Radboud Universiteit

Collective phenomena in strongly correlated systems: Dual Fermion and Dual Boson approaches

Mikhail Katsnelson

Main collaborators:

A. Rubtsov, A. Lichtenstein, H. Hafermann, E. van Loon, E. Stepanov, M. Lemeshko

Outline

- Motivation: correlations in itinerant-electron magnets, Van Hove scenario for high-Tc…
- Dual Fermions: general idea
- Dual Fermions: applications (Fermi condensate, spin polaron in cobaltates…)
- Dual Bosons for non-local interactions
- Dual Bosons: applications (plasmons in strongly correlated systems, long-range dipole-dipole interactions for ultracold gases…)

Key word: nonlocal (interactions and/or correlations)

Motivation I: Iron

After 15 years of use of LDA/GGA + DMFT

Itinerant-electron magnetism: Fe, Co, Ni

Nickel: seems to be DMFT metal (a broad circle of properties can be calculated with the same – and reasonable – *U* value)

Iron: qualitatively OK, quantitatively – not so impressive

Cobalt: intermediate case

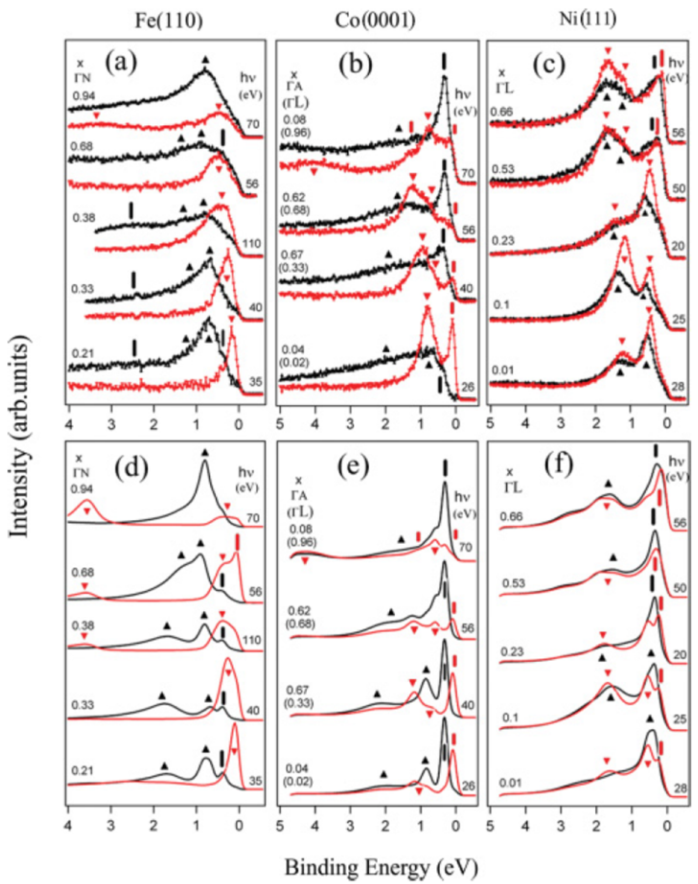
Important: *honest* comparison with ARPES, with matrix elements, surface effects, etc. Just from spectral density you cannot say anything!

ARPES for 3d metals

PHYSICAL REVIEW B 85, 205109 (2012)

Effects of spin-dependent quasiparticle renormalization in Fe, Co, and Ni photoemission spectra: An experimental and theoretical study

J. Sánchez-Barriga,[1] J. Braun,[2] J. Minár,[2] I. Di Marco,[3] A. Varykhalov,[1] O. Rader,[1] V. Boni,[4] V. Bellini,[5] F. Manghi,[4] H. Ebert,[2] M. I. Katsnelson,[6] A. I. Lichtenstein,[7] O. Eriksson,[3] W. Eberhardt,[1] H. A. Dürr,[1,8] and J. Fink[1,9]



Variation of U does not help too much for Fe

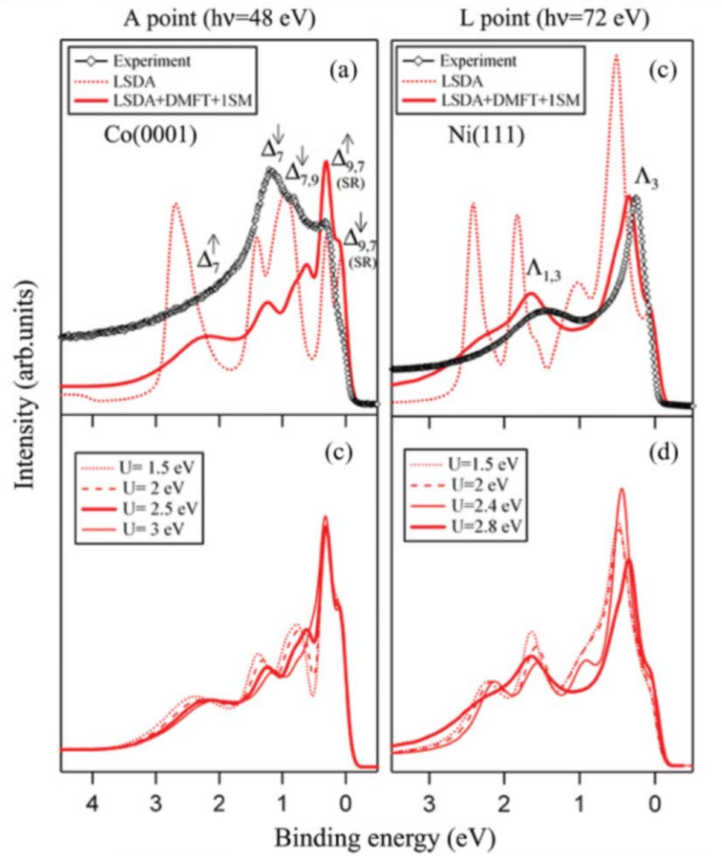


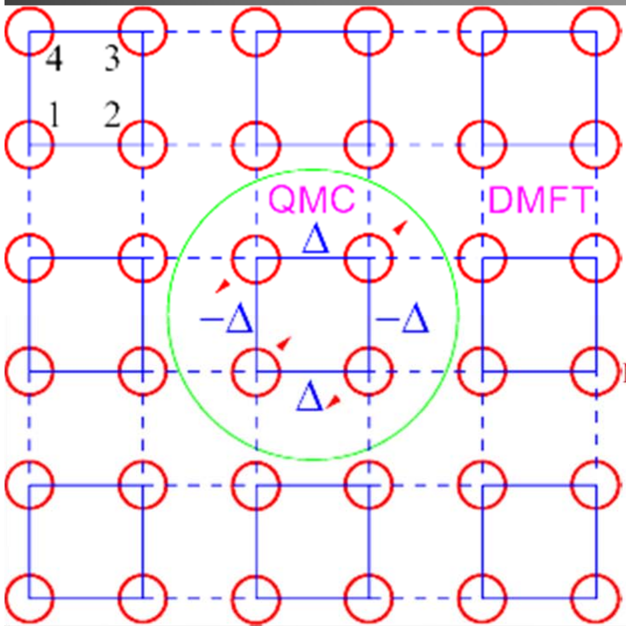
TABLE I. Values of the experimental and theoretical mass enhancement factors m^*/m_0 for majority spin states at high symmetry points of the BBZ of Fe, Co, and Ni, respectively. The theoretical values are derived for $U(\mathrm{Fe}) = 1.5$ eV, $U(\mathrm{Co}) = 2.5$ eV, $U(\mathrm{Ni}) = 2.8$ eV.

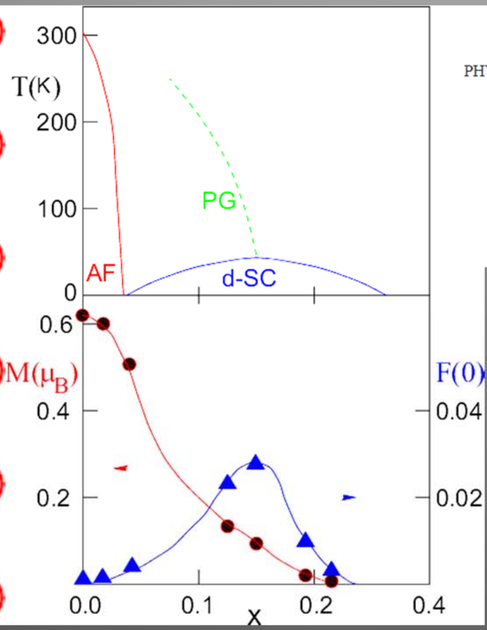
	Fe			Co			Ni	
	Expt.	Theory		Expt.	Theory		Expt.	Theory
Γ	1.7	1.2	Γ	1.26	1.31	Γ	2.0	1.8
N	1.1	1.2	A	1.29	1.31	Λ	1.9	1.8

Black – spin up, red – spin down
Upper panel – exper,lower - DMFT

Motivation II: High-T_c superconductors

d-wave paring itself is nonlocal effect (cannot be introduced on site)





RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 62, NUMBER 14 1 OCTOBER 2000-II

Antiferromagnetism and *d*-wave superconductivity in cuprates: A cluster dynamical mean-field theory

A. I. Lichtenstein[1] and M. I. Katsnelson[2]
[1]*University of Nijmegen, 6525 ED Nijmegen, The Netherlands*
[2]*Institute of Metal Physics, 620219 Ekaterinburg, Russia*
(Received 22 November 1999)

Cluster DMFT as the first step
Order parametrer on the bond rather than on site

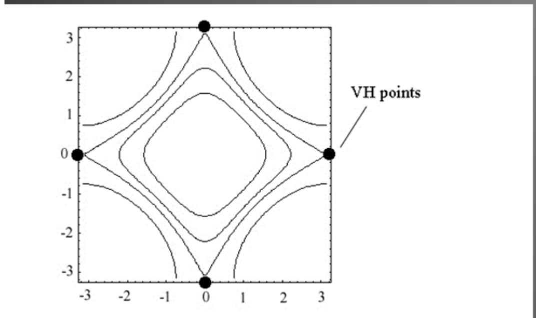
Important role of (antiferro)magnetic fluctuations, interplay of magnetism and superconductivity

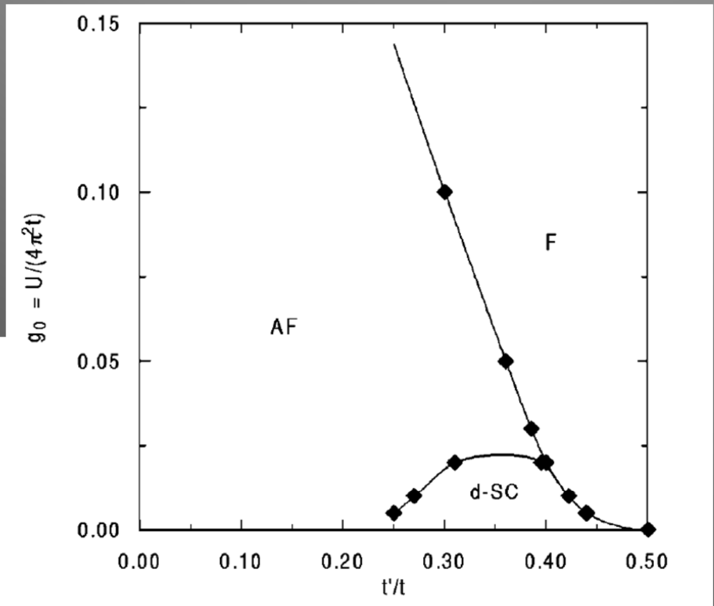
Pseudogap formation, node and antinode points at the Fermi surface, shadow Fermi surface etc. etc.

