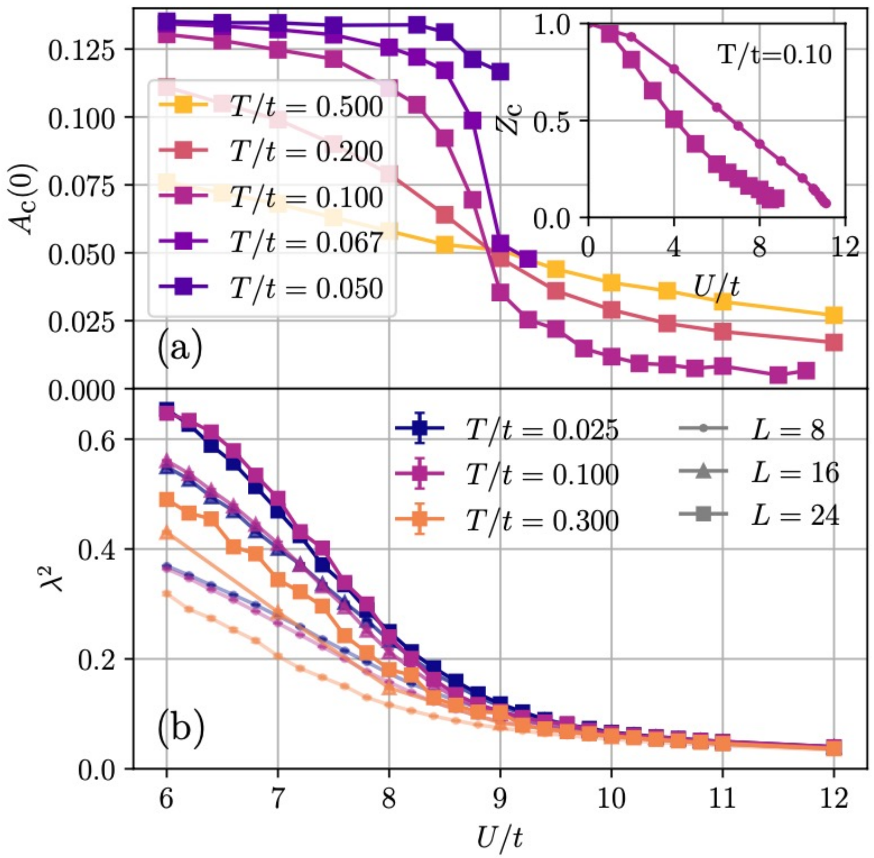




- In (D)MFT: transition from PM to 120° Heisenberg magnetism
- All methods agree at low coupling
- METTS and CDMFT show excellent agreement in E_{pot} and very good in E_{kin}

*A. Wietek, …, TS and A. Georges, Phys. Rev. X **11**, 041013 (2021)*

Metal-insulator crossover



CDMFT: spectral weight

$$A_c(\omega = 0) = -\frac{1}{\pi}\,\mathrm{Im}G_c(i\omega_n \to i0^+)$$

METTS: localization length

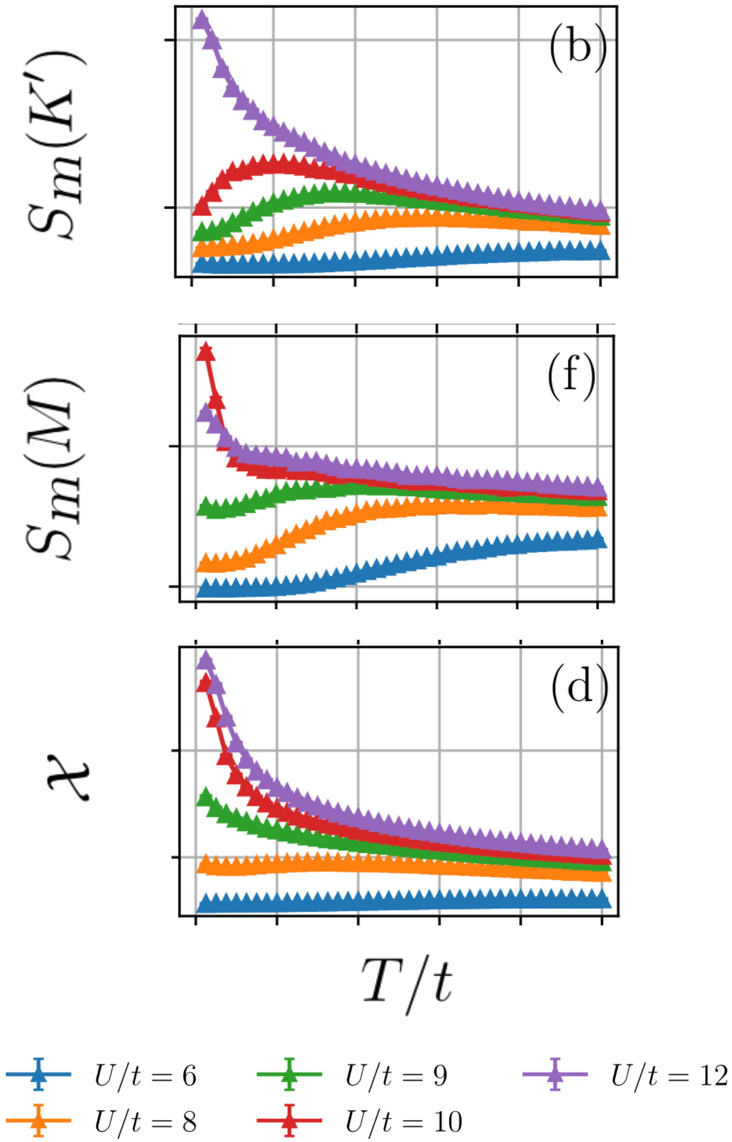
$$\lambda^2 = \frac{1}{N}\left(\langle X^2\rangle - \langle X\rangle^2\right)$$

