Mutli-Orbital Continuous-Time QMC for LDA+DMFT Studies of $LiNiO_2$

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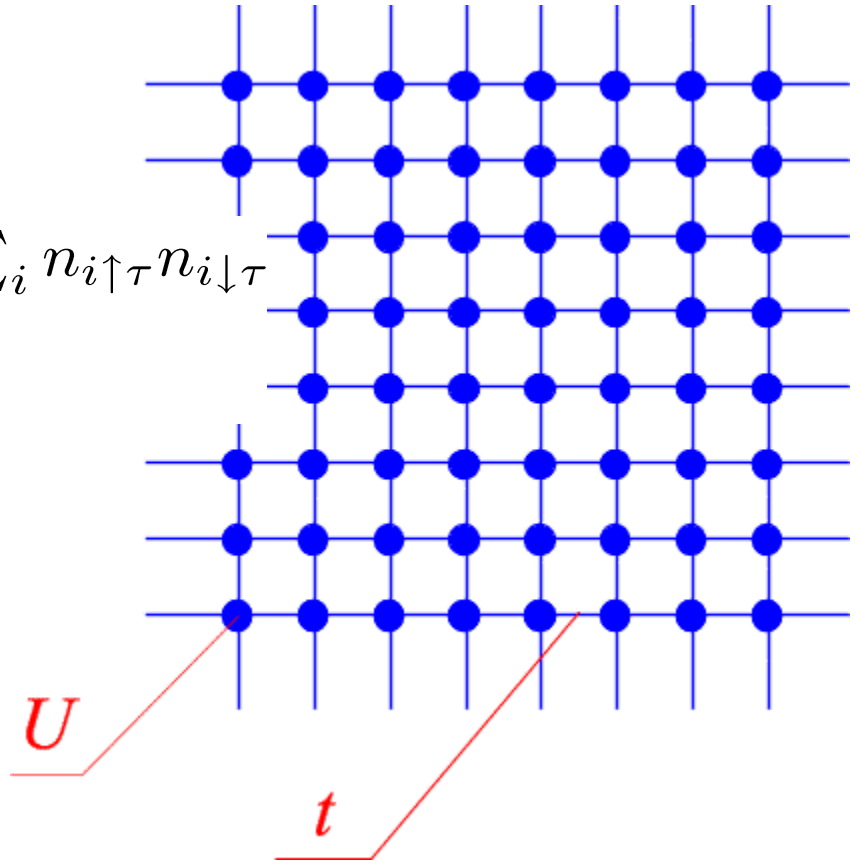
A problem of strong correlations

Example: Hubbard model

$$H = \sum_{k\sigma} (\epsilon_k - \mu)\, c^{\dagger}_{k\sigma} c_{k\sigma} + U \sum_i n_{i\uparrow\tau} n_{i\downarrow\tau}$$

$$\epsilon_k = -2t(\cos k_x + \cos k_y)$$



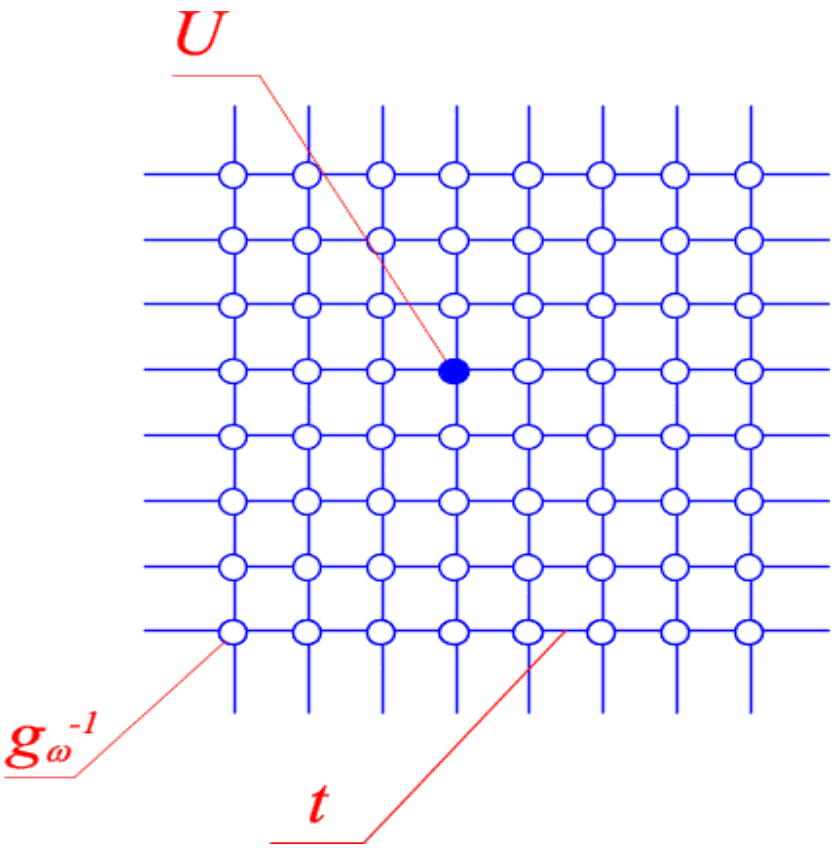
Real materials:

