Dynamical vertex approximation - a step beyond DMFT

Karsten Held*

IFP TU Wien

Prague, June 29, 2010

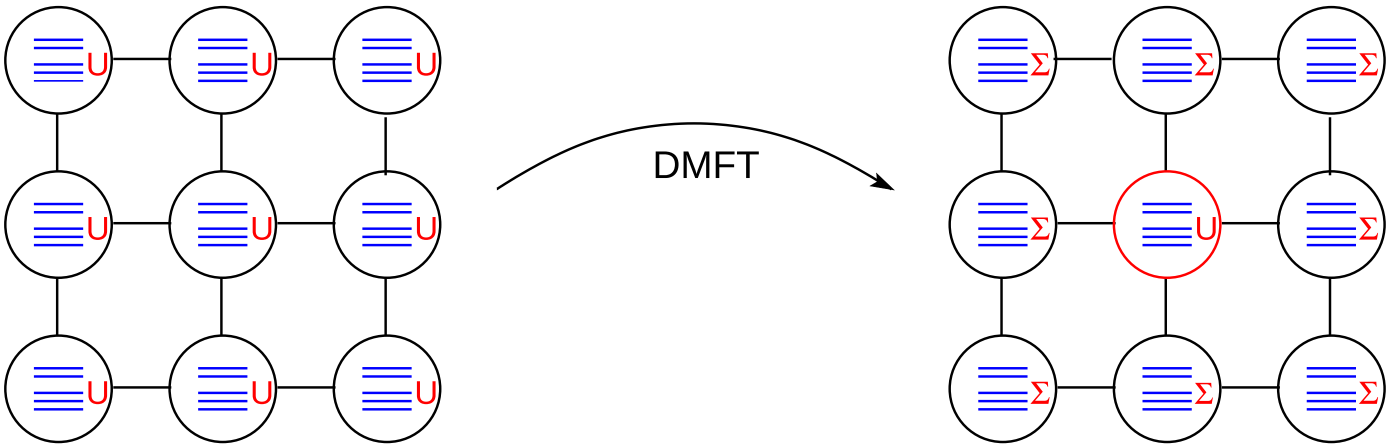
- Motivation
- Dynamical vertex approximation (DΓA)
- Effect of spin fluctuations in 3D and 2D
- Phase diagram and critical exponents
- NanoDΓA**

** with A. Toschi and A. Katanin PRB 75, 45118 (2007); PRB 80, 75104 (2009), Prog Theor Phys Suppl 176, 117 (2008)*

*** with A. Valli, G. Sangiovanni Phys. Rev. Lett. 104, 246402 (2010)*

Motivation

Dynamical mean field theory



Σ all topologically distinct, but local diagrams

Success story: quasiparticle renormalizations, magnetism, kinks ...

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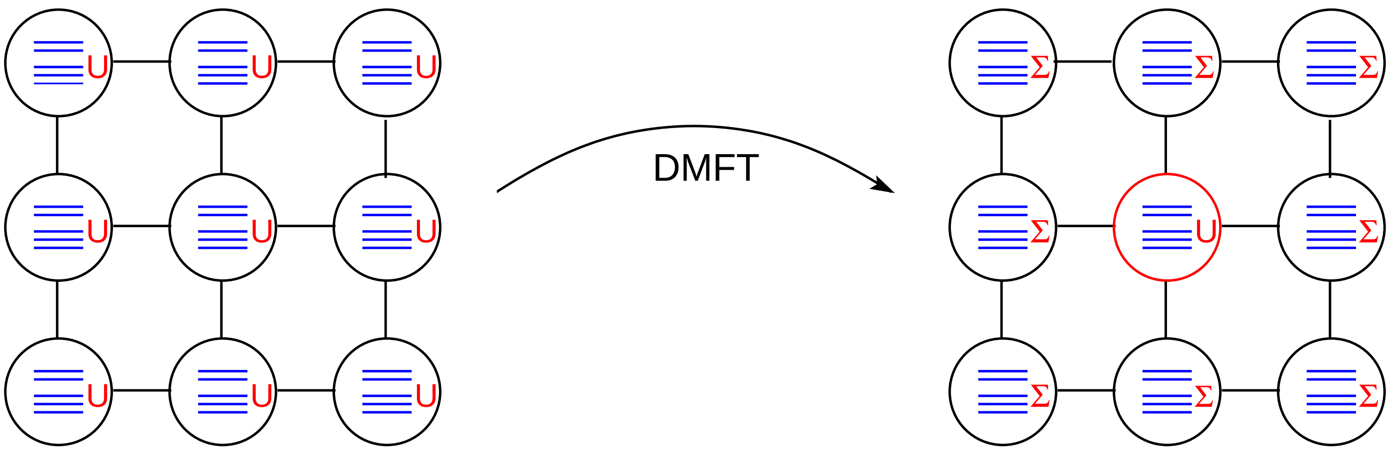

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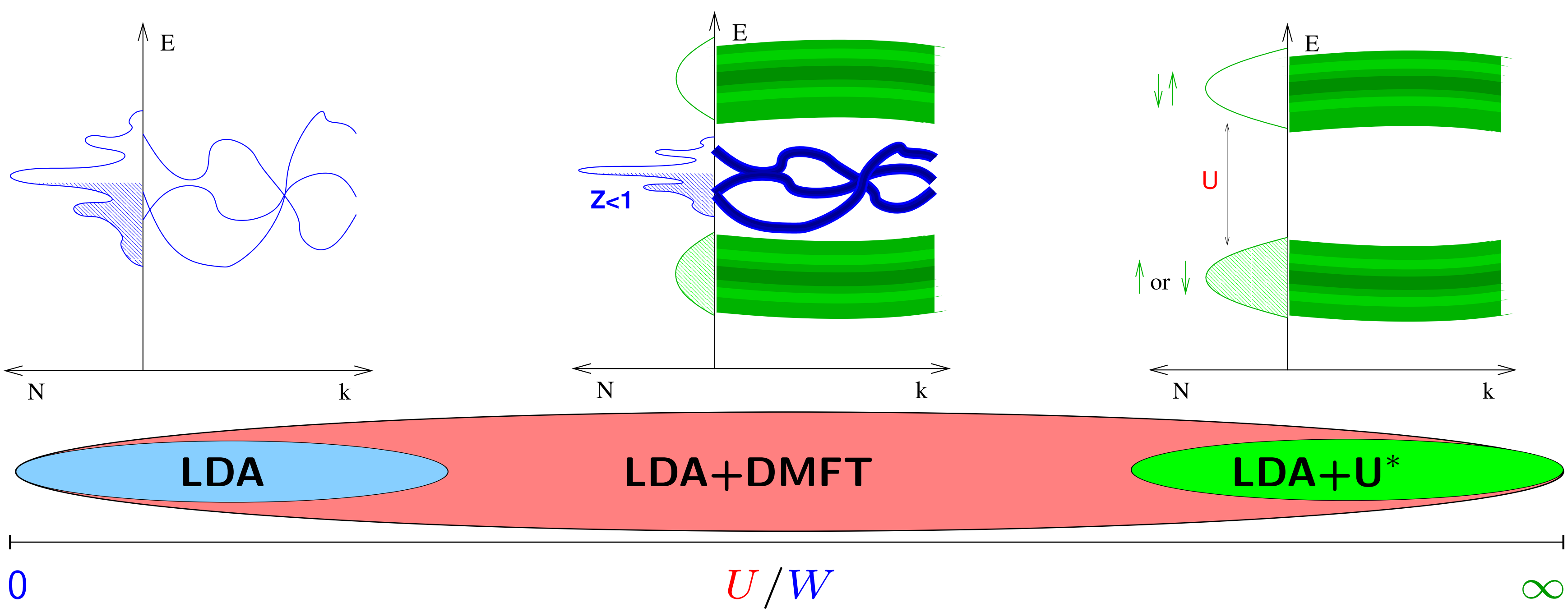

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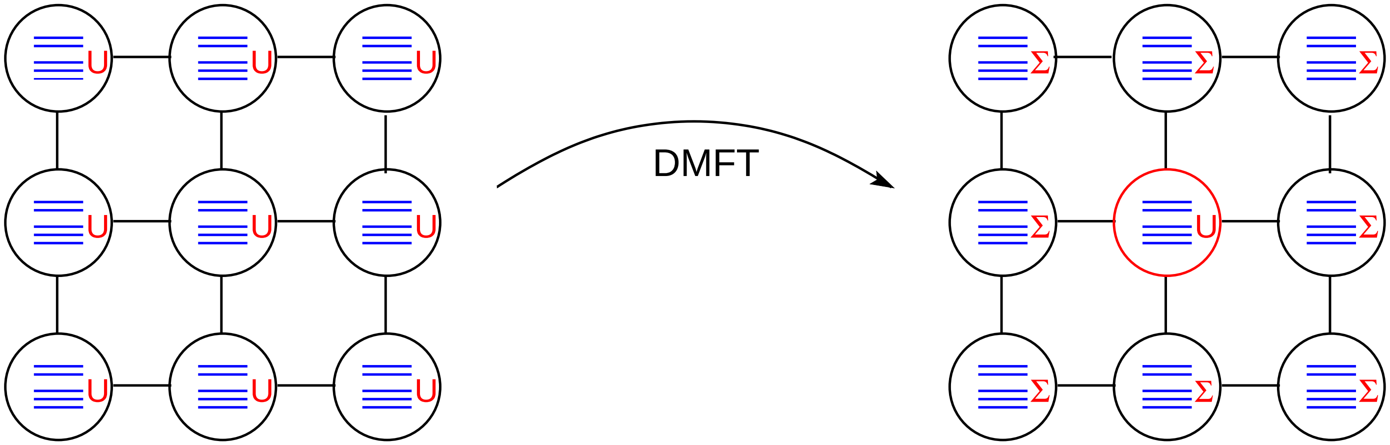


Σ all topologically distinct, but local diagrams

Success story: quasiparticle renormalizations, magnetism, kinks ...