Not enough – most interesting nonlocal correlation effects should be treated in k-space

Example: Van Hove filling and optimal doping in high-*Tc* superconductors (also – pseudogap, etc.)

Irkhin, Katanin & MIK, PRB 64, 165107 (2001); PRL 89, 076401 (2002)





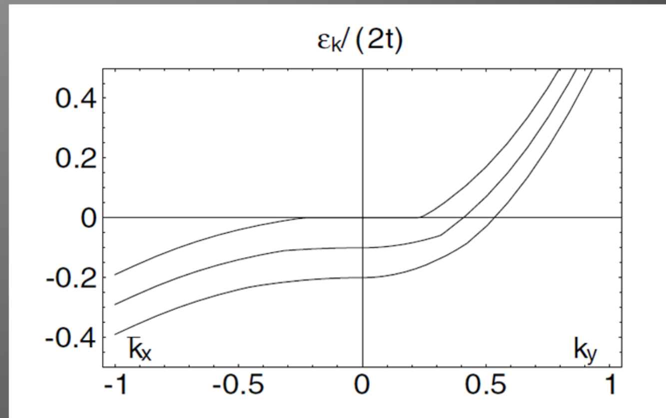
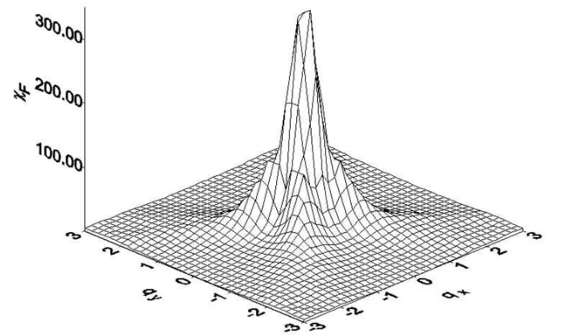
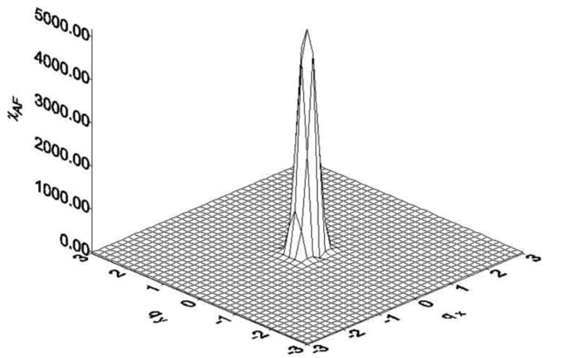


FIG. 1. Quasiparticle dispersion for $t'/t = -0.3$ and $U = 4t$ from RG approach. The values of the chemical potential are $\tilde{\mu} = 0, -0.2t, -0.4t$ (from top to bottom).

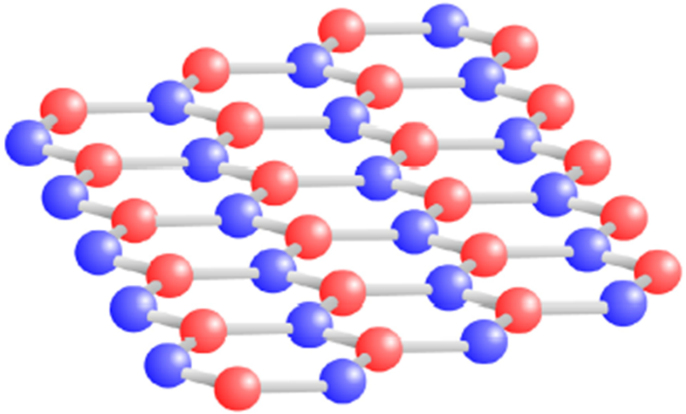


Parquet approx.



Flattering of the band (“fermion condensate”, NFL behavior in a broad range of doping)

Motivation III: Graphene



Crucially important!!!

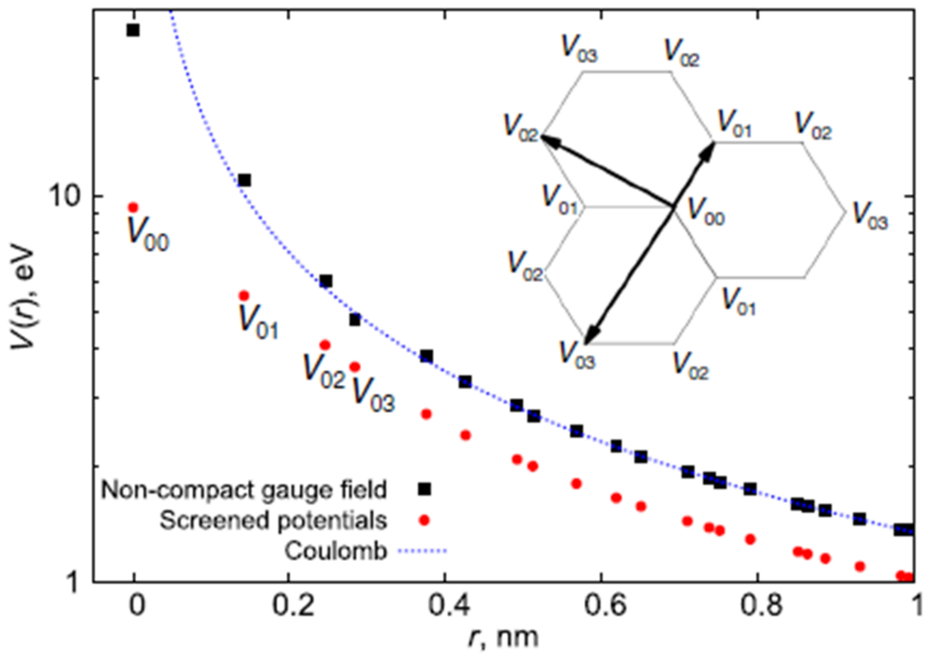
PRL 106, 236805 (2011) PHYSICAL REVIEW LETTERS week ending 10 JUNE 2011

Strength of Effective Coulomb Interactions in Graphene and Graphite

T. O. Wehling,[1] E. Şaşıoğlu,[2] C. Friedrich,[2] A. I. Lichtenstein,[1] M. I. Katsnelson,[3] and S. Blügel[2]

	Graphene		Graphite	
	Bare	cRPA	Bare	cRPA
$U_{00}^{A \text{ or } B}$ (eV)	17.0	9.3	17.5, 17.7	8.0, 8.1
U_{01} (eV)	8.5	5.5	8.6	3.9
$U_{02}^{A \text{ or } B}$ (eV)	5.4	4.1	5.4, 5.4	2.4, 2.4
U_{03} (eV)	4.7	3.6	4.7	1.9

Long-range interactions



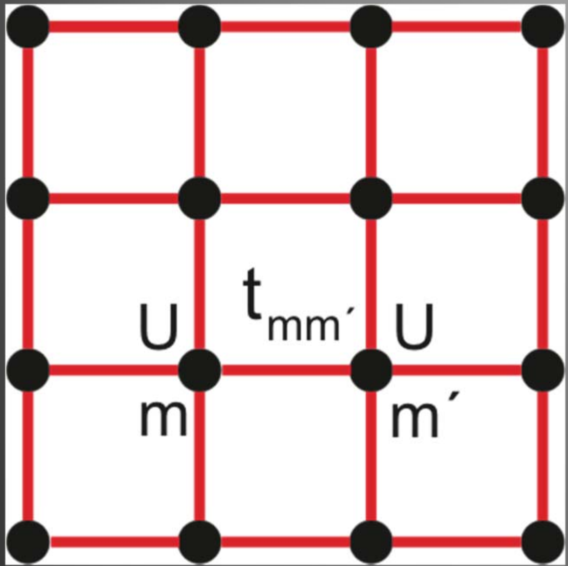
Logarithmic remormalization of effective mass due to long-range Coulomb interaction...

Phase diagram (semimetal vs excitonic insulator

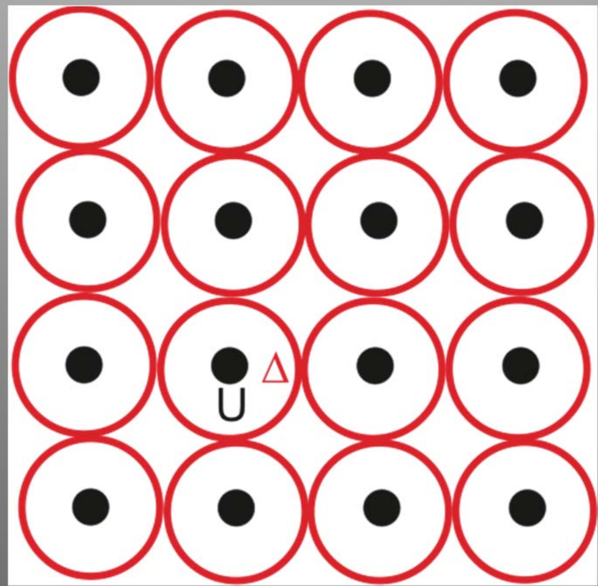
Renormalization of minimal conductivity...