- Have multiorbital bands
- Show spatial nonlocality (AF fluctuations, or van Hove points, etc.)

Electronic properties of $LiNiO_2$

- 6 t_{2g} and 1 e_g electron in Ni atom
- Mott insulator
- no spin or orbital ordering down to zero temperature (quantum liquid)

DMFT framework



DMFT condition:

$$g_\omega = \sum_k \frac{N^{-1}}{g_\omega^{-1} - \epsilon_k + \Delta_\omega}$$

Main routes

- Improve solvers for realistic description of multiorbital SIAM, including multiplet structure
- Describe spatial nonlocality (in particular, quantum-liquid state)

Weak-coupling CT-QMC: the idea

$$S = -(i\omega + \mu)\sum_{\omega s} c^{\dagger}_{\omega s} c_{\omega s} + U\int_0^{\beta} n_{\tau\uparrow} n_{\tau\downarrow} d\tau$$

W

Consider the series with respect to *W* (in the interaction representation)

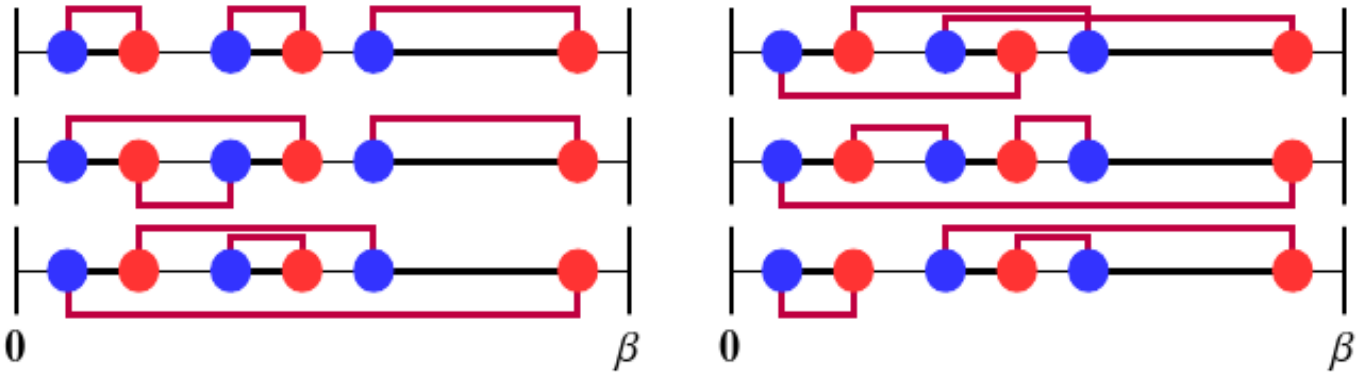
The series always converges for a finite fermionic system at finite temperature; it is possible to organize a random walk over the terms of whose series

A.N. Rubtsov, V. V. Savkin, and A. I. Lichtenstein,
Phys. Rev. B 72 035122 (2005).