Not included:

non-local correlations

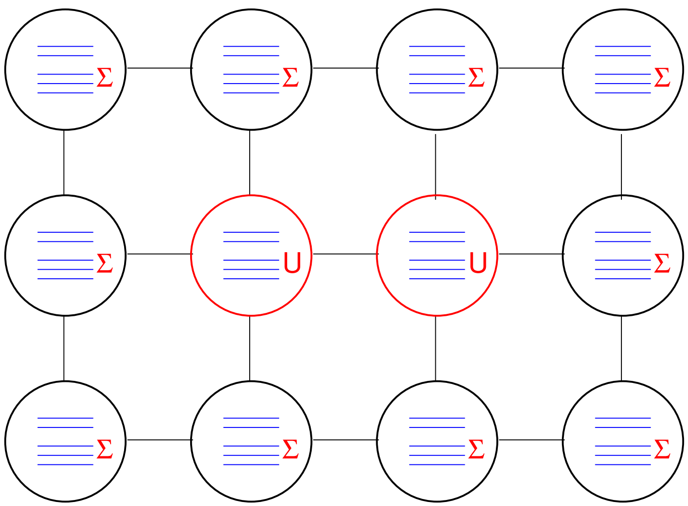
p-, d-wave superconductivity, pseudogaps, spin Peierls

magnons, (quantum) critical behavior ...

k-dependent Σ

beyond DMFT

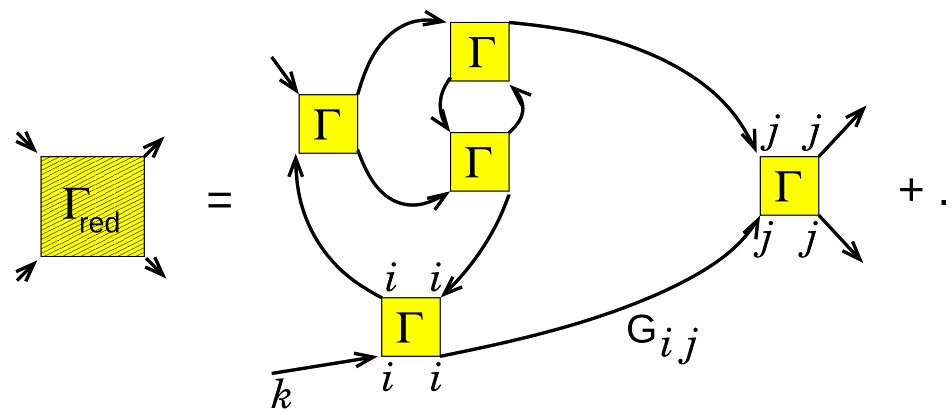
cluster extensions of DMFT



- non-local short-range correlations
- d/p-wave superconductivity

Hettler *et al.*'98, Lichtenstein Katsnelson'00,
Kotliar *et al.*'01, Potthoff'03

diagrammatic extensions of DMFT



dynamical vertex approximation

- short and long-range correlations
- (para-)magnons, criticality ...

Kusunose cond-mat/0602451
Toschi, Katanin, KH cond-mat/0603100
Slezak *et al.* cond-mat/0603421

cf. dual Fermions: Rubtsov *et al.*'08
cf. DMFT+spin-Fermion Kuchinskii *et al.*'05

Dynamical vertex approximation (DΓA)

DMFT: all (topological distinct) local diagram for Σ

Generalization: all local diagrams for $\mathbf{n}$-particle fully irreducible vertex Γ

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construct Σ (local and non-local diagrams)

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$n = \infty \rightarrow$ exact solution

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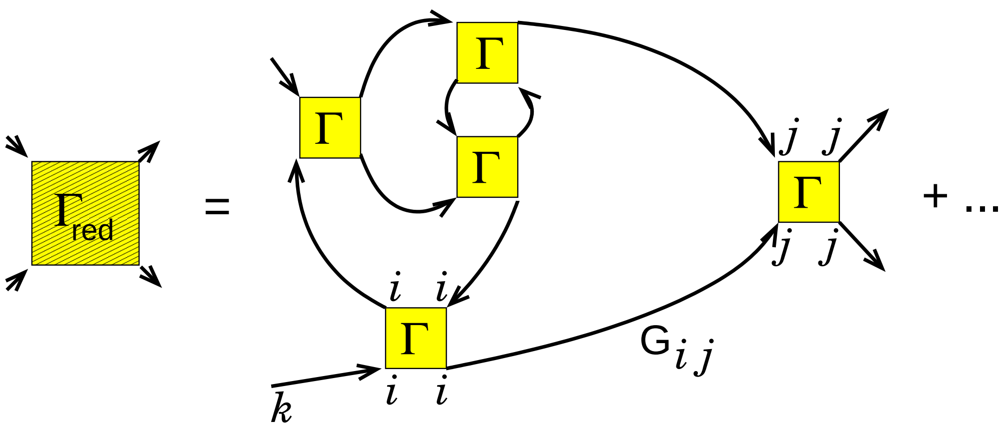

local Γ, non-local G

$\longrightarrow$

non-local reducible vertex Γ_{red}

via parquet equations

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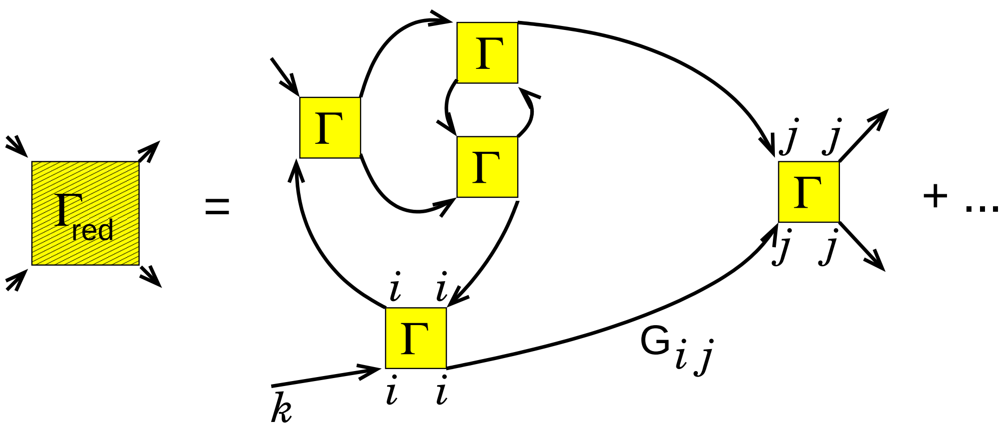

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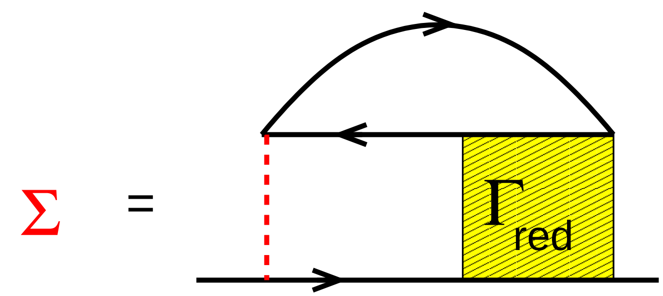

$\Gamma_{\rm red}$

$\longrightarrow$

non-local Σ

exact relation (eq. of motion)

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$\dots$

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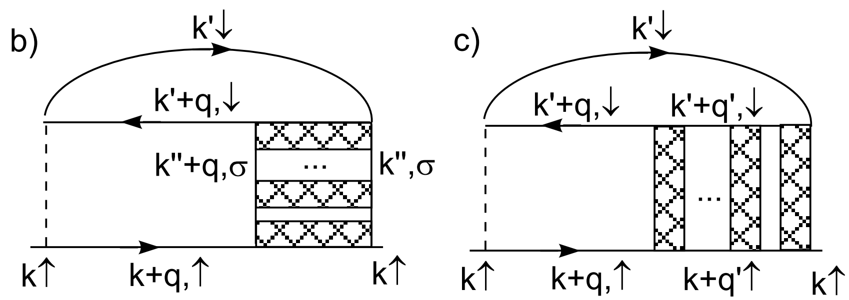
First step: restriction to ladder diagrams

Σ =



lines: non-local G

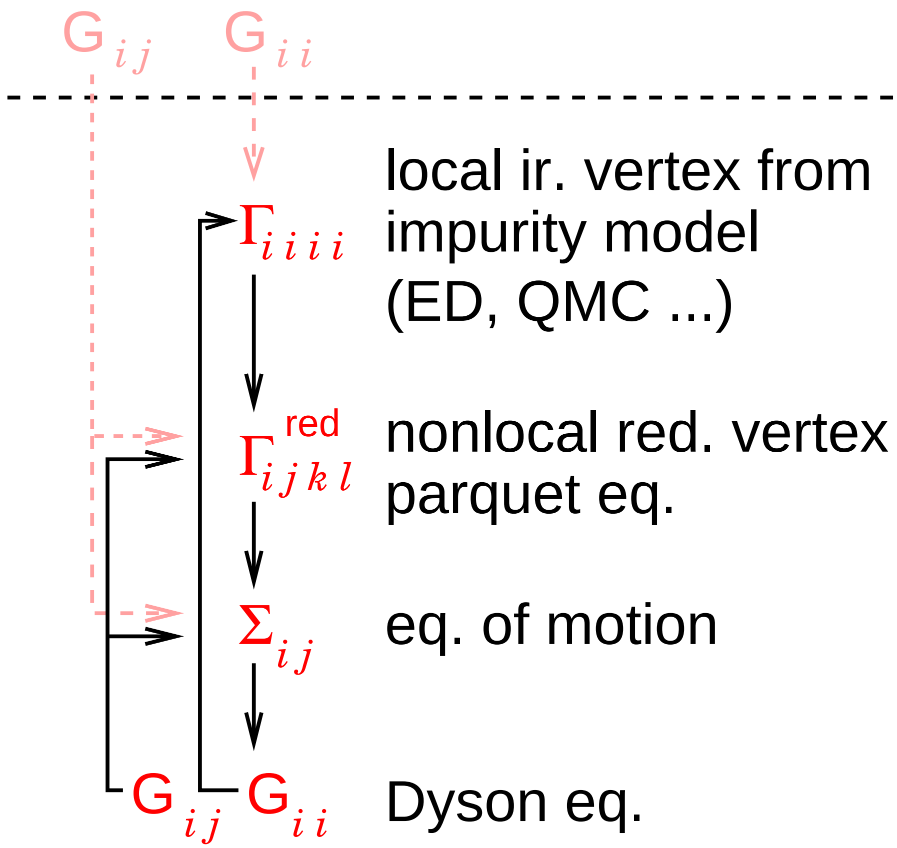
crosshatched: local irreducible vertex in spin/charge channels

$\Gamma_{\rm S,C}(\nu,\nu',\omega) = \chi_{0,\rm loc}^{-1} - \chi_{\rm S,C}^{-1}$