Non-local correlations: DMFT-and beyond

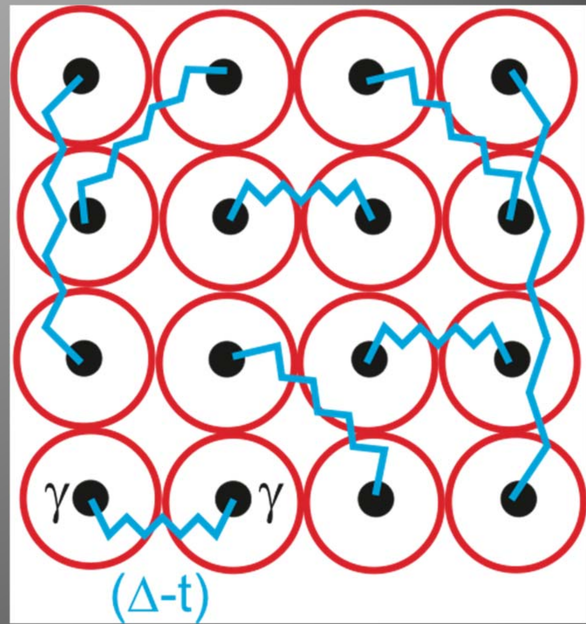
Lattice



DMFT



DF



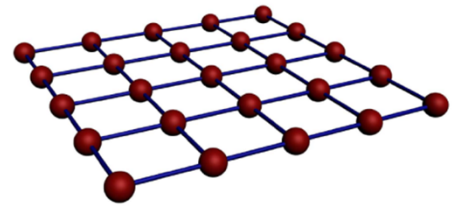
Start from
Correlated Lattice:
QMC has large
“sign” problem

Find the optimal
Reference System:
Dynamical Mean Field
Bath hybridization

Expand around
DMFT solution
Dual Fermions

Beyond DMFT: Dual Fermion scheme

General Lattice Action $H = h + U$

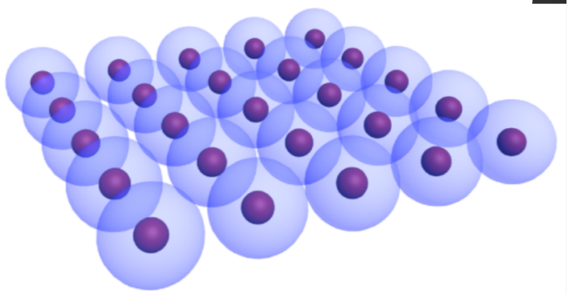


$$S[c^*,c] = \sum_{\omega k m m' \sigma} \left[h_k^{mm'} - (i\omega+\mu)1\right] c^*_{\omega k m \sigma} c_{\omega k m' \sigma} + \frac{1}{4} \sum_{i\{m,\sigma\}} \int_0^\beta U_{1234} c_1^* c_2^* c_3 c_4 d\tau$$

Reference system: Local Action with hybridization Δ_ω

$$S_{loc} = \sum_{\omega m m' \sigma} \left[\Delta_\omega^{mm'} - (i\omega+\mu)1\right] c^*_{\omega m \sigma} c_{\omega m' \sigma} + \frac{1}{4} \sum_{i\{m,\sigma\}} \int_0^\beta U_{1234} c_1^* c_2^* c_3 c_4 d\tau$$

Lattice-Impurity connection:



$$S[c^*,c] = \sum_i S_{loc}[c_i^*, c_i] + \sum_{\omega k m m' \sigma} \left(h_k^{mm'} - \Delta_\omega^{mm'}\right) c^*_{\omega k m \sigma} c_{\omega k m' \sigma}.$$

Sum over momenta in Δ-terms cancels sum over sites!

A. Rubtsov, MIK, A. Lichtenstein, PRB **77**, 033101 (2008)

Dual Fermions II

Gaussian path-integral

$$\int D[\vec{f}^*,\vec{f}]\,\exp(-\vec{f}^*\hat{A}\vec{f}+\vec{f}^*\hat{B}\vec{c}+\vec{c}^*\hat{B}\vec{f})=\det(\hat{A})\exp(\vec{c}^*\hat{B}\hat{A}^{-1}\hat{B}\vec{c})$$

with

$$\begin{aligned} A &= g_\omega^{-1}(\Delta_\omega - h_k)g_\omega^{-1} \\ B &= g_\omega^{-1} \end{aligned}$$

new action:

$$S_d[f^*,f] = -\sum_{k\omega}\mathcal{G}_{k\omega}^{-1} f_{k\omega}^* f_{k\omega} + \frac{1}{4}\sum_{1234}\gamma_{1234}^{(4)} f_1^* f_2^* f_4 f_3 + \ldots$$

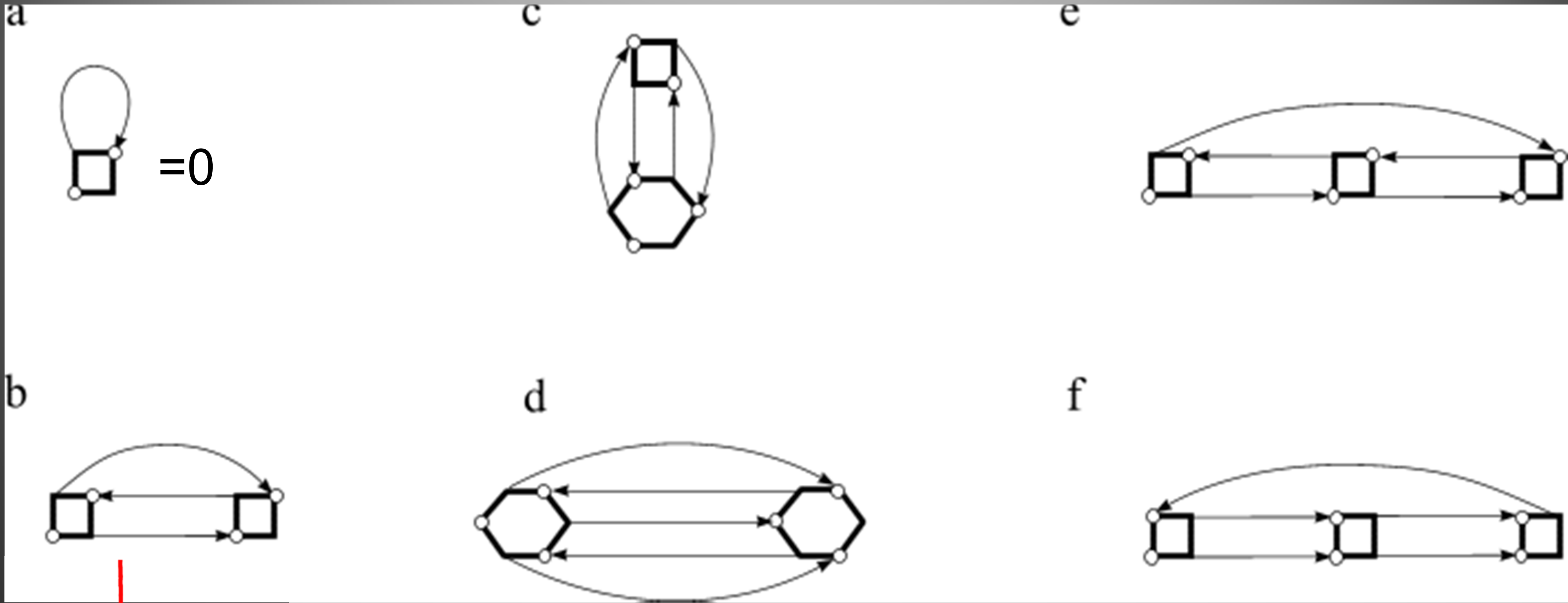
Diagrammatic:

$$\mathcal{G}_{k\omega} = G_{k\omega}^{DMFT} - g_\omega$$

$$\gamma_{1234}^{(4)} = g_{11'}^{-1} g_{22'}^{-1}\left(\chi_{1'2'3'4'} - \chi_{1'2'3'4'}^{0}\right) g_{3'3}^{-1} g_{4'4}^{-1}$$

g_ω and $\chi_{\nu,\nu',\omega}$ from DMFT impurity solver

Basic diagrams for dual self-energy



Lines - dual Green's function.

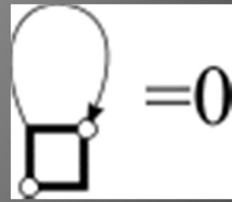
$$\tilde{G}^0_\omega(\mathbf{k}) = \left[g_\omega^{-1} + \Delta_\omega - t_\mathbf{k}\right]^{-1} - g_\omega$$

$$\tilde{\Sigma}^{(b)}_{12}(\mathbf{k}) = -\frac{1}{2}\left(\frac{T}{N}\right)^2 \sum_{\mathbf{k}_1\mathbf{k}_2} \sum_{345678} \gamma_{1345} \tilde{G}_{57}(\mathbf{k}_1) \tilde{G}_{83}(\mathbf{k}_2) \tilde{G}_{46}(\mathbf{k}+\mathbf{k}_2-\mathbf{k}_1) \gamma_{6728}$$

Condition for Δ and relation with DMFT

To determine Δ, we require that Hartree correction in dual variables vanishes. If no higher diagrams are taken into account, one obtains DMFT

$G^d = G^{DMFT} - g$



$$\frac{1}{N}\sum_{\mathbf{k}} \tilde{G}^0_\omega(\mathbf{k}) = 0 \quad \Longleftrightarrow \quad \frac{1}{N}\sum_{\mathbf{k}} G^{\rm DMFT}_\omega(\mathbf{k}) = g_\omega$$

Higher-order diagrams give corrections to the DMFT self-energy, and already the leading-order correction is nonlocal

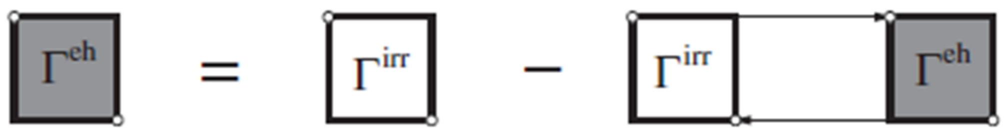
$$\Sigma(k,\omega) = \Sigma_{DMFT}(\omega) + \Sigma_d(k,\omega)/[1+g\Sigma_d(k,\omega)]$$

PRL **102,** 206401 (2009) PHYSICAL REVIEW LETTERS week ending 22 MAY 2009

Efficient Perturbation Theory for Quantum Lattice Models

H. Hafermann,[1] G. Li,[2] A. N. Rubtsov,[3] M. I. Katsnelson,[4] A. I. Lichtenstein,[1] and H. Monien[2]

Ladder summation for four-leg Vertex only – approximation by default

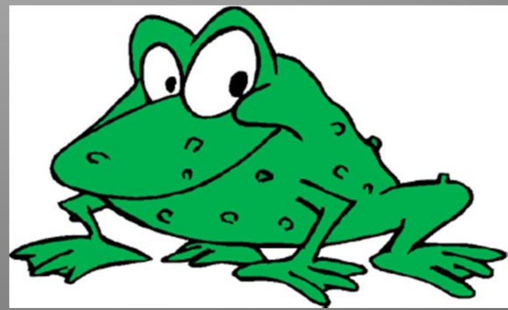


Why do we do this?

Hamiltonian action with local in time,
but large (tall and beatiful) U

(troubles,
troubles)

Non-Hamiltonian action with retarded
V, formally including all orders
of interaction (but negligible!)