Strong-coupling CT-QMC

$$S = S_{at} + \Delta_{\tau-\tau' s s'} c^{\dagger}_{s\tau} c_{s'\tau'}$$

The idea is to expand in hybridization



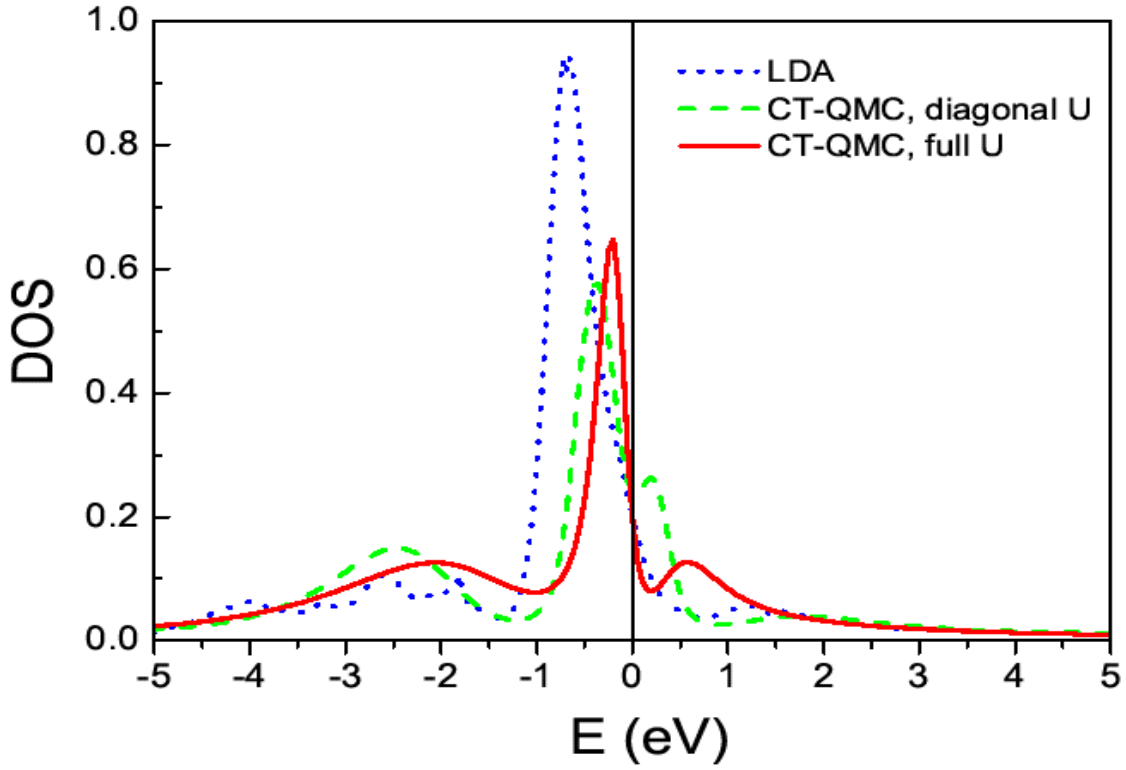
It's possible to sum up all the diagrams for a given operator set. One obtains:

$$Z = Z_0 \sum_{k=0}^{\infty} \frac{1}{k!} Tr \left\langle c^{+}_{\sigma}(\tau) c_{\sigma}(\tau') \ldots c^{+}_{\sigma'}(\tau) c_{\sigma'}(\tau') \right\rangle_{\text{at}} \det[\Delta(\tau-\tau')]$$

P. Werner et al, Phys.Rev.Lett.**97**, 076405(2006)

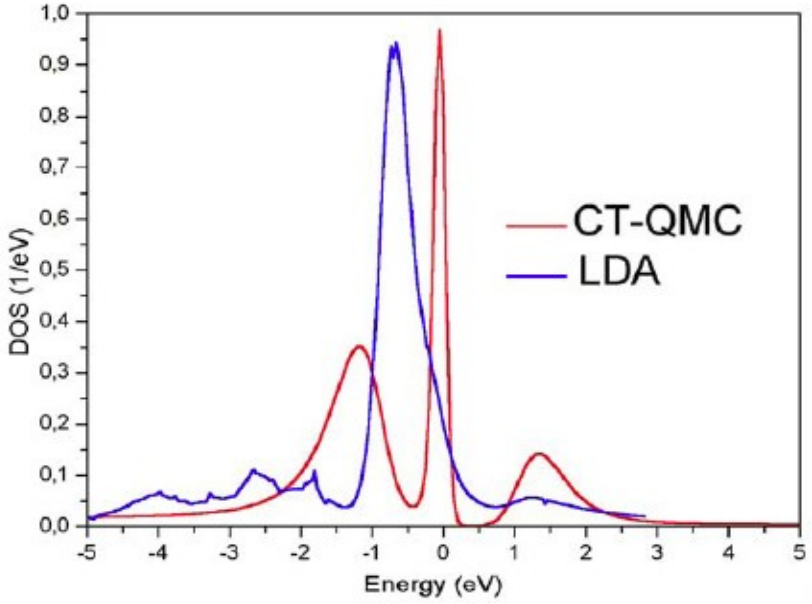
5-orbital model with off-diagonal interaction