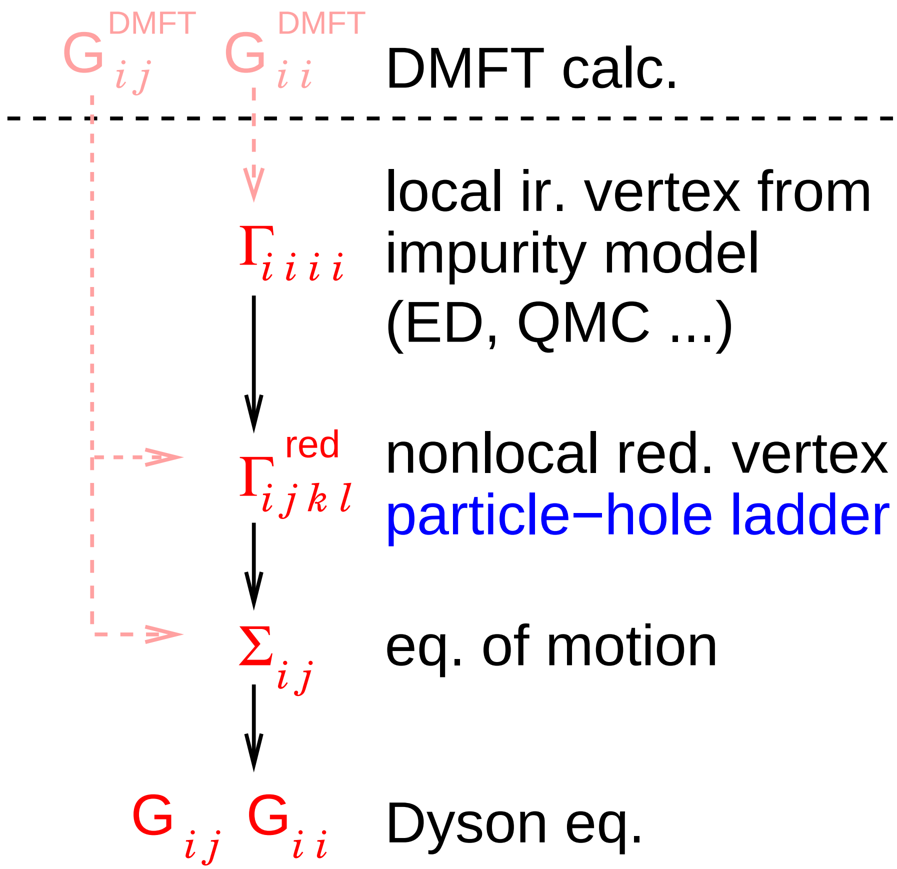
magnons, spin-fluctuations at (A)FM phase transition

G_{ij} from DMFT

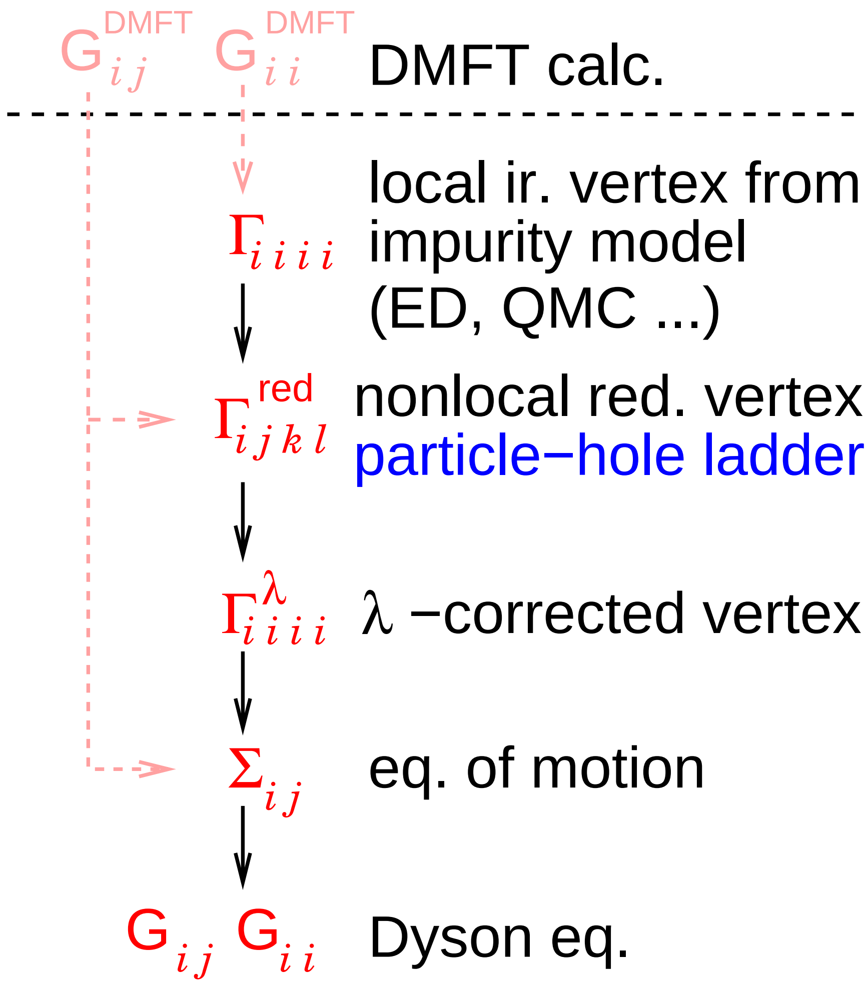
DΓA algorithm (full version)



DΓA algorithm (restriction to ph ladders)



DΓA algorithm (Moriyaesque λ correction)



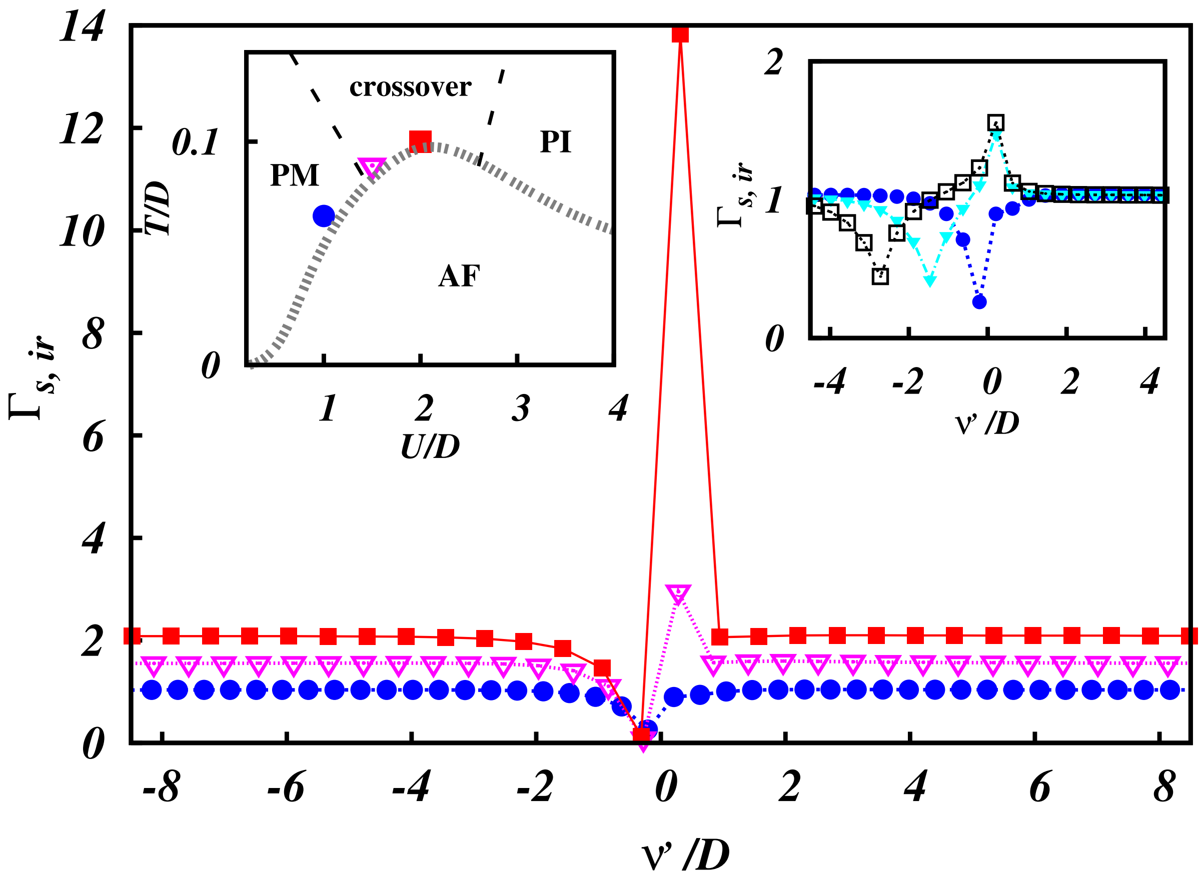
$$\chi^s_{\mathbf{q}\omega} \longrightarrow \left[(\chi^s_{\mathbf{q}\omega})^{-1} + \lambda\right]^{-1}.$$

λ adjusted by sum rule: $$-\int_{-\infty}^{\infty} \frac{d\nu}{\pi} \mathrm{Im}\Sigma_{\mathbf{k},\nu} = U^2 n(1-n/2)/2$$

Results: 3D Hubbard model without λ correction

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

cubic lattice, exact diagonalization as impurity solver



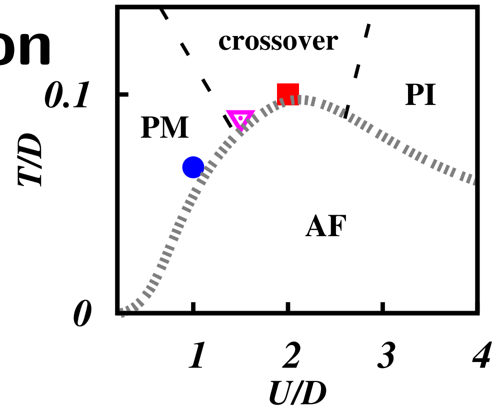
eff. bandwidth ≡ 2D

$\omega = 0$

$\nu = \pi T$

$\Gamma_{\mathrm{s,ir}}(\nu, \nu', \omega)$ strongly frequency dependent

Results: 3D Hubbard model w/o λ correction



Σ and A for $\mathbf{k} = (\pi/2, \pi/2, \pi/2)$ (on Fermi surface)

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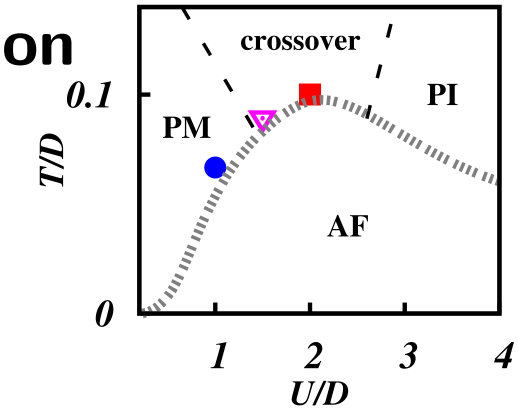