Transformation of a beautiful princess
to an ugly frog

1. DMFT is now our zeroth-order approx., all nonlocal effects are already there in the best possible way

2. There is a very efficient way to calculate all correlators for the impurity problem by CTQMC

3. Simplest sequences of diagramms are good enough (sometimes)

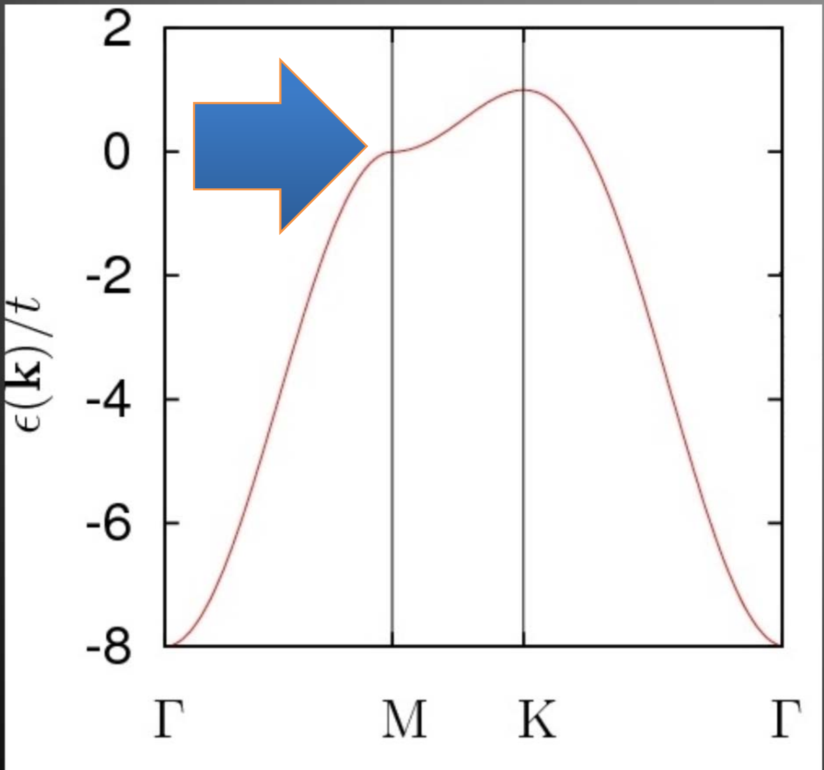
Triangular Lattice- VHS

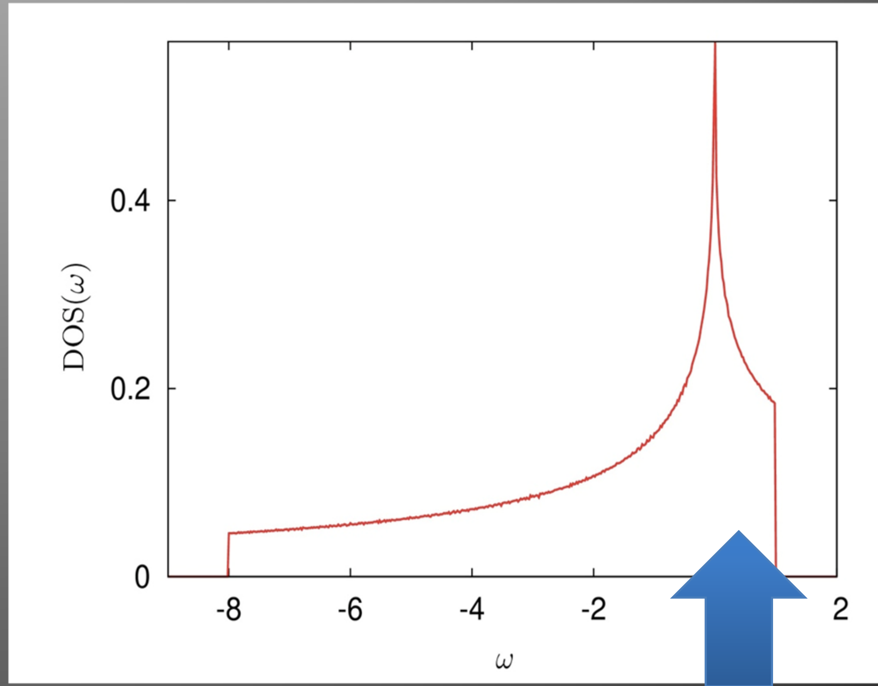
PRL **112,** 070403 (2014) PHYSICAL REVIEW LETTERS week ending 21 FEBRUARY 2014

Fermi Condensation Near van Hove Singularities Within the Hubbard Model on the Triangular Lattice

Dmitry Yudin,[1] Daniel Hirschmeier,[2] Hartmut Hafermann,[3] Olle Eriksson,[1] Alexander I. Lichtenstein,[2] and Mikhail I. Katsnelson[4,5]

$$\varepsilon_{\mathbf{k}} = -2t\left(\cos k_x + 2\cos\frac{k_x}{2}\cos\frac{k_y\sqrt{3}}{2}\right) - \mu$$





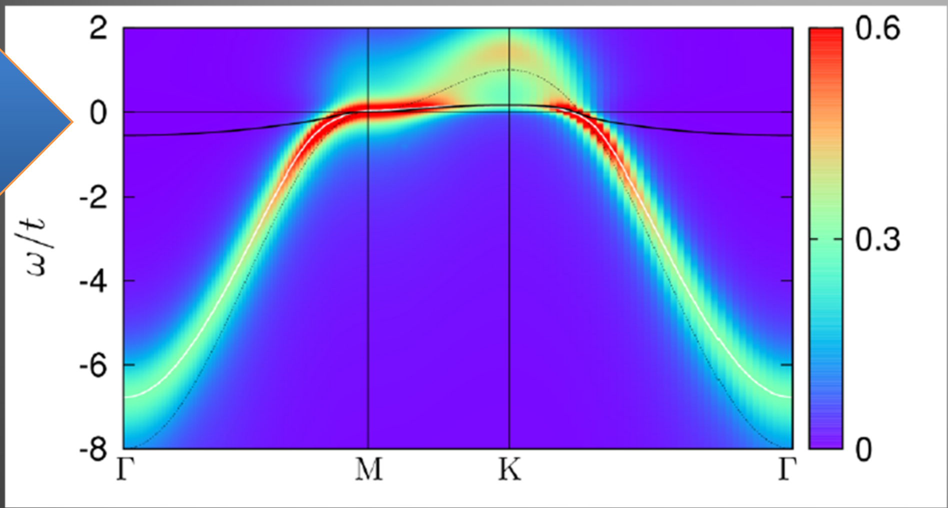
$$N(\varepsilon) = \frac{1}{\pi^2 t\sqrt{3}} K\left(\frac{1}{2} + \frac{|\varepsilon| + 2t - \varepsilon^2/4t}{4\sqrt{t\,(|\varepsilon| + t)}}\right) \sim_{|\varepsilon|/t \ll 1} N_0 \log\left(\frac{2t}{|\varepsilon|}\right)$$

$$N_0 = \sqrt{3}/(2\pi^2 t)$$

Van Hove sinqularity at filling n=2/3

Extended van Hove singularity: Fermion Condensate

Spectral Function

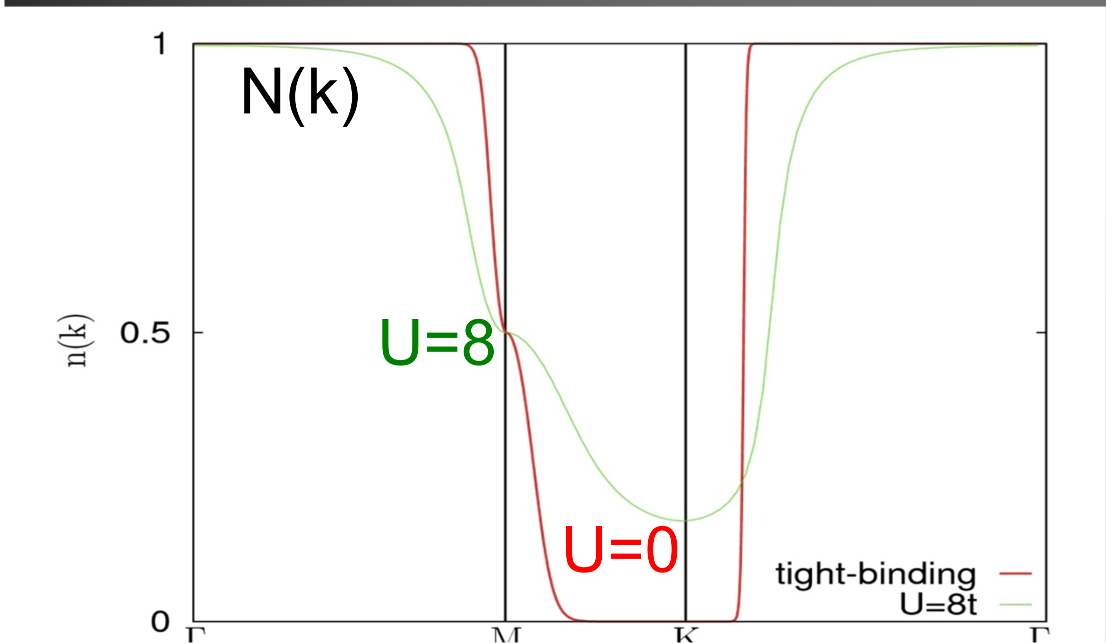


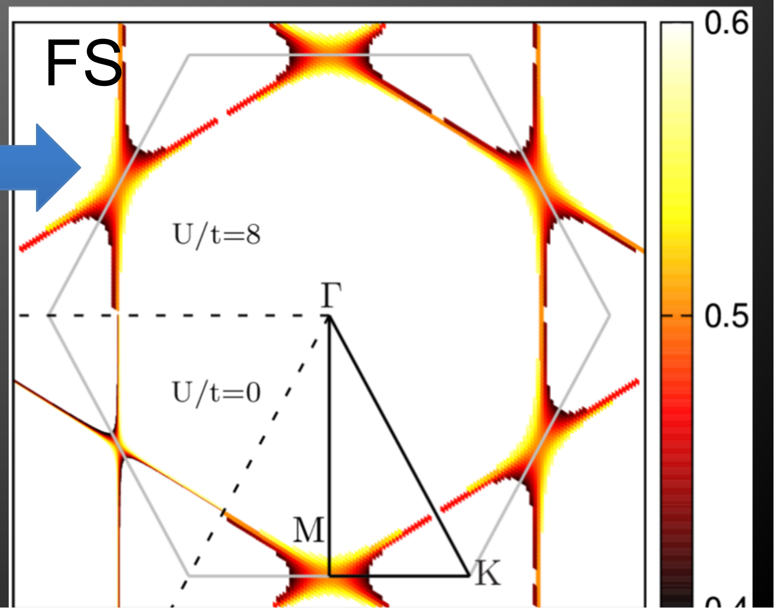
Ladder DF approx.