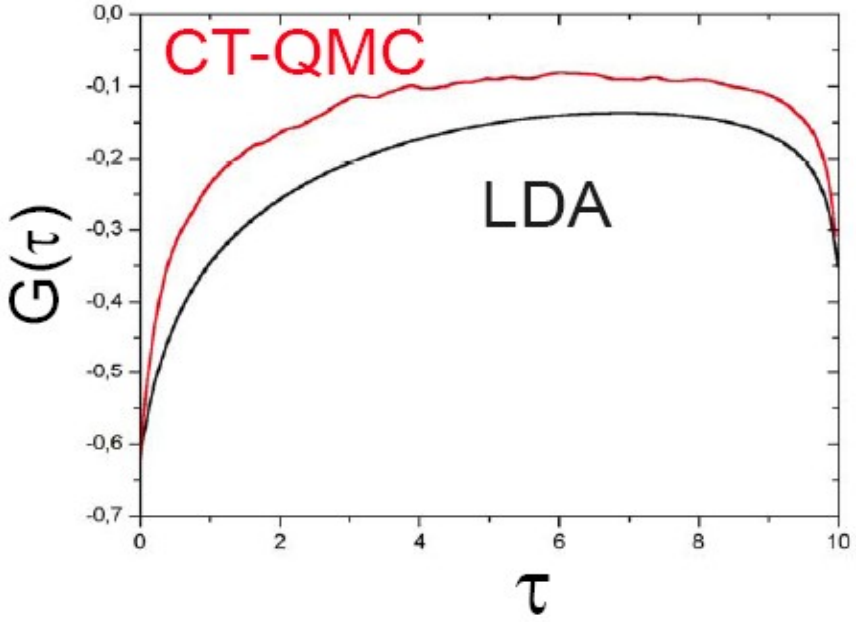
Co atom in Cu substrate



E. Gorelov, T. O. Wehling, A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein
PRB 2009

5-orbital model with off-diagonal interaction

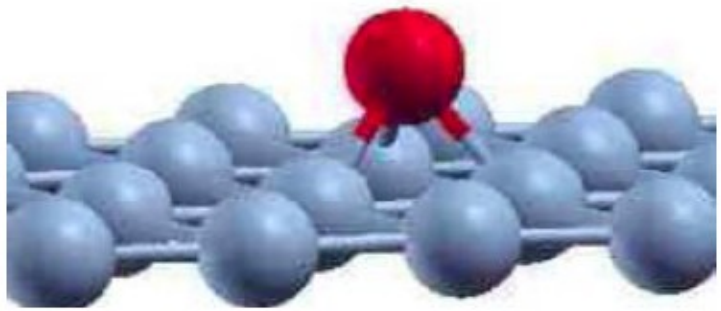




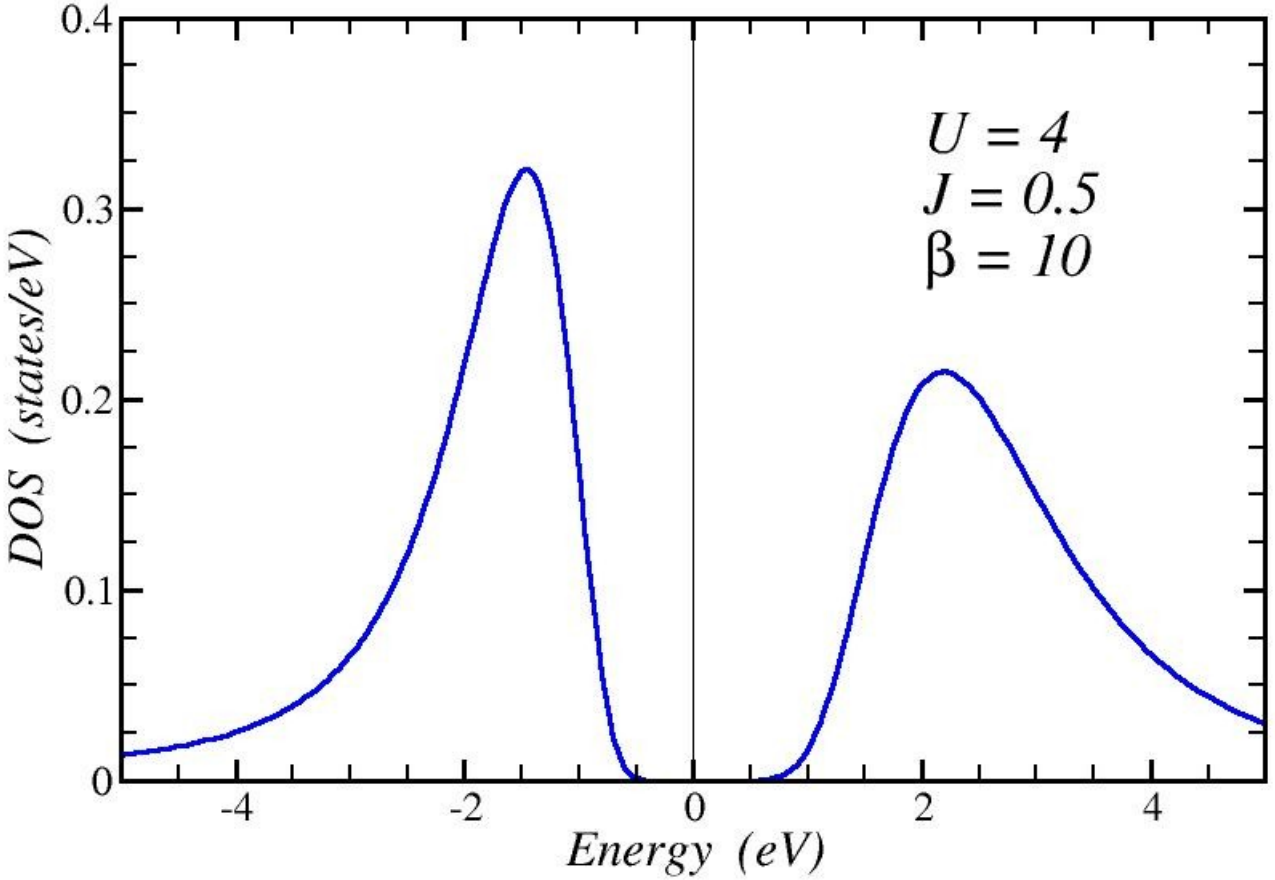
Co atom on Cu substrate

U=4, J=0.9, T~1/40 W

E. Gorelov et al,
Phys. Rev. B **80**, 155132 (2009)



2-orbital DMFT with off-diagonal interaction for e_g states of $LiNiO_2$



Dual-fermion approach for nonlocality of strong correlations

Methodologically, dual-fermion technique is a perturbation expansion on top of the dynamical mean-field theory

For a system with localized nonlinearity

$$S[c,c^*] = -\sum_{i\omega,\sigma}(\mu + i\omega)c^*_{i,\omega,\sigma}c_{i,\omega,\sigma} + U\int_0^\beta n_{i,\uparrow,\tau}n_{i,\downarrow,\tau}d\tau + \sum_{\omega k\sigma}\epsilon_k c^*_{\omega k\sigma}c_{\omega k\sigma}$$