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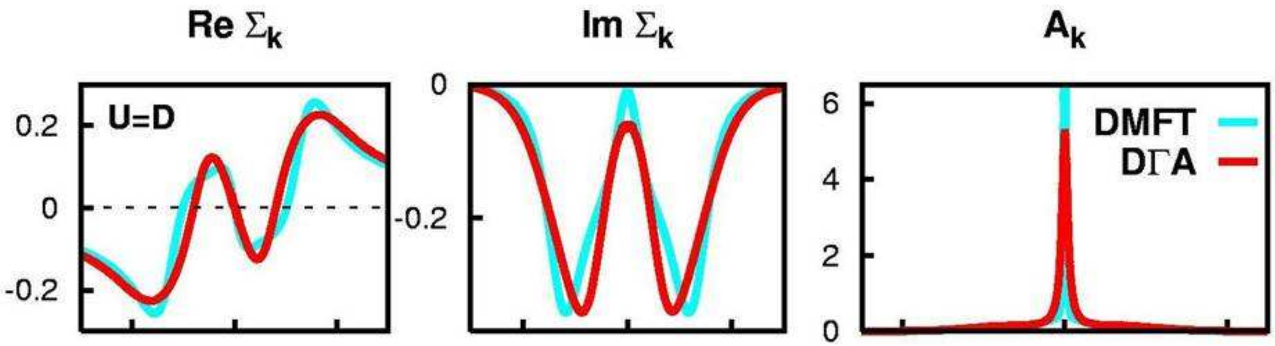

←

weak damping of QP peak

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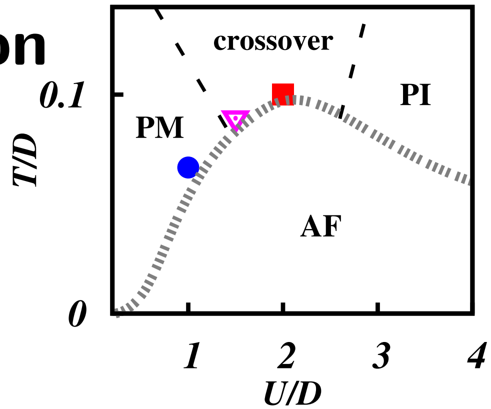

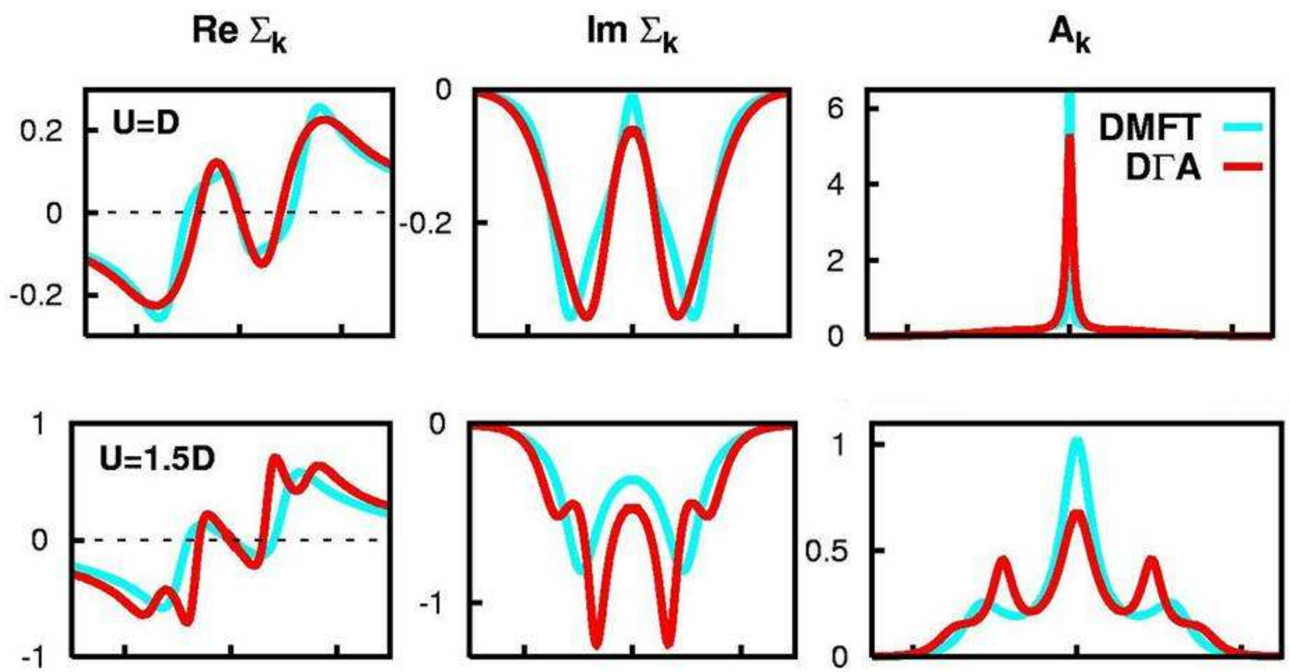

weak damping of QP peak

QP-damping strongly enhanced

Results: 3D Hubbard model w/o λ correction

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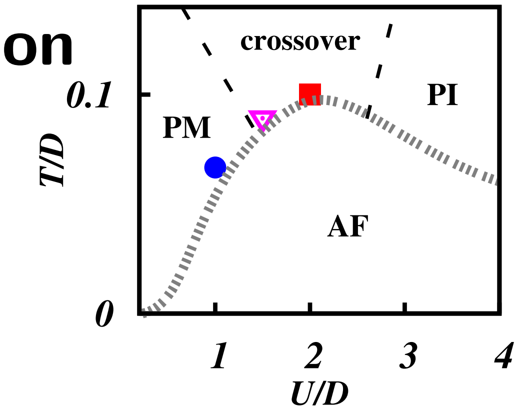
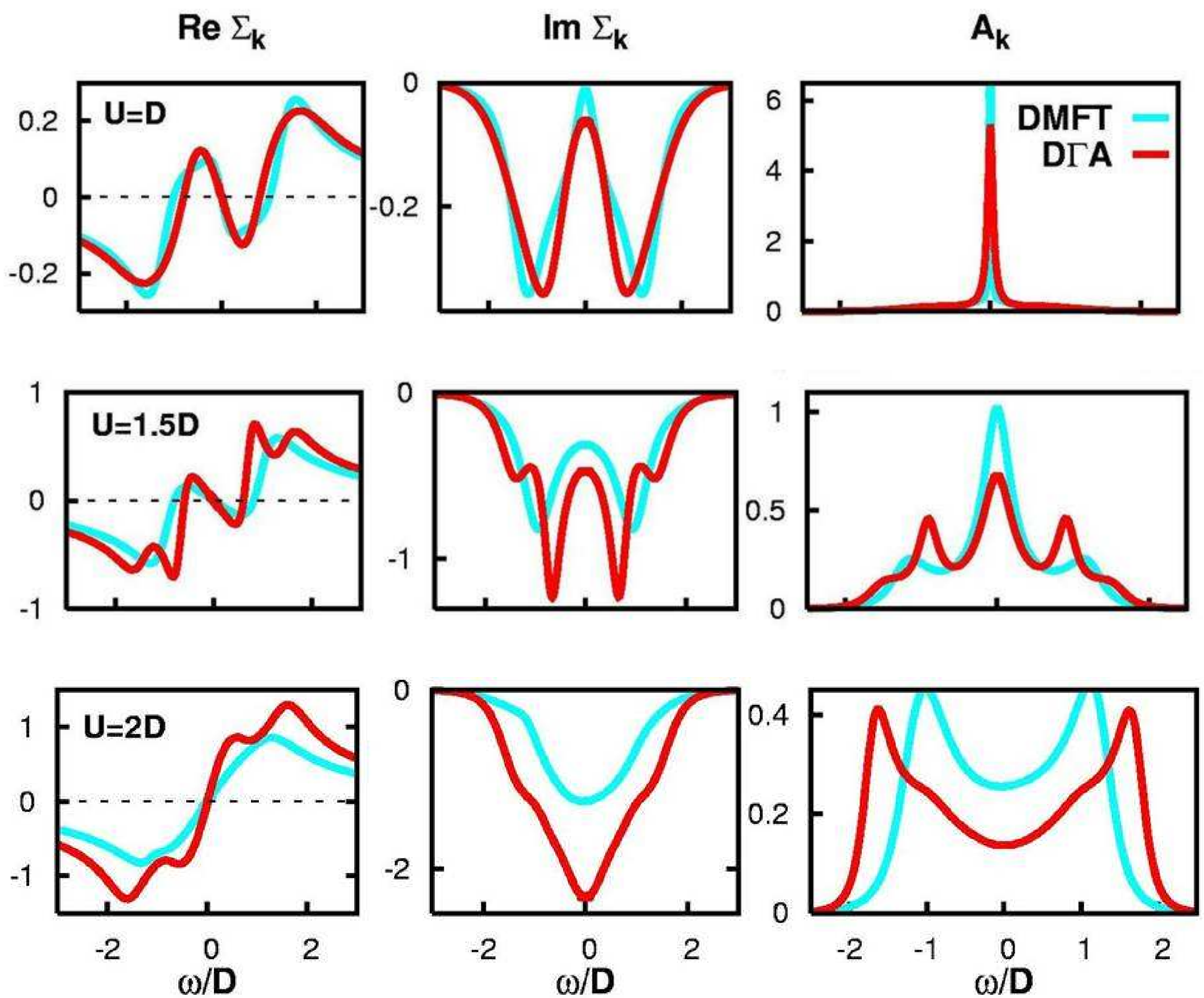




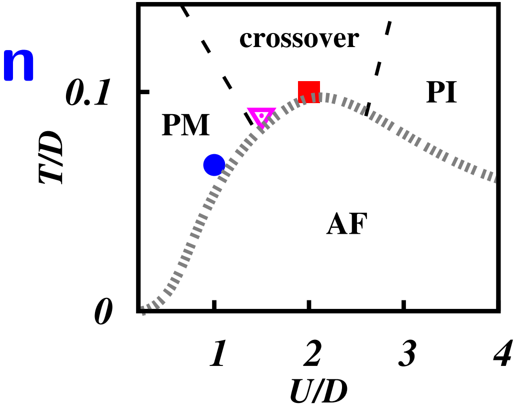
weak damping of QP peak

QP-damping strongly enhanced

more insulating

Results: 3D Hubbard model with λ correction

Σ and A for $\mathbf{k} = (\pi/2, \pi/2, \pi/2)$ (on Fermi surface)