$U/t = 8$ and $T/t = 0.05$

The effect survives at relatively high temperatures, may be suitable for the observation in optical lattices

Microscopic realization of the fermion condensate



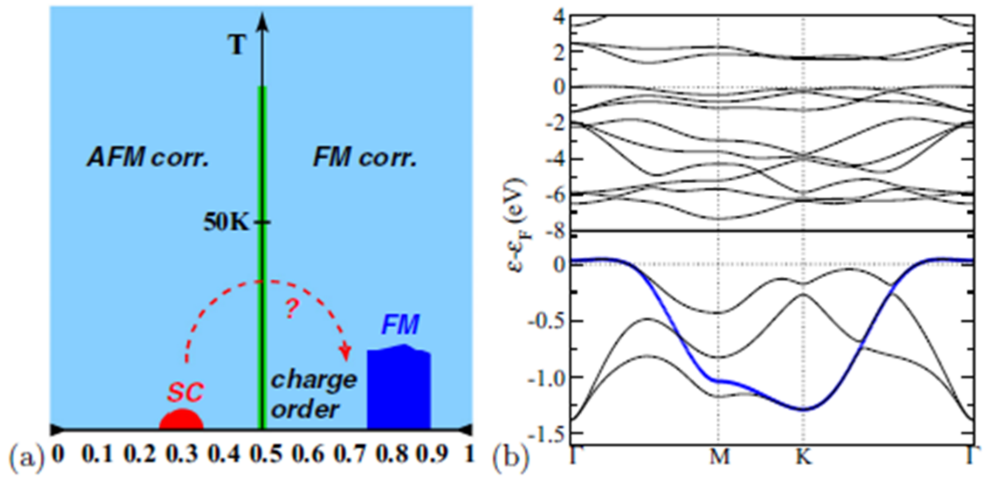


Dual Fermions for Real Materials: Layered Cobaltate

PHYSICAL REVIEW B **91**, 155114 (2015)

From Hubbard bands to spin-polaron excitations in the doped Mott material Na_xCoO_2

Aljoscha Wilhelm,[1] Frank Lechermann,[1] Hartmut Hafermann,[2] Mikhail I. Katsnelson,[3] and Alexander I. Lichtenstein[1]



The model: mapping on a_{1g} band only (blue). Giant VHS – should be the main effect. Dual fermions in ladder approximation

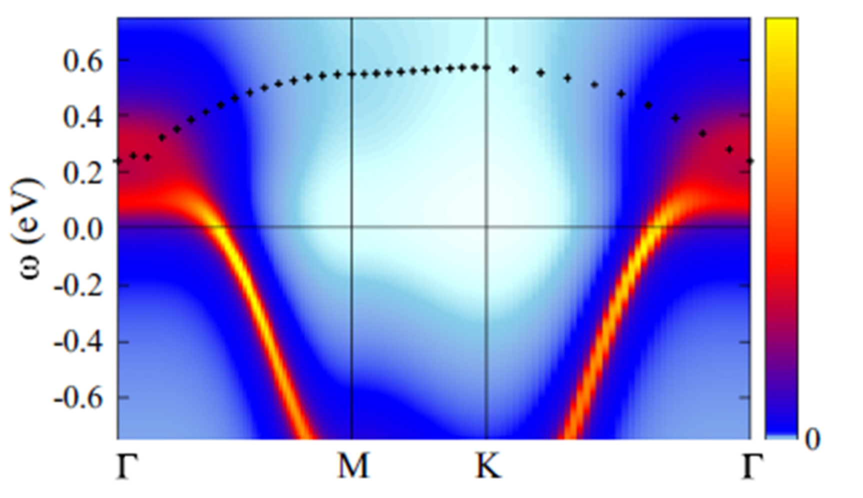
Physics: bound state (spin polaron) in FM *t-J* model (MIK 1982)

$$|\Psi\rangle = \sum_{ij,i\neq j} \psi_{ij} |ij\rangle$$

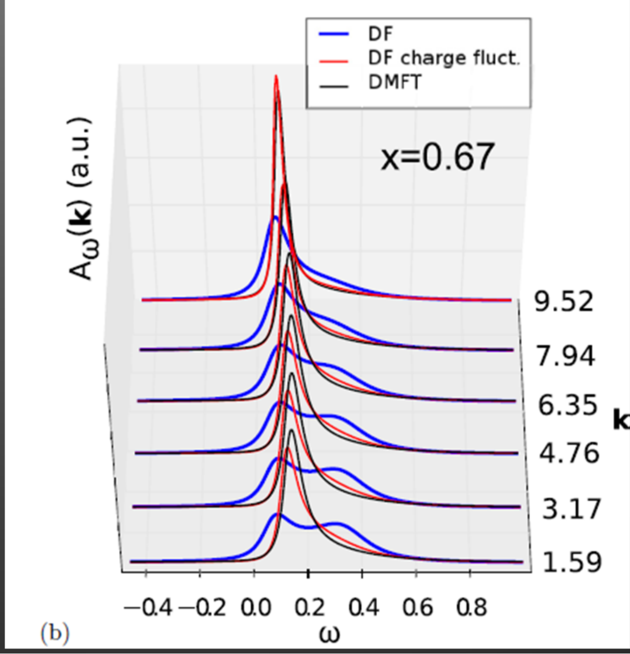
$$c^{\dagger}_{i\sigma} S^{-}_{j} |\mathrm{FM}\rangle \equiv |ij\rangle$$

$$E\psi_{ij} = \sum_{k\neq j} t_{ik}\psi_{kj} + t_{ij}\psi_{ji} + \sum_{k\neq i} J_{jk}(\psi_{ij} - \psi_{ik})$$

t - hopping
J - exchange



Band splitting beyond DMFT



Non-local Coulomb interactions

Dual boson approach to collective excitations in correlated fermionic systems

A.N. Rubtsov[a], M.I. Katsnelson[b], A.I. Lichtenstein[c,*]

Annals of Physics 327 (2012) 1320–1335

General non-local action for solids:

$$S = \sum_r S_{at}[c_r^\dagger, c_r] + \sum_{r,R\neq 0,\omega,\sigma} \varepsilon_R c^\dagger_{r\omega\sigma} c_{r+R\omega\sigma} + \sum_{r,R\neq 0,\Omega} V_{R\Omega} \rho^*_{r\Omega} \rho_{r+R\Omega}$$

Atomic action with local Hubbard-like interaction

$$S_{at} = -\sum_{\omega\sigma} (i\omega + \mu) c^\dagger_{\omega\sigma} c_{\omega\sigma} + \int_0^\beta U c^\dagger_\uparrow c_\uparrow c^\dagger_\downarrow c_\downarrow d\tau$$

Bosonic charge and spin variables:

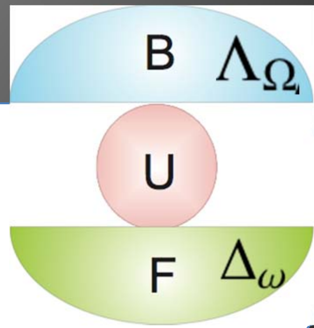
$$\rho_j \equiv \sum_{\sigma\sigma'} c^\dagger_\sigma s^j_{\sigma\sigma'} c_{\sigma'} - \bar{\rho}, \qquad j = \{0, x, y, z\}$$

Dual Bosons for non-local Interactions

Separate local and non-local effective actions:

$$S = \sum_r S_{imp}[c_r^\dagger, c_r] + \sum_{\omega,k,\sigma} (\varepsilon_k - \Delta_{\omega\sigma})\, c^\dagger_{\omega k\sigma} c_{\omega k\sigma} + \sum_{\Omega,k} (V_{\Omega k} - \Lambda_\Omega)\, \rho^*_{\Omega k}\rho_{\Omega k}$$

Impurity action with fermionic and bosonic bathes (CT-QMC)



$$S_{imp} = S_{at} + \sum_\omega \Delta_\omega c^\dagger_\omega c_\omega + \sum_\Omega \Lambda_\Omega \rho^*_\Omega \rho_\Omega$$

Dual boson-fermion transformation: $c^\dagger \Rightarrow f^\dagger$ $\rho^* \Rightarrow \eta^*$

$$\tilde{S} = -\sum_{\omega k} \tilde{\mathcal{G}}^{-1}_{\omega k} f^\dagger_{\omega k} f_{\omega k} - \sum_{\Omega k} \tilde{X}^{-1}_{\Omega k} \eta^*_{\Omega k} \eta_{\Omega k} + \sum_i \tilde{U}[\eta_i, f_i, f_i^\dagger]$$

Dual Bosons for non-local Interactions II

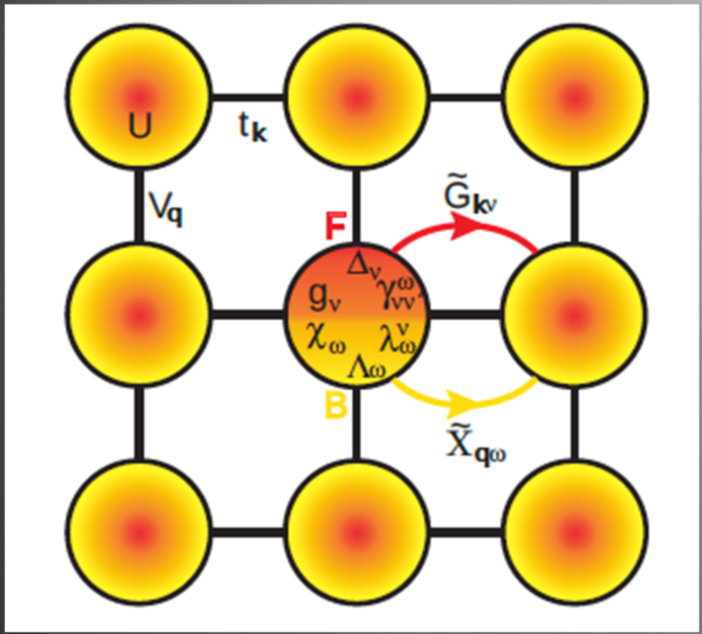


Figure 1. (Color online) Sketch of the DB formalism. The original action with parameters U, $V_\mathbf{q}$ and $t_\mathbf{k}$ is replaced by an auxiliary impurity problem with fields Δ_ν, Λ_ω. The expectation values of this impurity model (g_ν, χ_ω, $\gamma_{\nu\nu'\omega}$ and $\lambda_{\nu\omega}$) enter a *dual* theory in terms of $\tilde{G}$ and $\tilde{X}$.

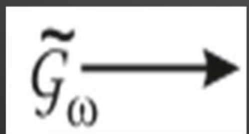
$$\tilde{G}^{(0)}_{\mathbf{k}\nu} = [g_\nu^{-1} + \Delta_\nu - \varepsilon_k]^{-1} - g_\nu,$$
$$\tilde{X}^{0}_{\mathbf{q}\omega} = [\chi_\omega^{-1} + \Lambda_\omega - V_q]^{-1} - \chi_\omega.$$

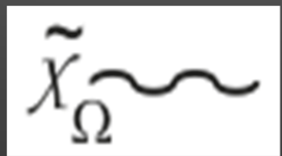
$$g_\nu = -\langle c_\nu c_\nu^* \rangle_{\text{imp}},$$
$$\chi_\omega = -\langle \rho_\omega \rho_{-\omega} \rangle_{\text{imp}}$$

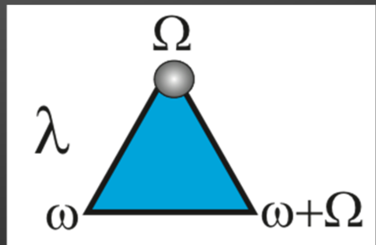
Technically: Hubbard-Stratonovich transformation

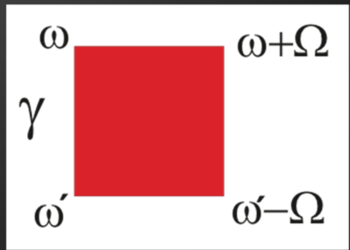
$$\int D[c^\dagger, c]\, e^{c^\dagger E c} = \int D[c^\dagger, c] \det(\alpha_f^{-1} E \alpha_f^{-1}) \int D[f^\dagger, f]\, e^{-f^\dagger \alpha_f E^{-1} \alpha_f f + f^\dagger \alpha_f c + c^\dagger \alpha_f f}$$
$$\int D[\rho^*, \rho]\, e^{\rho^* W \rho} = \int D[\rho^*, \rho] \det(\alpha_b W^{-1} \alpha_b) \int D[\eta^*, \eta]\, e^{-\eta^* \alpha_b W^{-1} \alpha_b \eta + \eta^* \alpha_b \rho + \rho^* \alpha_b \eta}$$