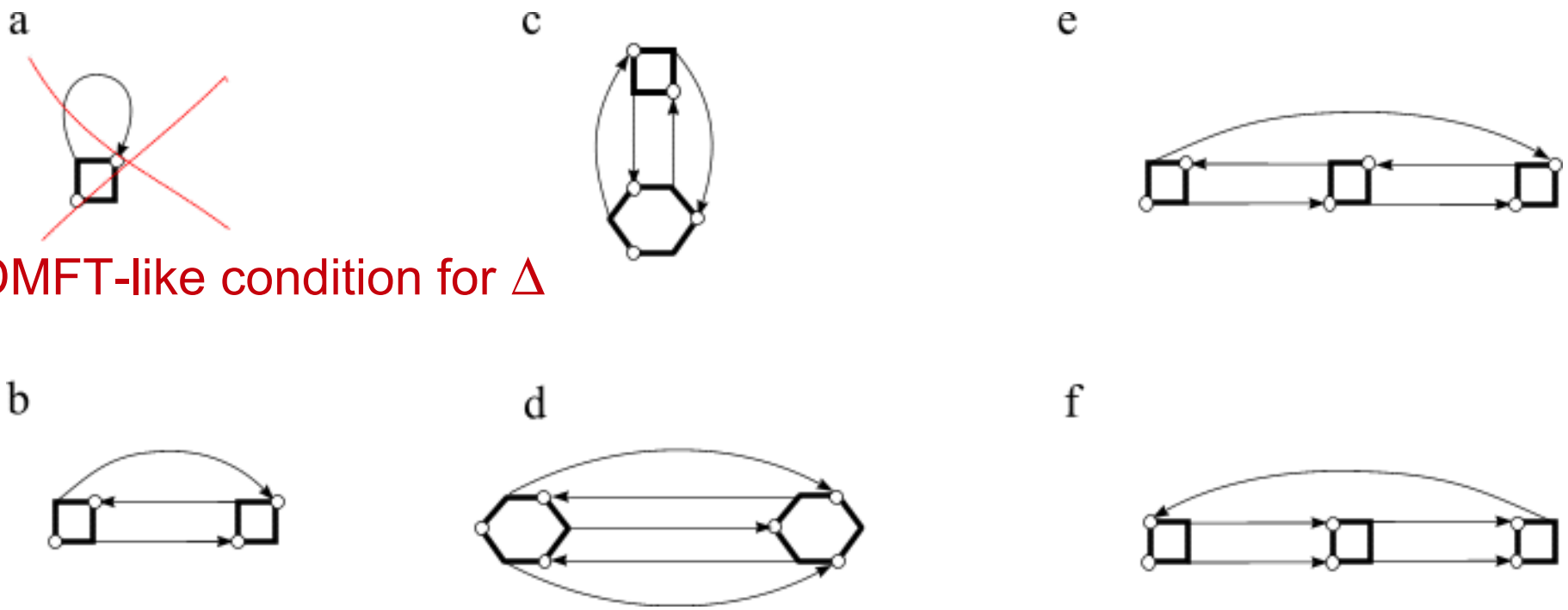
there is an exact mapping to the dual system

$$S[f,f^*] = \sum_{\omega k\sigma} g_\omega^{-2}\left((\Delta_\omega - \epsilon_k)^{-1} + g_\omega\right) f^*_{\omega k\sigma}f_{\omega k\sigma} + \sum_i V_i$$

where *g* is the Green's function of the DMFT-like impurity problem;
Tailor coefficients for V are higher vertex parts of that impurity problem

$$V[f_i,f_i^*] = -\gamma^{(4)}_{1234}f^*_1 f_2 f^*_3 f_4 + \gamma^{(6)}_{123456}f^*_1 f_2 f^*_3 f_4 f^*_5 f_6 + \ldots$$

Low-order diagrams for the dual self energy



DMFT-like condition for Δ

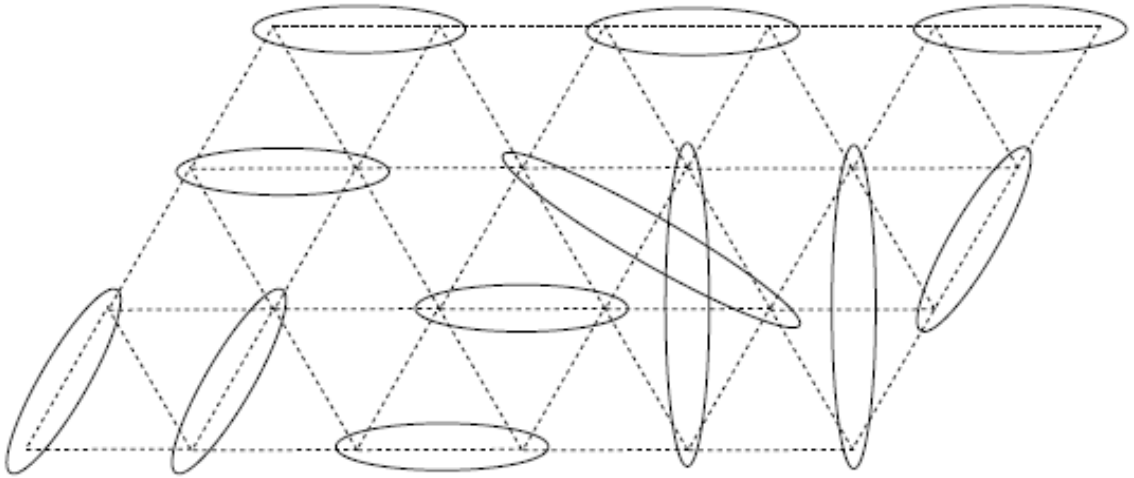
Once the problem is solved in new variables, its easy to return to the initial ones: there is an exact relation between lattice Green's functions