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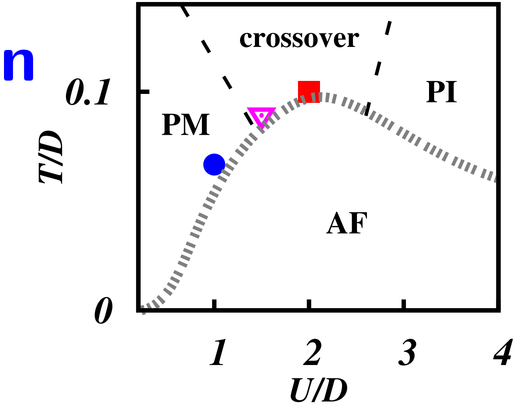
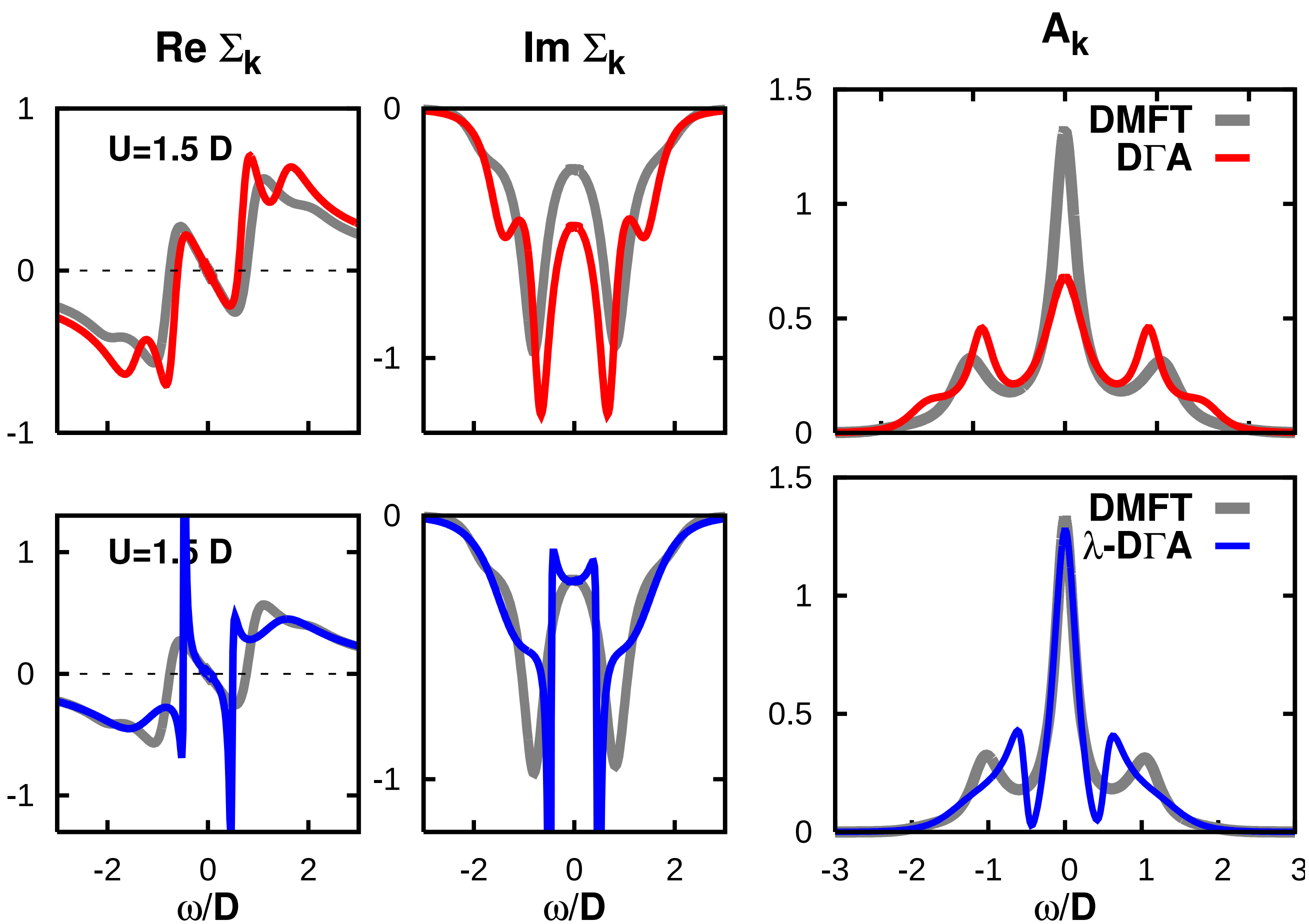
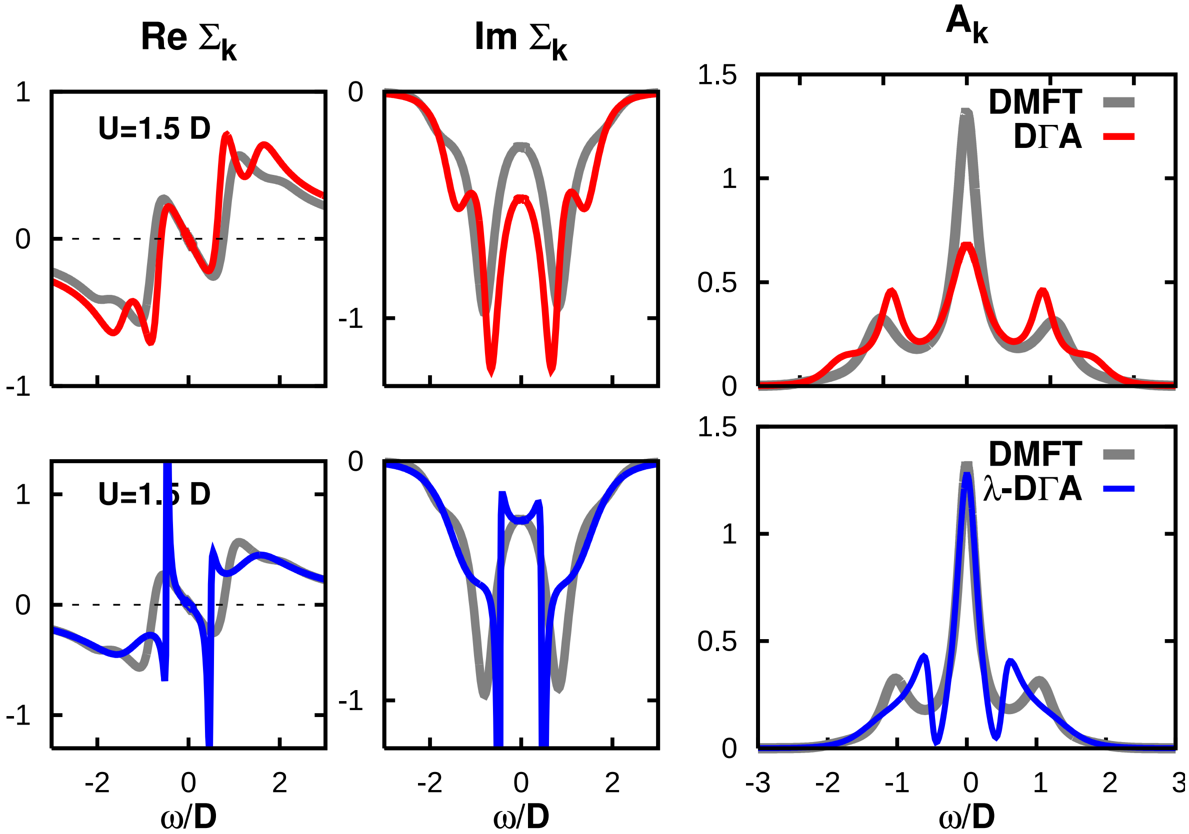