Diagrams:



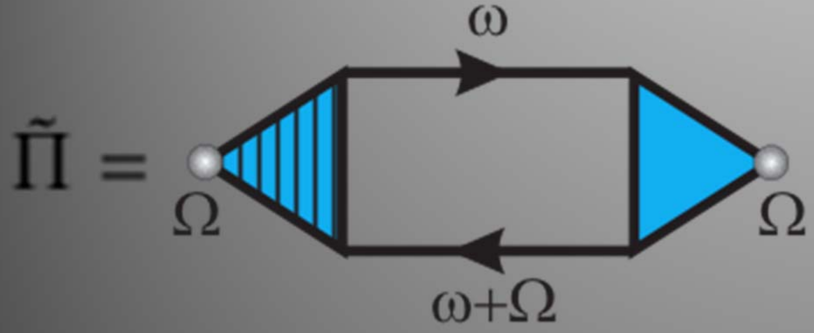




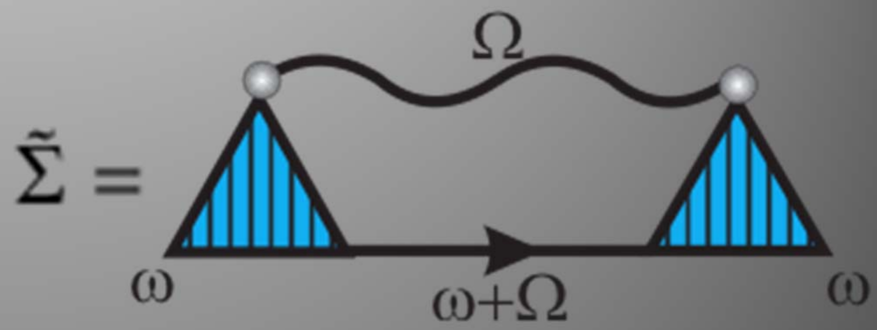


Diagrammatic scheme

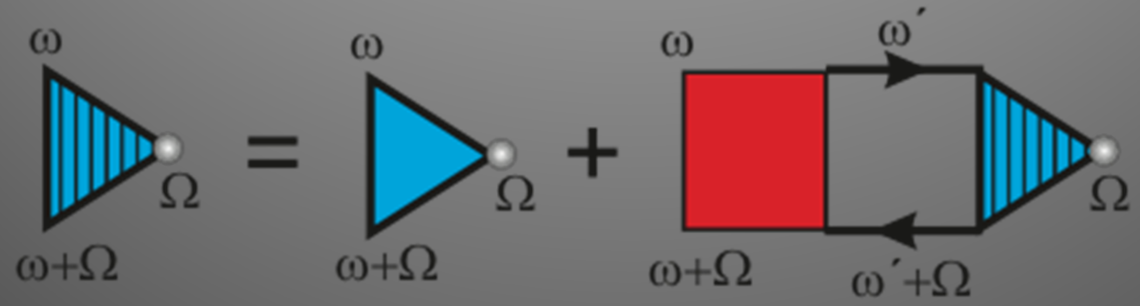
Bosonic Selfenergy



Fermionic Selfenergy

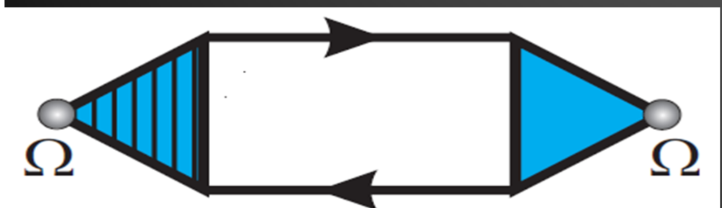


Renormalized vertex:

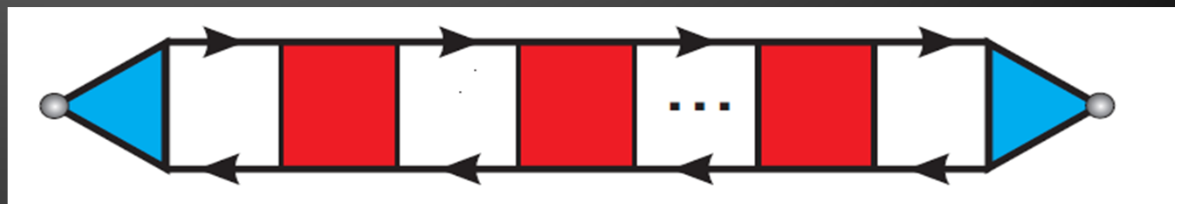


Fermionic and Bosonic Green Functions

Ladder summation:



= sum of



Conservation laws

Charge conservation law $$\Omega^2 \langle \rho\rho \rangle_{\Omega K} = K^2 \langle jj \rangle_{\Omega K}$$

As a consequence $$\langle \rho\rho \rangle_{K=0} = 0 \text{ at any finite frequency}$$

In 3D for metals $$\langle \rho\rho \rangle_{\omega, K\to 0} \propto \frac{K^2}{\Omega^2 + \Omega_p^2}$$ Ω_p is the plasma frequency

Exact G and no vertex $$\chi^0_{\Omega K} = -\sum_{k\omega} \mathcal{G}_{\omega k} \mathcal{G}_{\omega+\Omega k+K}$$

$$\chi^0_{\Omega K} = -\sum_{\omega k} \left(\frac{1}{i\omega - \varepsilon_k - \Sigma_\omega} - \frac{1}{i(\omega+\Omega) - \varepsilon_{k+K} - \Sigma_{\omega+\Omega}} \right) \frac{1}{i\Omega + \Sigma_\omega - \Sigma_{\omega+\Omega}}$$

If Sigma is nonlinear in energy – charge conservation is Violated (Baym 1962)
Vertex is absolutely necessary, charge conservation is provided by Ward identity (cf. Edwards & Hertz, 1973 for magnons in the Hubbard model)

Very nontrivial: DB with ladder summation is fine in this sense (but not with the lowest-order diagram only) - analytical proof and numerical check

Plasmons in strongly correlated materials

PRL 113, 246407 (2014) PHYSICAL REVIEW LETTERS week ending 12 DECEMBER 2014

Plasmons in Strongly Correlated Systems: Spectral Weight Transfer and Renormalized Dispersion

E. G. C. P. van Loon,[1,*] H. Hafermann,[2] A. I. Lichtenstein,[3,4] A. N. Rubtsov,[5,6] and M. I. Katsnelson[1,4]

$$H = -t \sum_{\langle ij \rangle} c^\dagger_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{\mathbf{q}} V_{\mathbf{q}} \rho_{\mathbf{q}} \rho_{-\mathbf{q}}$$

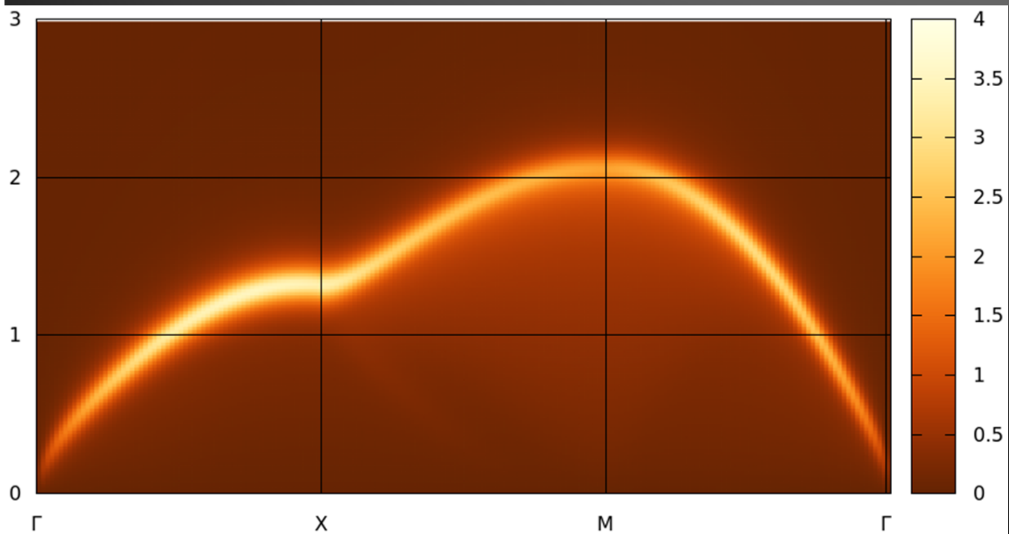
2D system (square lattice), half filling, NN approx.,long-range Coulomb interaction is added to the Hubbard model

$$U + V_0/|\mathbf{q}|$$

$$V_0 = 2\pi e^2/\kappa$$

Spectral function for plasmons (measured by EELS) $-\mathrm{Im}\, \epsilon_E^{-1}(\mathbf{q})$

Weak correlations – random phase approximation (RPA)



Well-defined plasmon branch (some broadening at large ***q*** due to Landau damping)

$\omega_p(\mathbf{q}) \propto \sqrt{q}$ at small ***q***

“Normal” behavior

Plasmons in strongly correlated materials II

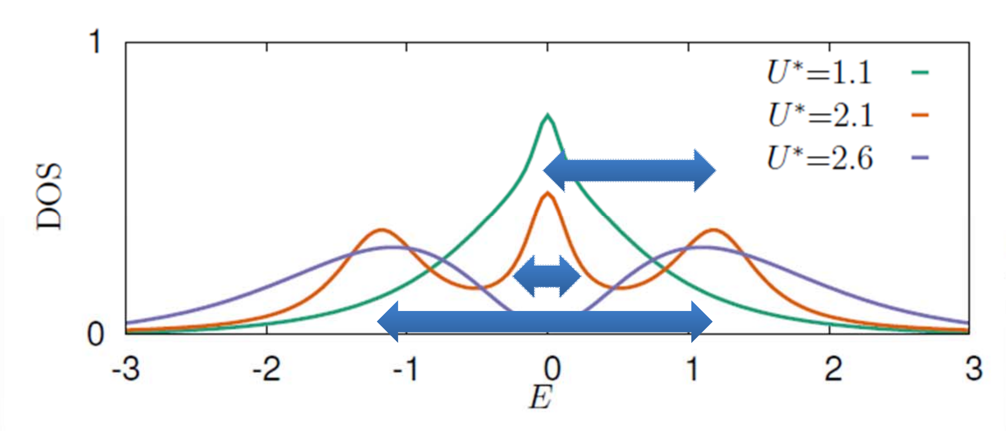


Figure 2. Local density of states (DOS) of the two-dimensional Hubbard model with long-range Coulomb interaction calculated within EDMFT. The local interaction U^* moves spectral weight from the quasi-particle peak at the Fermi energy to the Hubbard bands at $E \sim \pm U^*/2$. For sufficiently large U^*, the system is a Mott insulator.