Technically,

dual-fermions is a good couple to CT-QMC,

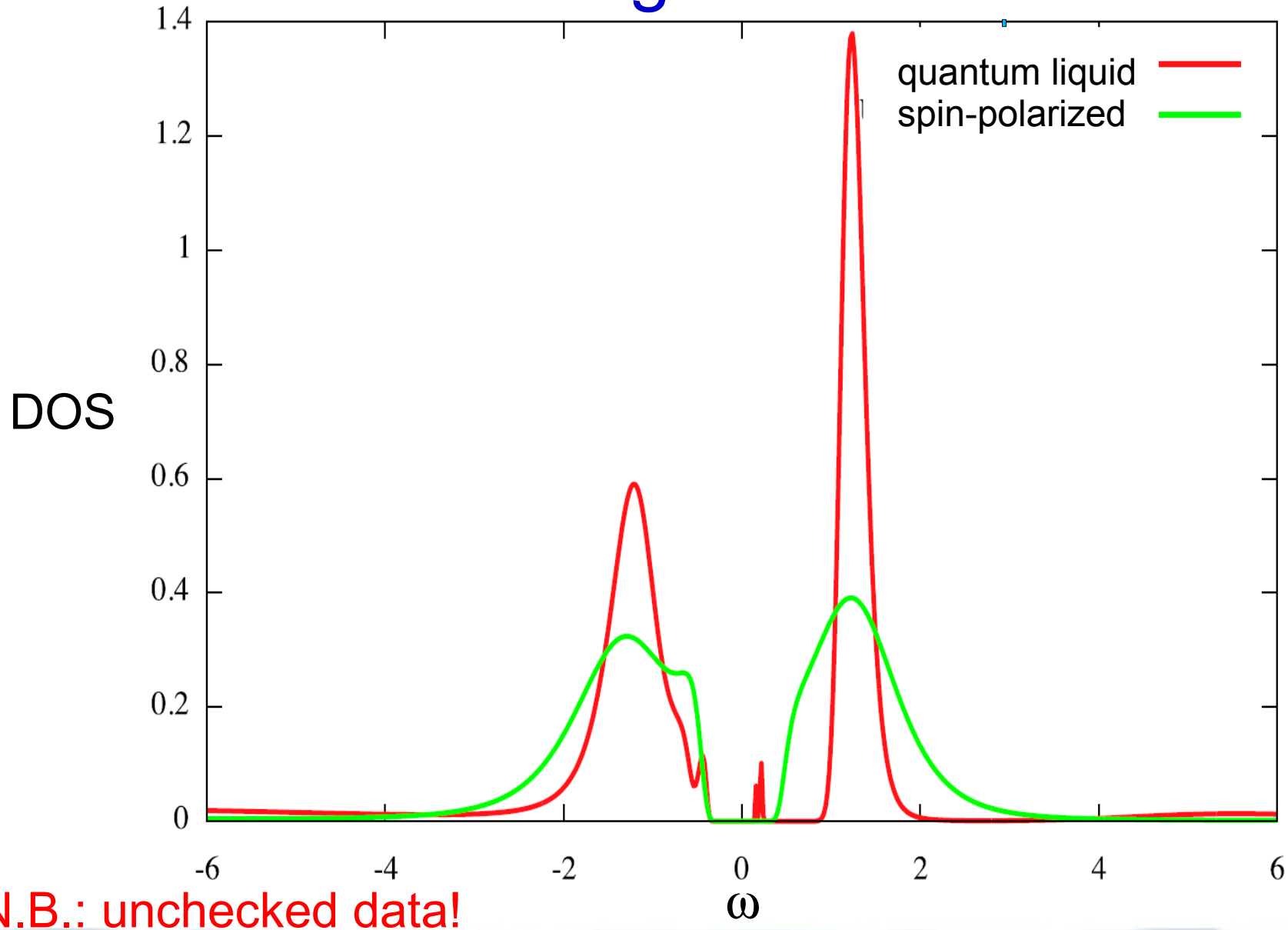
because the diagram calculation requires vertex parts of the impurity problem in Matsubara domain

Quantum liquid of singlets at triangular lattice



Picture from “Quantum spin liquids ” by Gregoire Misguich

Single-electron DOS for Hubbard model at triangular lattice



N.B.: unchecked data!