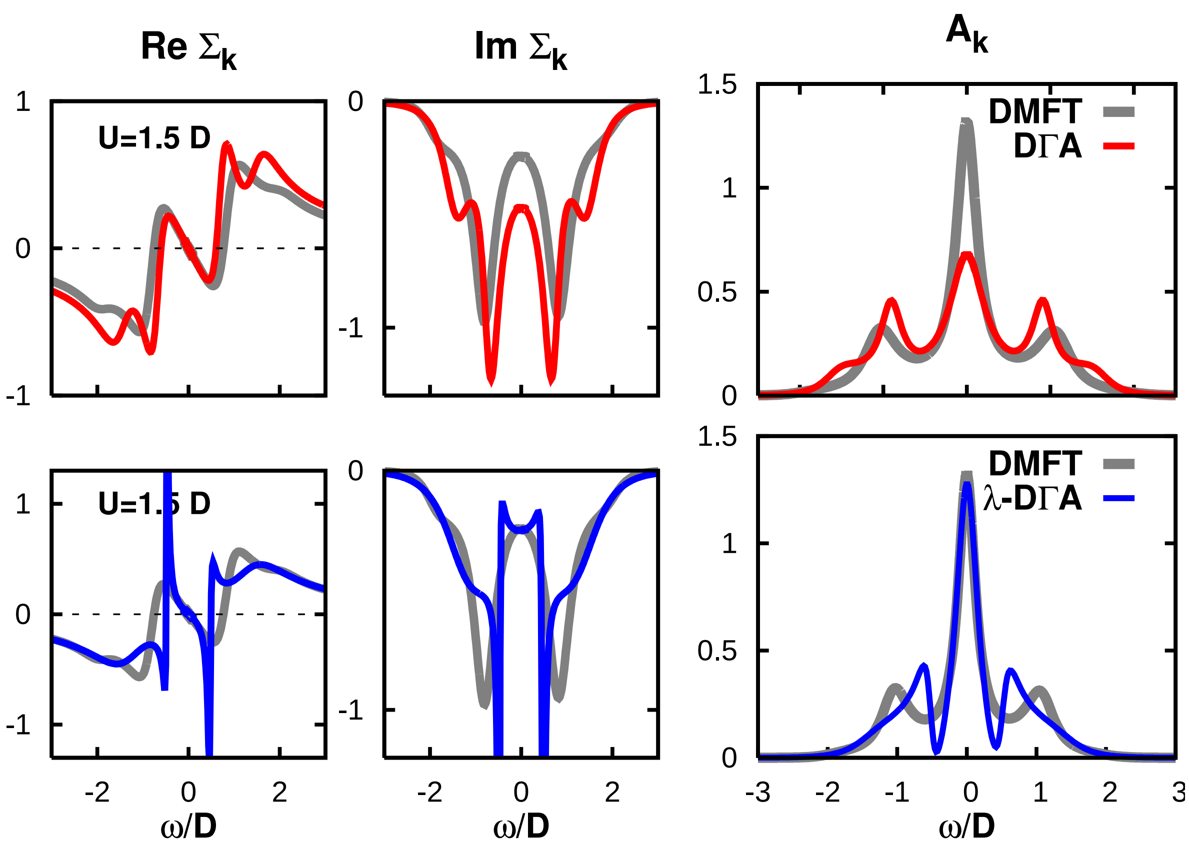
Comparison with/without λ correction



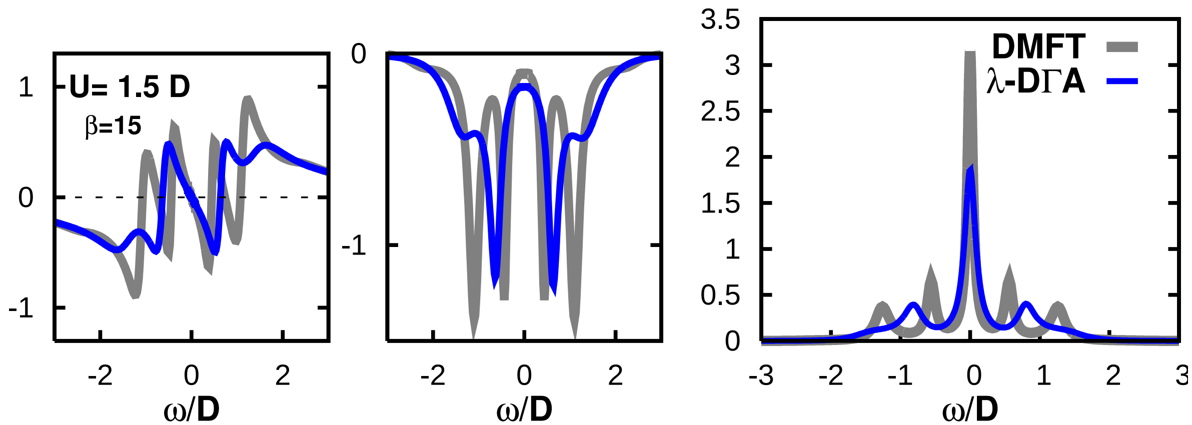
now far away from T_N! $(T = 0.09)$



Re Σ_k
Im Σ_k
A_k
U=1.5 D
U=1.5 D
DMFT
DΓA
DMFT
λ-DΓA
ω/D
ω/D
ω/D

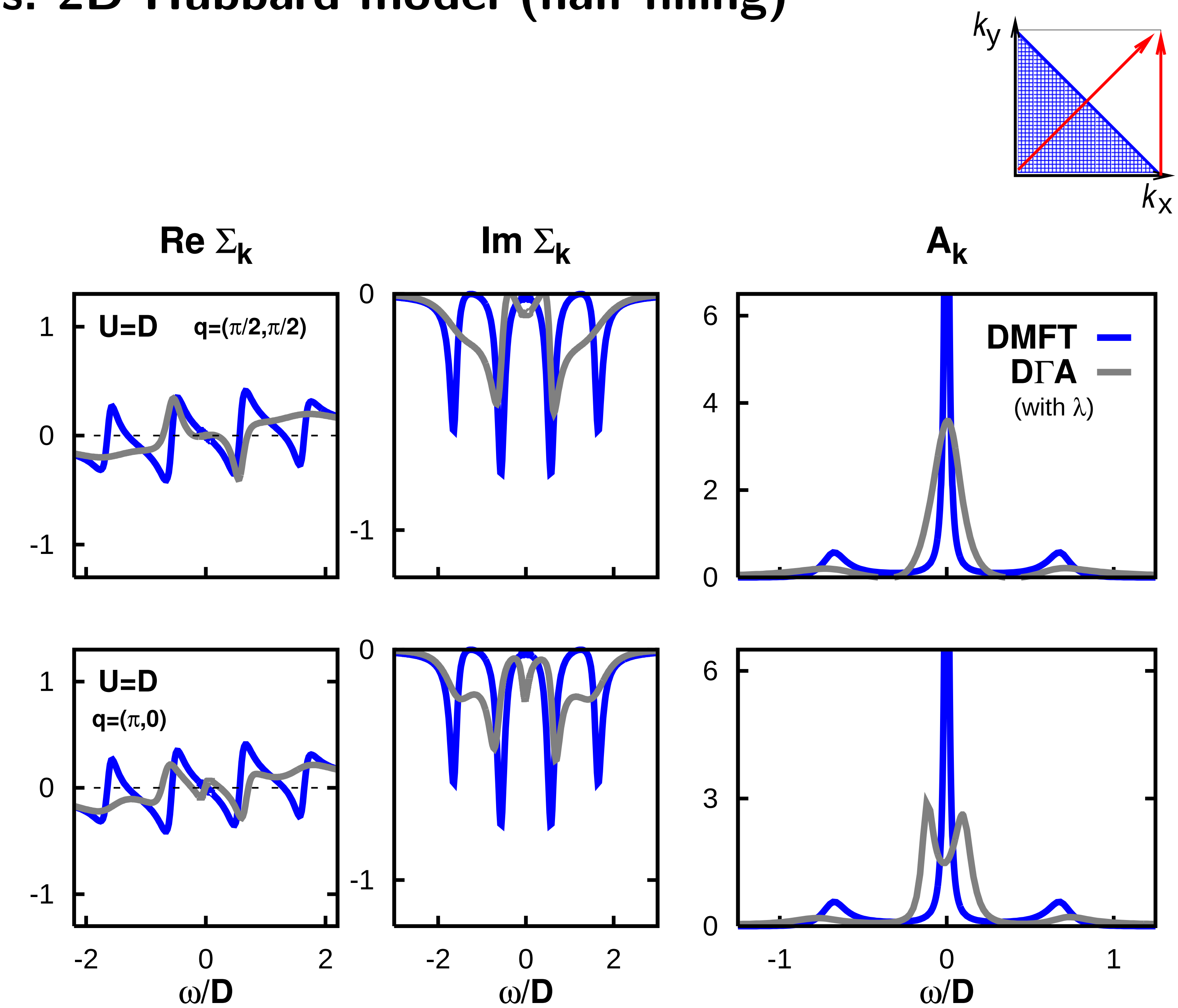


Reducing T towards T_N **λ corrected T ($T = 0.067$)**



similar results as without λ correction but at a lower T

Results: 2D Hubbard model (half-filling)



nodal
$\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$

anti-nodal
$\mathbf{k} = (\pi, 0)$

anisotropic pseudogap

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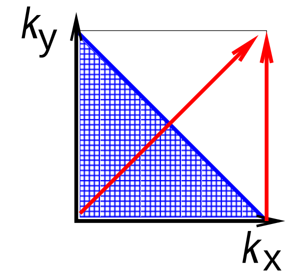
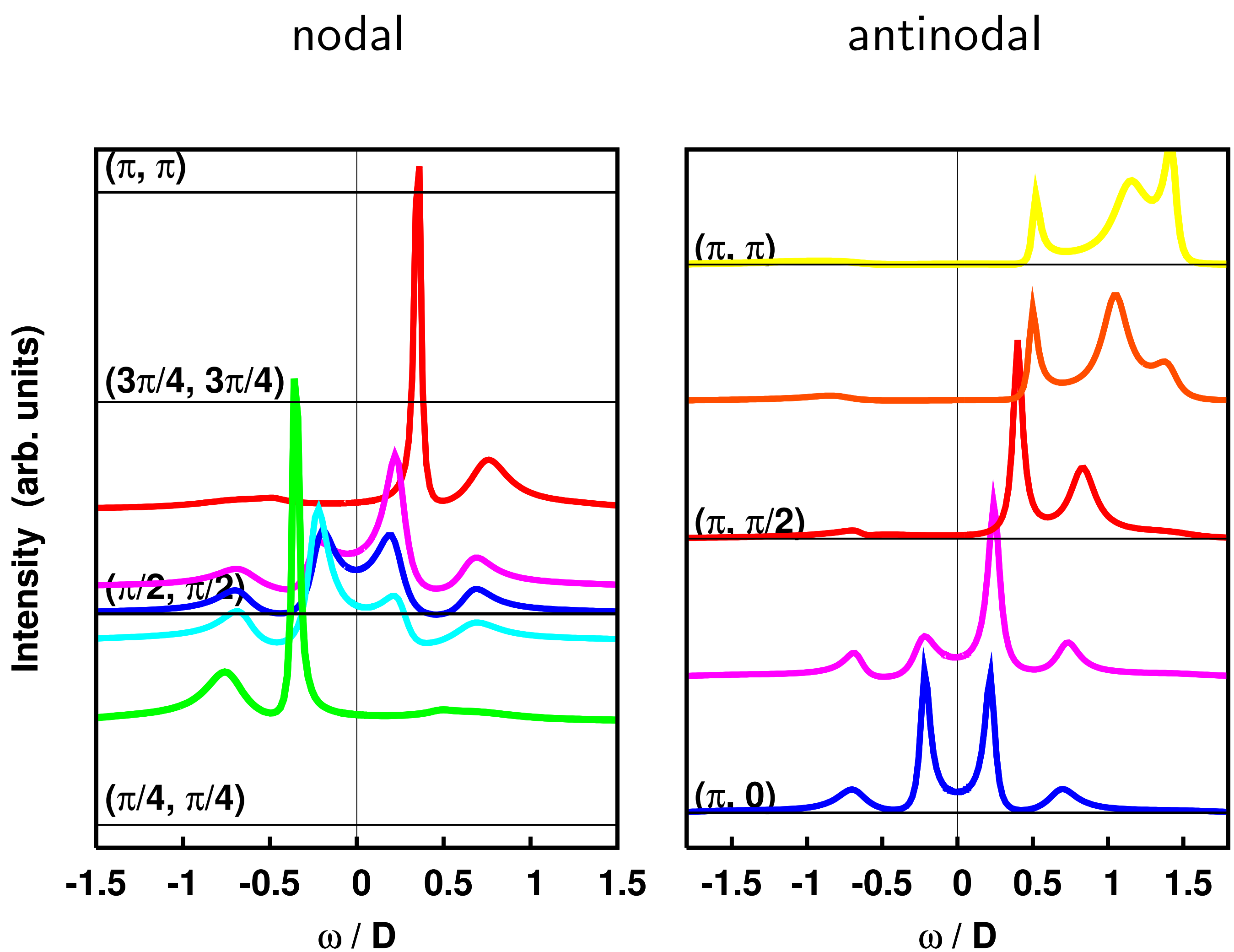
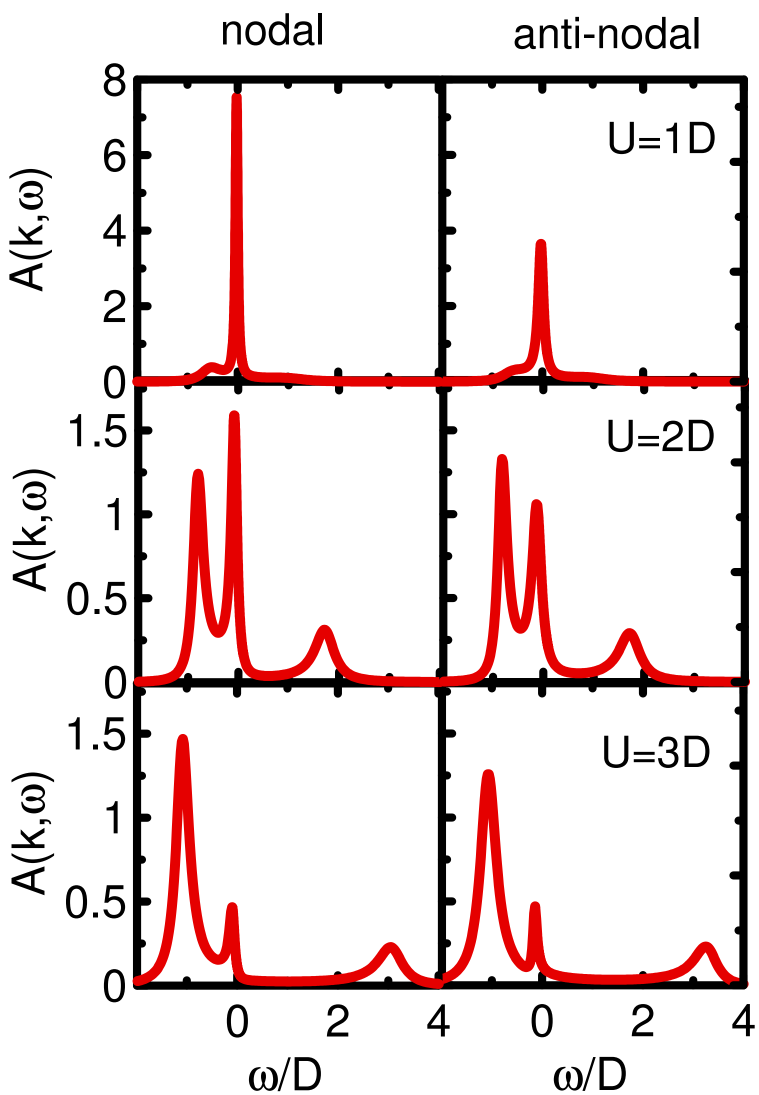