Several types of e-h excitations which can form plasmons?!

Ladder dual boson approximation

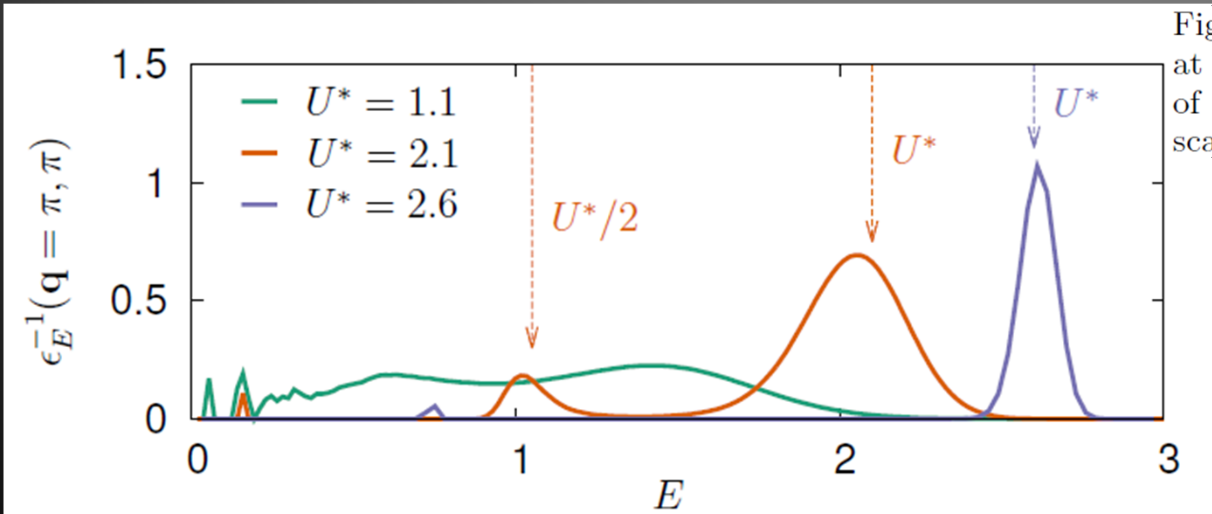


Figure 4. A cross section of the EELS ($-\operatorname{Im}\epsilon^{-1}$) of Fig. 3 at the M point, $\mathbf{q} = (\pi, \pi)$. The interaction causes a transfer of spectral density. The arrows indicate the typical energy scales U^* and $U^*/2$.

One can expect spectral density transfer for plasmons

Plasmons in strongly correlated materials III

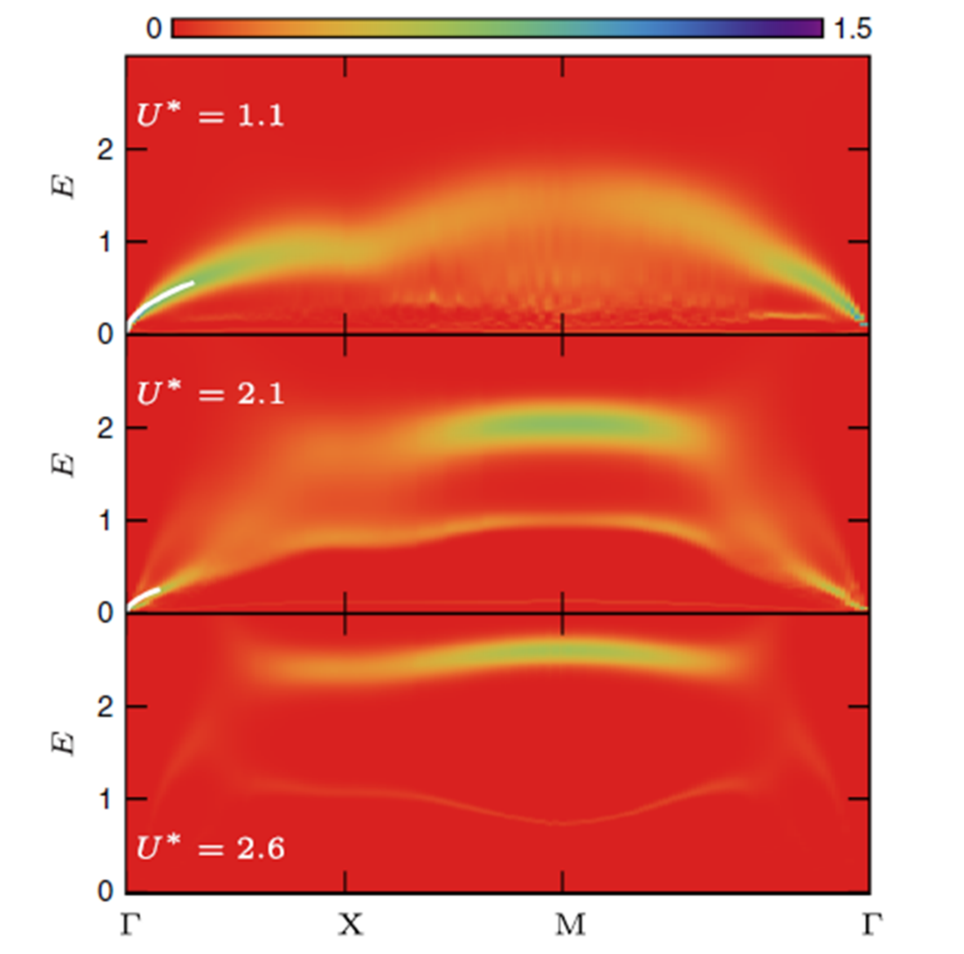
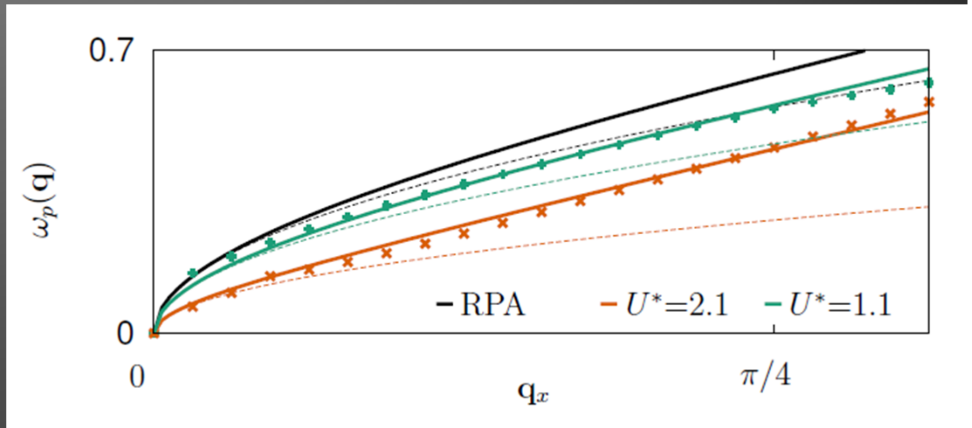


FIG. 3 (color online). Inverse dielectric function $-\mathrm{Im}\epsilon_E^{-1}(\mathbf{q})$ of the 2D Hubbard model with long-range Coulomb interaction for different values of the effective local interaction U^* across the Mott transition. The spectra show a transition from itinerant to localized behavior. The interaction causes a spectral weight transfer as well as a renormalization of the long-wavelength plasmon dispersion. The dispersion relation $\omega_p(\mathbf{q})^2 = \alpha V_0 q$ is shown in white.

In Mott insulator phase
no plasmons at small ***q***

In strongly correlated
metals spectral density
transfer



Change of plasmon dispersion
(rather linear than square root,
except very small ***q***)

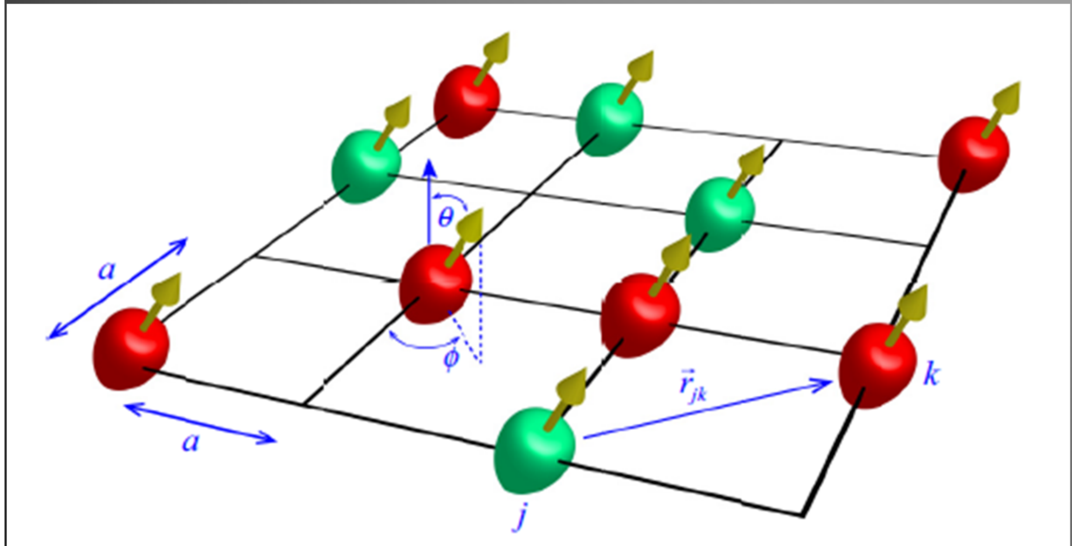
Ultracold gases in optical lattices

RAPID COMMUNICATIONS

PHYSICAL REVIEW B **92**, 081106(R) (2015)

Ultralong-range order in the Fermi-Hubbard model with long-range interactions

Erik G. C. P. van Loon,[1] Mikhail I. Katsnelson,[1] and Mikhail Lemeshko[2,*]



$$H = -t\sum_{\langle jk\rangle\sigma} c^\dagger_{j\sigma}c_{k\sigma} + \frac{U}{2}\sum_j n_j n_j + \frac{1}{2}\sum_{jk} V^d_{jk} n_j n_k$$

$$V^d_{jk} = c_d[1 - 3(\hat{r}_{jk}\cdot\hat{d})^2]/(r_{jk}/a)^3$$

	c_d (Hz)		
	$a = 1064$ nm	$a = 532$ nm	$a = 266$ nm
^{23}Na^{40}K [15,16]	926	7.4×10^3	59.3×10^3
^{40}K^{87}Rb [11,12]	40	321	2.6×10^3
^{161}Dy [7]	1	8.6	68.7
^{167}Er [9,55]	0.5	4.2	33.8
^{53}Cr [5]	0.4	3.1	24.8

Phase diagram of dipoles in 2D square lattice from (ladder) DB, calculation of charge susceptibility from the side of high temperatures

Ultracold gases in optical lattices II

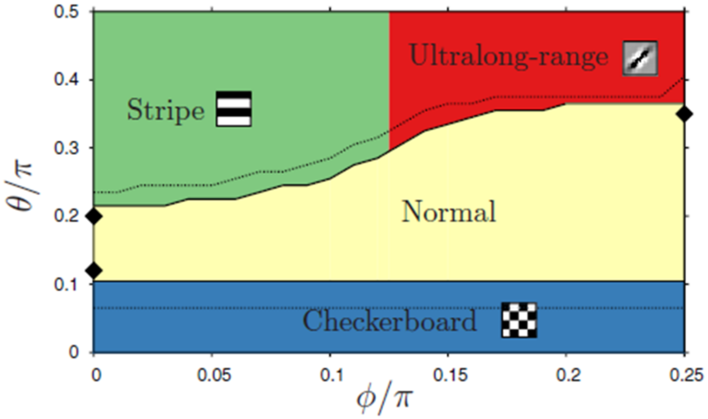


FIG. 2. (Color online) Phase diagram as a function of the dipole orientation at $U = 4t$, $c_d = 2t$, and filling $\langle n \rangle \approx 0.9$. The dotted lines show the phase boundaries at the reduced dipolar coupling, $c_d = 1.8t$. The black diamonds show the angles selected for Fig. 4.