Metal-insulator crossover at U/t≅9 from CDMFT and METTS

*ek, …, TS and A. Georges, Phys. Rev. X **11**, 041013 (2021)*

*H. T. Dang et al., Phys. Rev. B **91**, 155101 (2015)*

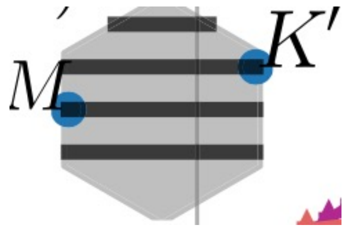
Magnetism and chirality: a METTS perspective



Magnetic structure factor

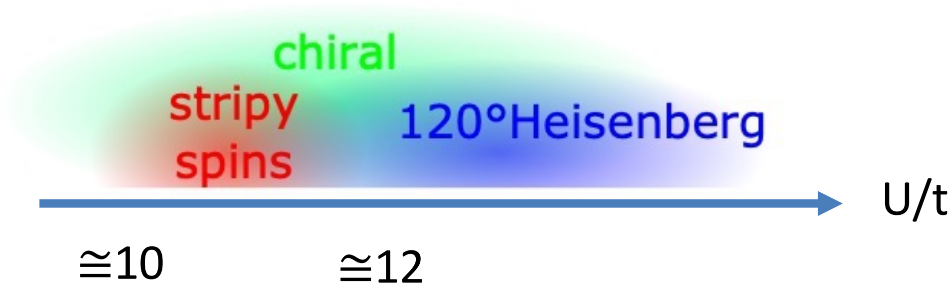
$$S_{\mathrm{m}}(\boldsymbol{k}) = \frac{1}{N} \sum_{l,m=1}^{N} \mathrm{e}^{i\boldsymbol{k}\cdot(\boldsymbol{r}_l - \boldsymbol{r}_m)} \langle \vec{S}_l \cdot \vec{S}_m \rangle$$

Chiral-chiral correlator



$$\mathcal{X} = \frac{1}{N} \sum_{\mu,\nu \in \triangle} \langle \chi_\mu \chi_\nu \rangle$$

$$\chi_\mu = \vec{S}_l \cdot (\vec{S}_m \times \vec{S}_n)$$



*A. Wietek, …, TS and A. Georges, Phys. Rev. X **11**, 041013 (2021)*

Acknowledgements























PHYSICAL REVIEW X **11,** 011058 (2021)

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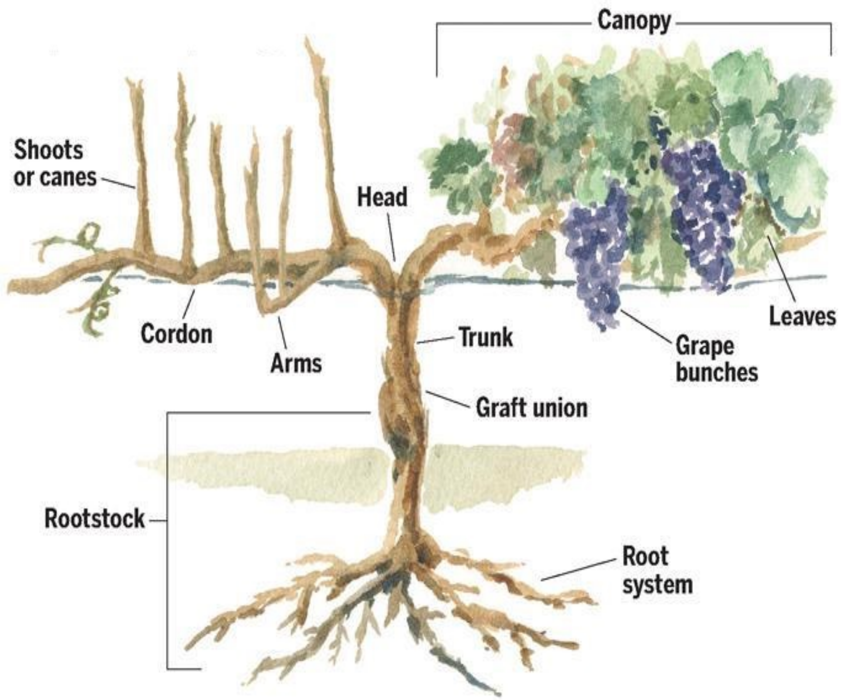

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…uncharted (model) territory

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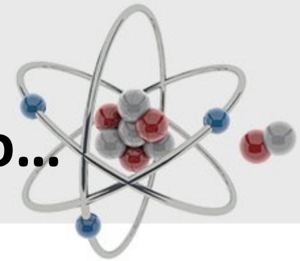

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- **Handshake** of Green function and wave-function based methods
- Agreement of CDMFT and METTS
- Intriguing **metal-insulator crossovers and magnetic ordering tendencies**

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Physical Review X **11**, 041013 (2021)

…a simple (?) test case

- Extensive **comparison of state-of-the-art quantum many-body** methods
- Metallic regime with fairly long-ranged correlations
- **Non-Fermi-liquid behavior** due to perfect nesting

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