$U = D, \beta = 16$

Results: 2D Hubbard model (off half-filling)



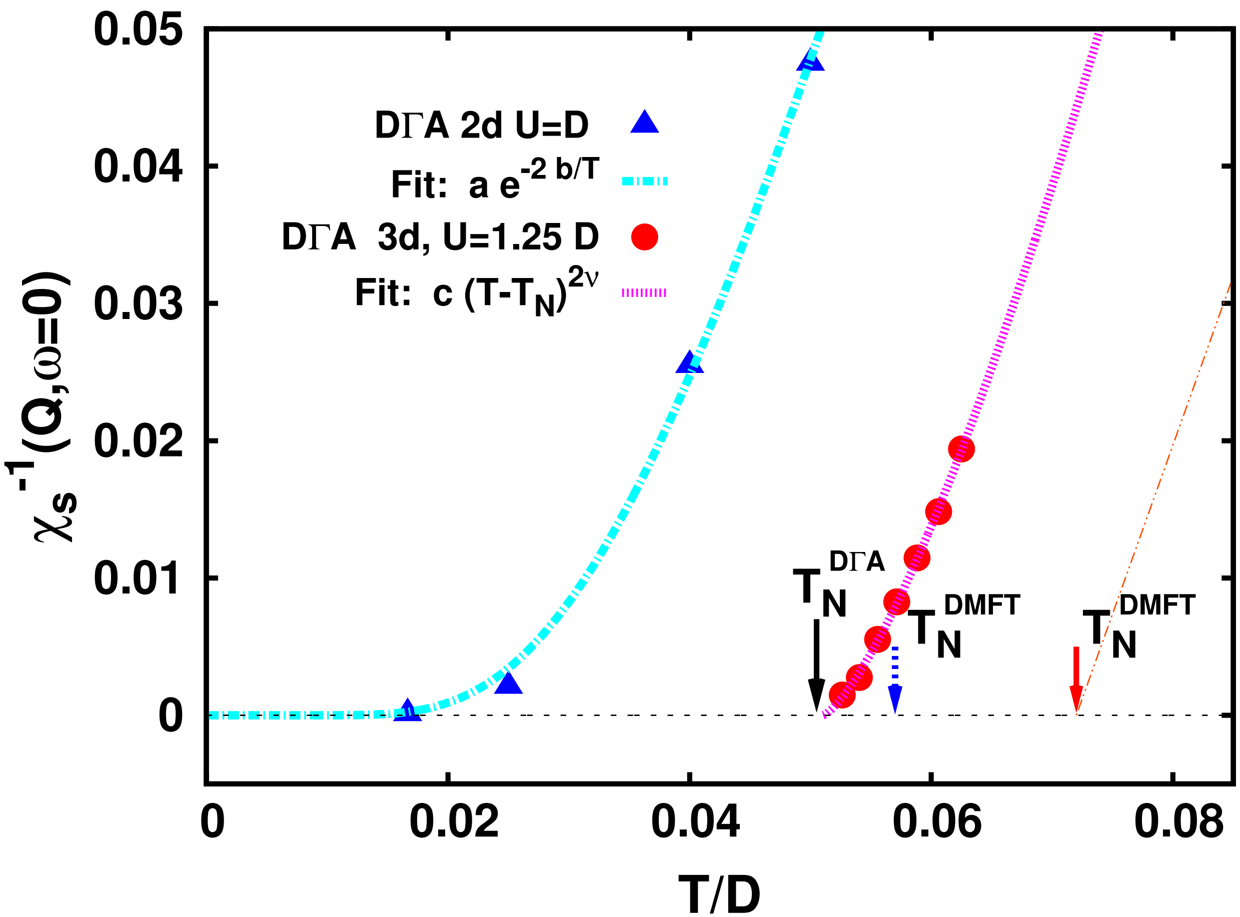
$t'/t = 0.3$
$n = 0.8$
$\beta = 100/D$

less anisotropic
at strong coupling

Critical exponents

Toschi, Katanin, KH '09

Antiferromagnetic phase transition in half-filled Hubbard model



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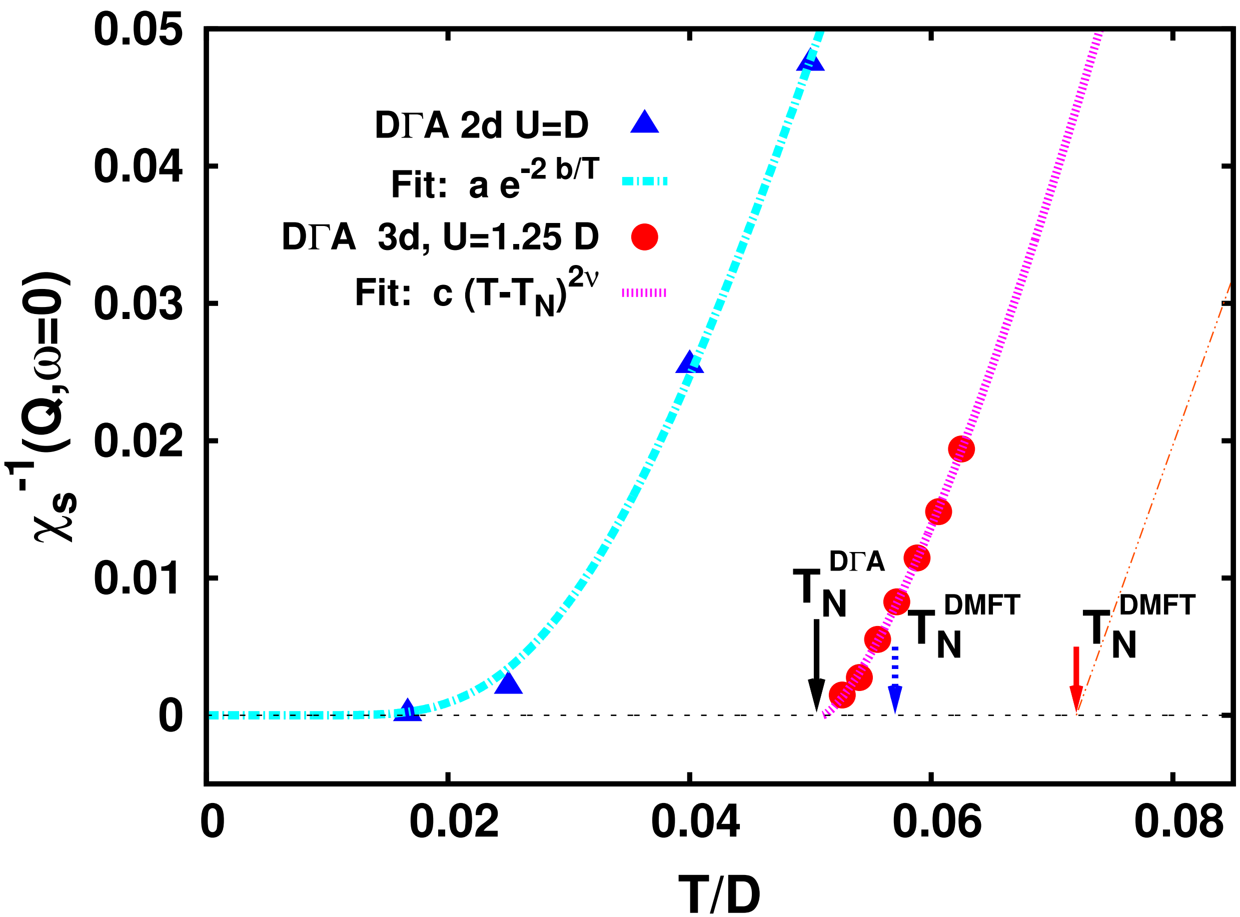

2D: Mermin-Wagner theorem fulfilled!

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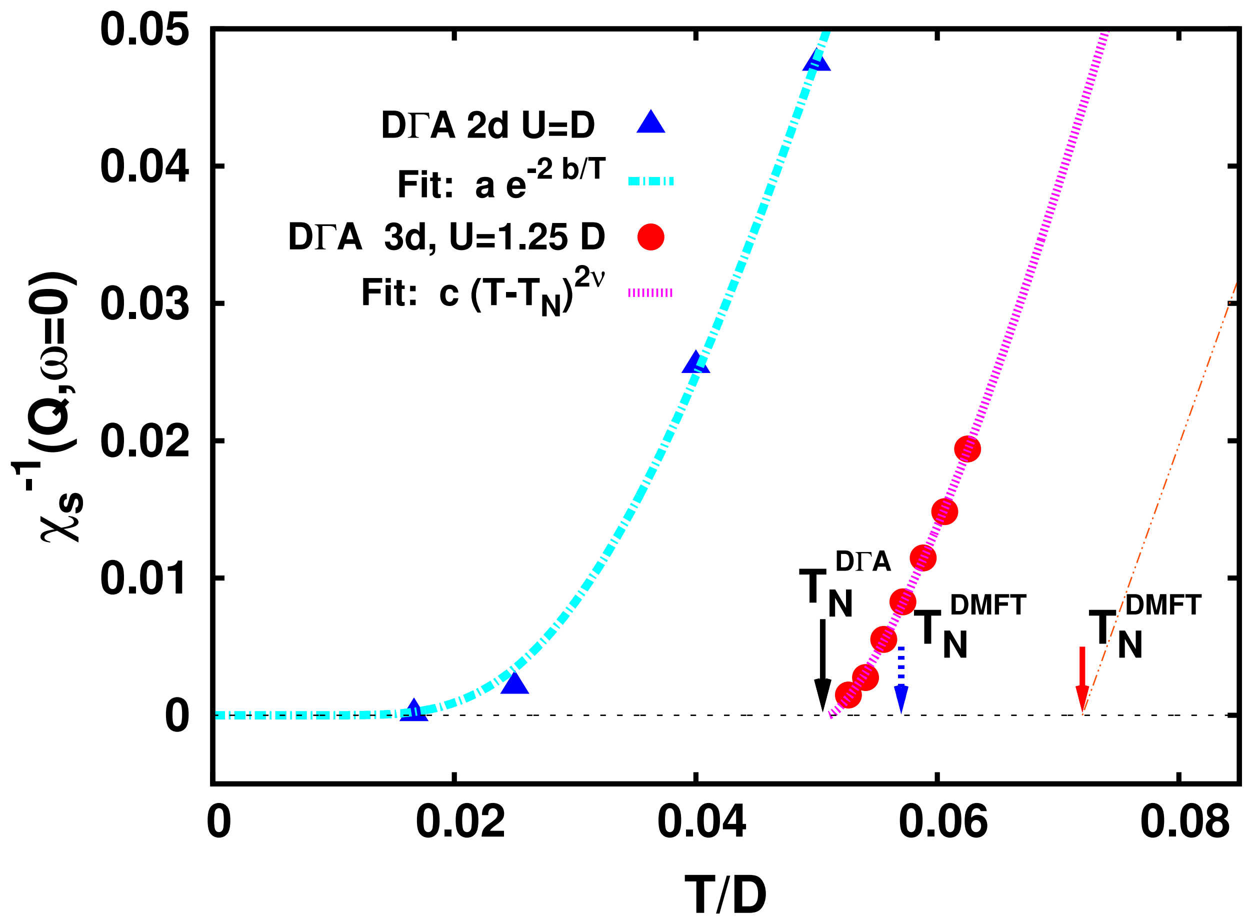

2D: Mermin-Wagner theorem fulfilled!