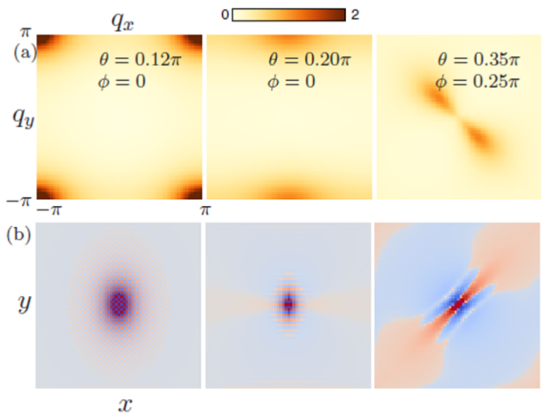


FIG. 4. (Color online) (a) Momentum-space susceptibility at selected points of the phase diagram, Fig. 2. (b) The corresponding density correlation function in real space: given a particle in the center of the figure, red indicates a higher probability to find a particle at x, y and blue a lower probability. Each pixel corresponds to a lattice site.

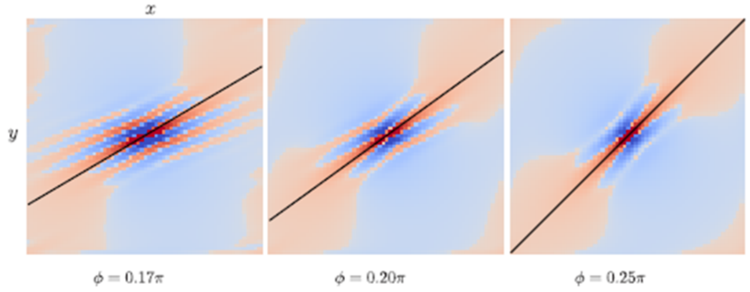


FIG. 5. (Color online) Real-space density correlation function as in Fig. 4(b), at fixed $\theta = 0.35\pi$, for three values of ϕ. The areas of high and low density follow the angle ϕ (black line).

Exotic phases with "ultra-long-range order"

$T = t/(4k_B)$ Corresponds to real experimental conditions (about 10 nK)

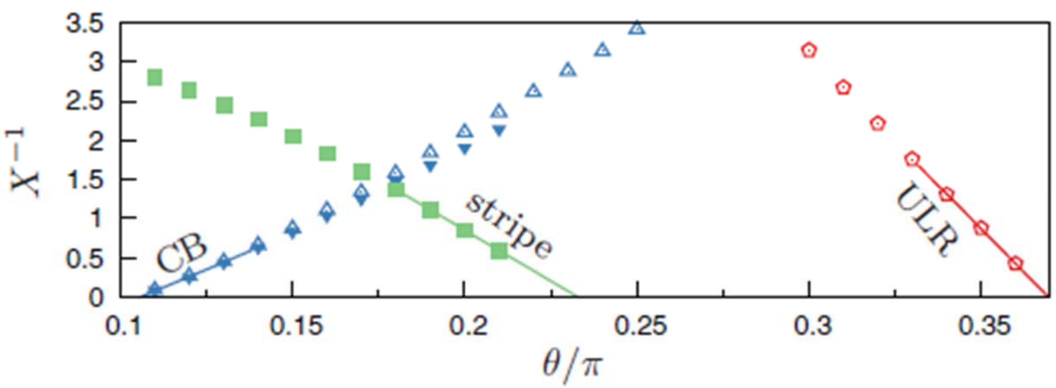


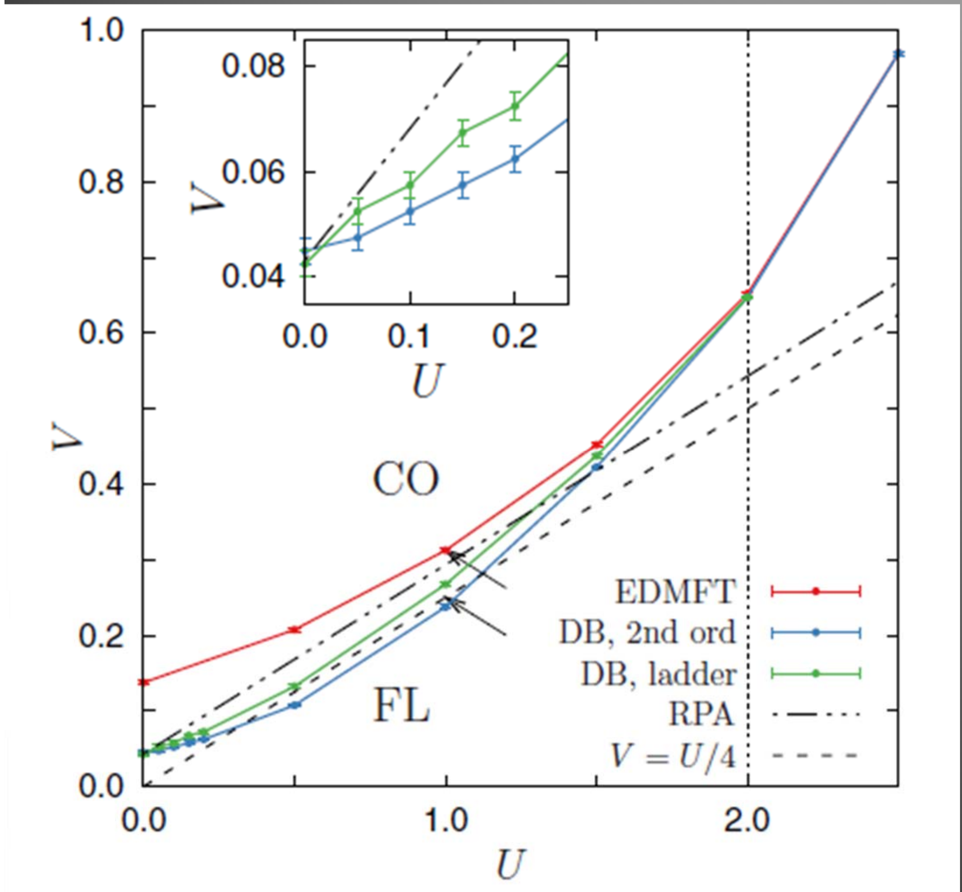
FIG. 3. (Color online) Inverse charge susceptibility in the normal phase, for the same parameters as in Fig. 2. The blue triangles show the divergence of the susceptibility at the checkerboard point, $\mathbf{q}_{CB} = (\pi,\pi)$, as θ is lowered, both for $\phi = 0$ (filled triangles) and $\phi = 0.25\pi$ (empty triangles). The green squares show the divergence of the $\mathbf{q}_{stripe} = (0,\pi)$ susceptibility as θ increases at $\phi = 0$ and the red pentagons show the $\mathbf{q}_* \approx (0.21\pi, -0.21\pi)$ susceptibility at $\phi = 0.25\pi$. The dashed lines show a linear extrapolation of the inverse susceptibility.

Charge ordering

PHYSICAL REVIEW B **90**, 235135 (2014)

Beyond extended dynamical mean-field theory: Dual boson approach to the two-dimensional extended Hubbard model

Erik G. C. P. van Loon,[1] Alexander I. Lichtenstein,[2] Mikhail I. Katsnelson,[1] Olivier Parcollet,[3] and Hartmut Hafermann[3]



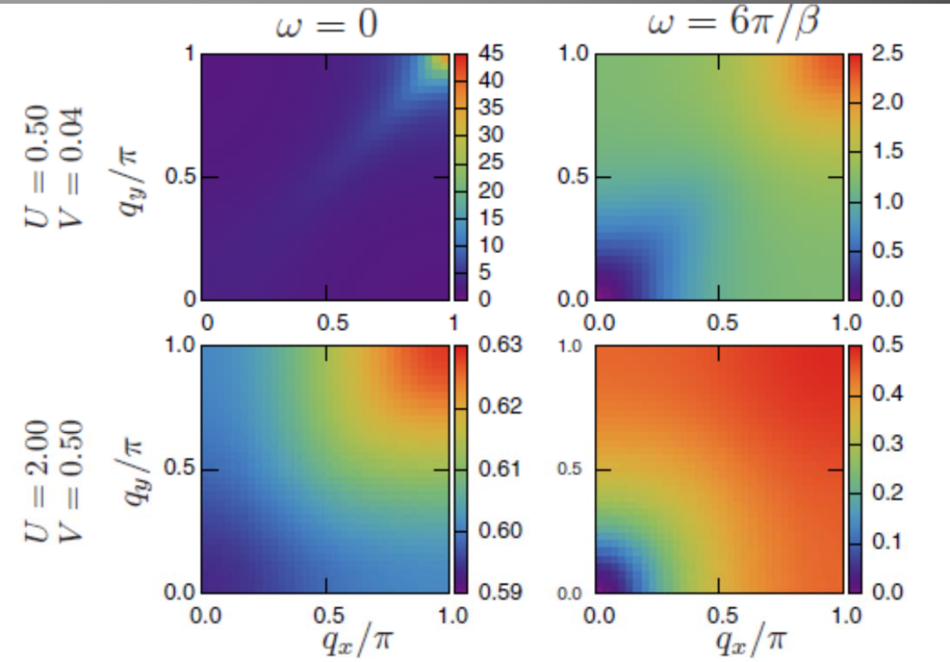


FIG. 17. (Color online) Momentum dependence of the physical polarization $\Pi_{\mathbf{q}\omega}$ for fixed Matsubara frequencies $\omega = 0$ (left column) and $\omega = 6\pi/\beta$ (right column) in the ladder approximation. In EDMFT, this quantity is a constant.

Charge ordering U-V model, T = 0.02
Square lattice

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y),$$

$$V_{\mathbf{q}} = 2V(\cos q_x + \cos q_y).$$

$$4t = 1$$

Summary

- DF is an efficient scheme to describe long-range non-local correlation effects. Improvement of DMFT
- DB allows to consider collective excitations (like plasmons, magnons) and “external” bosons on equal footing – looks promising! Improvement of EDMFT