3D: critical exponent $\nu = 0.67 \pm 0.05$ agrees with Heisenberg model $\nu = 0.707...$

Critical exponents

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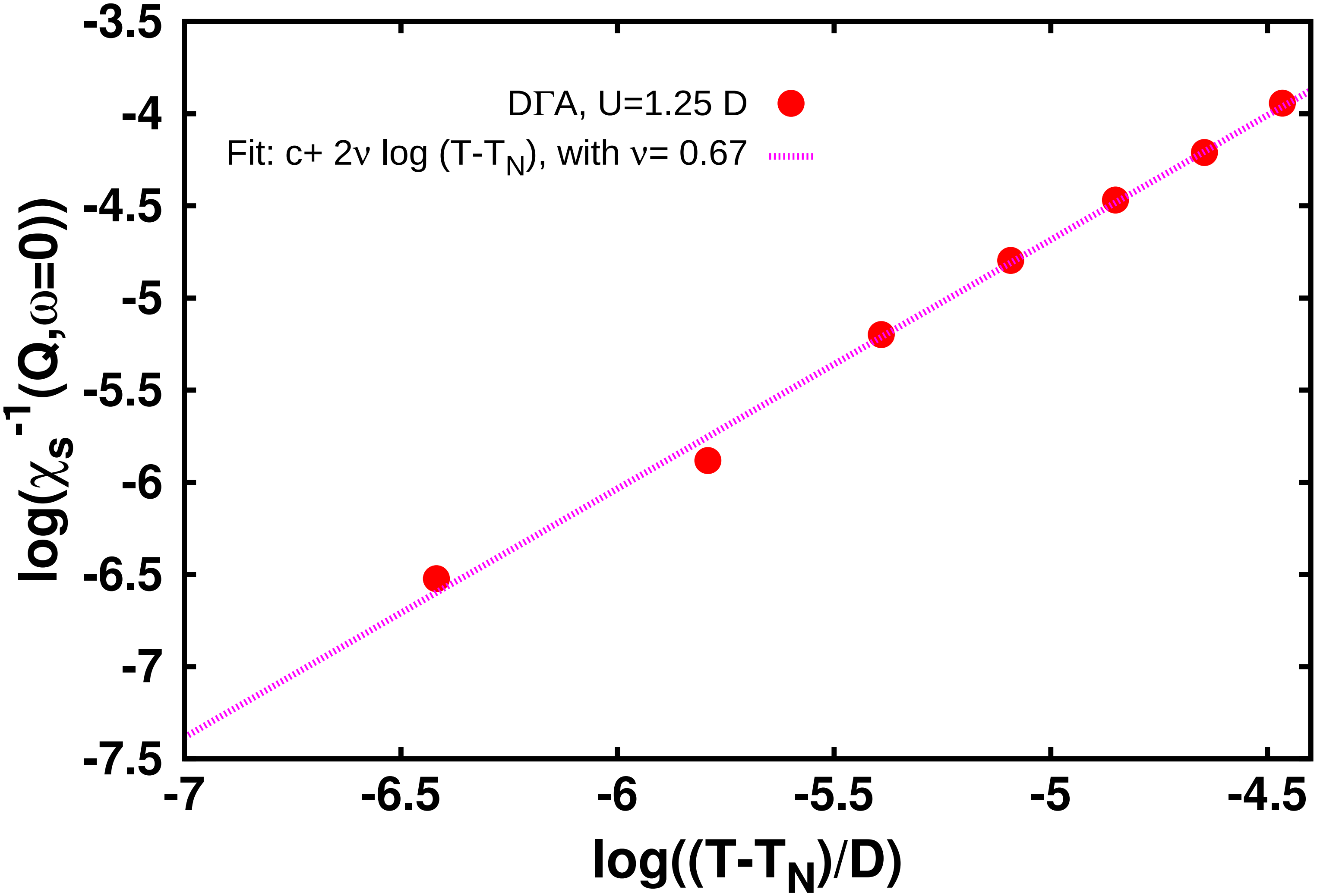
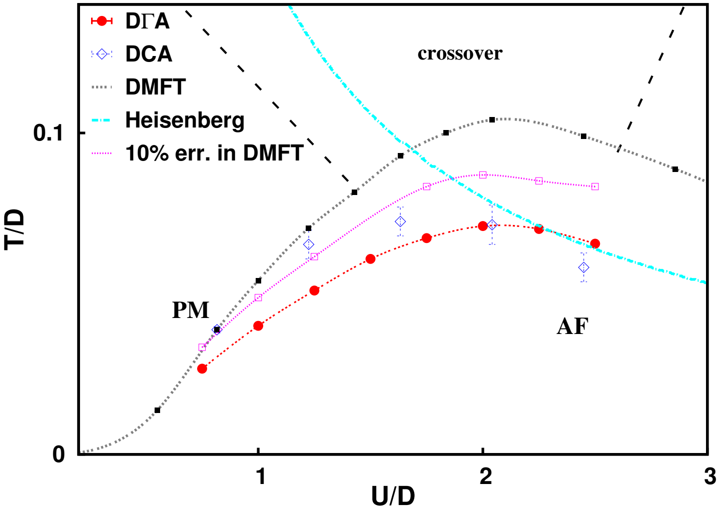
Logarithmic plot



Phase diagram

Rohringer, Toschi, Katanin, KH'10



DΓA for nanoscopic systems

Valli, Sangiovanni, Gunnarsson, Toschi, KH PRL'10

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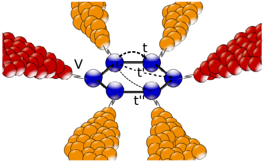
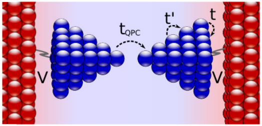
How can we calcualte somewhat larger nanosystems?





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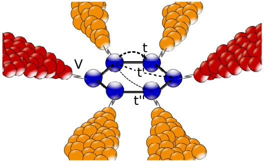
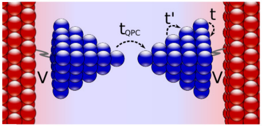
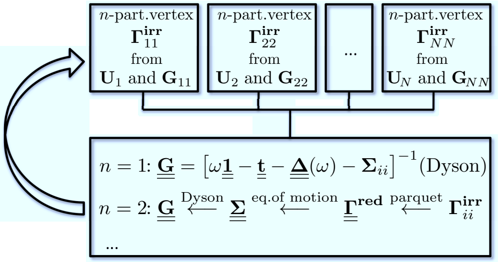
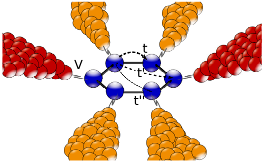






Validation against exact QMC solution

Valli, Sangiovanni, Gunnarsson, Toschi, KH PRL'10



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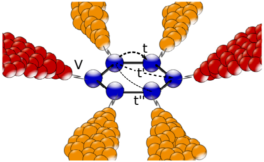
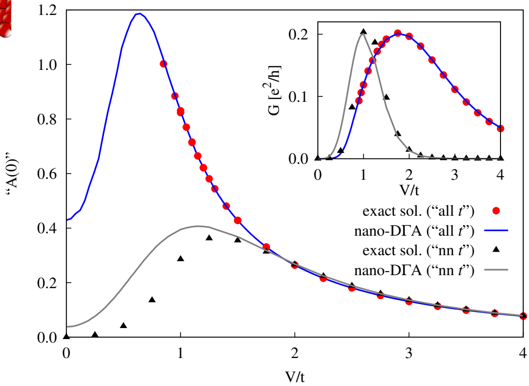
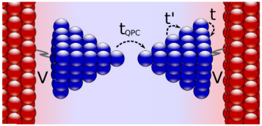




good agreement already on DMFT level
many neighbors, V favorable

Quantum point contact (104 atoms)

Valli, Sangiovanni, Gunnarsson, Toschi, KH PRL'10



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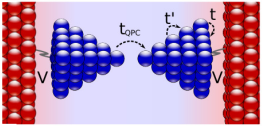
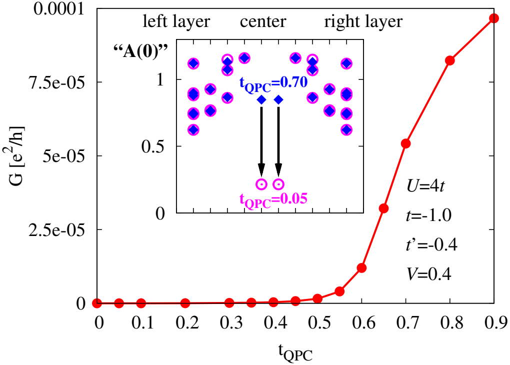
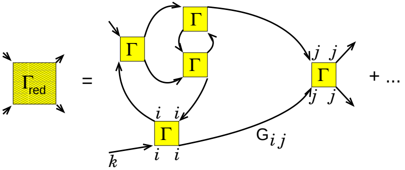




- Mott "transition" of atoms forming QPC
- expensive DΓA part scales linearly with system size
- DΓA vertex includes weak localization ...

Conclusion

- DΓA assumption: local 2-particle irreducible Γ



- DΓA can access short- and long-range correlations
- Results: 3D: Mott transition modified by AF fluctuations
  3D: critical exponent $\nu \approx 0.7$
  2D: pseudogap, Mermin Wagner fulfilled
- DΓA for nanoscopic systems

Outlook

- Physics: magnons, AFM & superconductivity, QCP
- Realistic multi-orbital calculations with LDA+DΓA