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Screening in strongly correlated materials

Michele Casula
Centre de Physique Theorique, Ecole Polytechnique, CNRS, 91128 Palaiseau, France

and

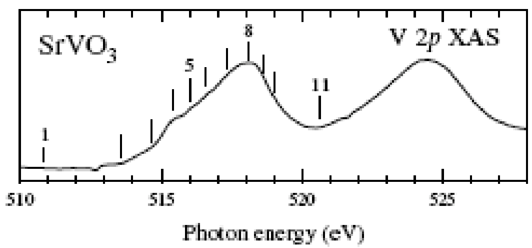
Silke Biermann
Centre de Physique Theorique, Ecole Polytechnique, CNRS, 91128 Palaiseau, France
CREST

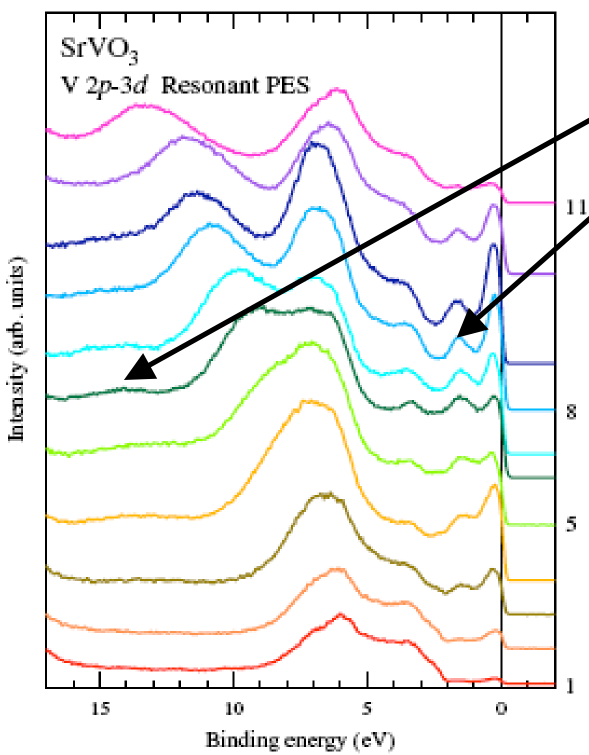
Outline

- Screening effects in correlated compounds
  - Electron Photoemission Spectroscopy
  - RPA screening of Hubbard U
- DMFT impurity solver with on site retarded interaction
- Application to the one-band symmetric dynamic Hubbard model
  - "Phase diagram"
  - Comparison with the static case
- Application to more realistic systems
  - Three-band dynamic Hubbard model for SrVO3
- Conclusions and perspectives

Satellites in electron photoemission spectroscopy

$SrVO_3$ V $2p$-$3d$ Resonant-PES



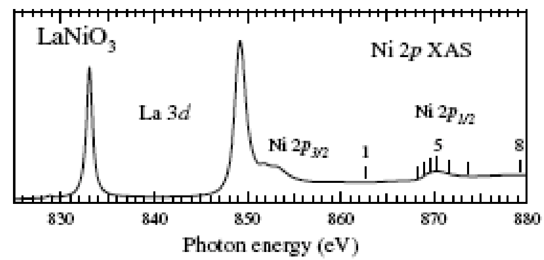


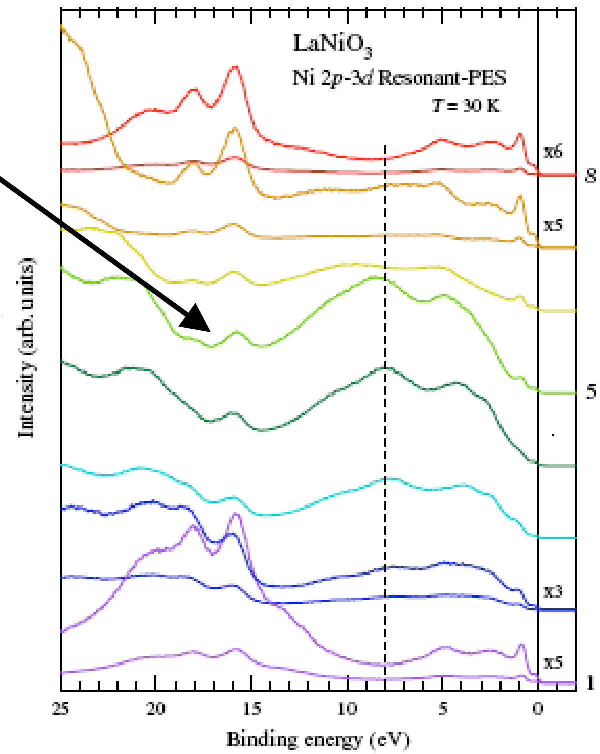
Satellites

- single particle excitations
- many-body correlation effects (i.e. 2-body resonances)
- **plasmon contributions (screening effects)**

Data by Eguchi, Chainani *et al.*

$LaNiO_3$ Ni $2p$-$3d$ Resonant-PES





On site screened repulsion

- Strong correlation related to localized d or f shells
- Multi-band Hubbard model valid to describe d or f electrons around the Fermi level
- Which U?
- Screening coming from the other electrons into the model
- RPA screening:

$$P = P_d + P_r;$$

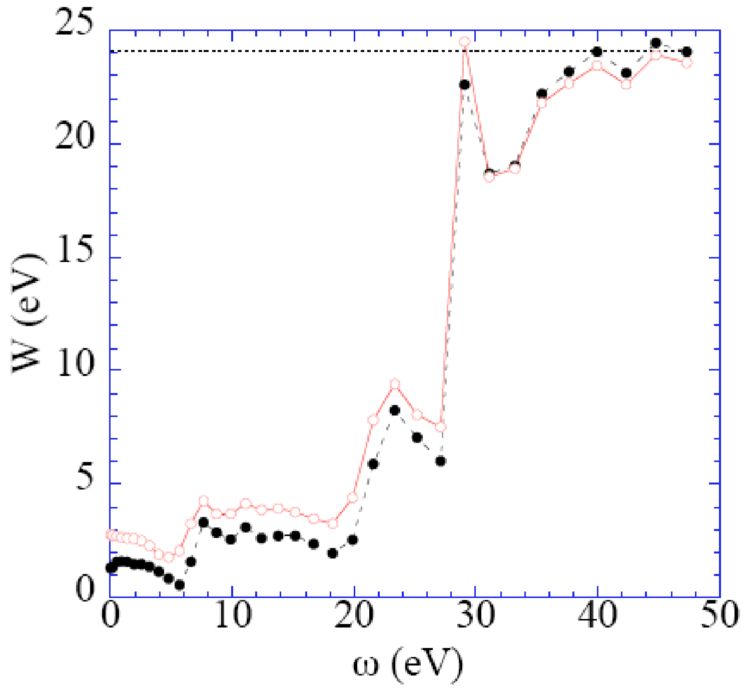
$$\boxed{W_r(\omega) = v[1 - P_r(\omega)v]^{-1}}$$

- Important consequences:

1. **«Strong» frequency dependence** even at low energy scale
2. **Static value very different from the unscreened** (infinite frequency) limit (usually one order of magnitude)
3. Frequency dependence can be mapped into **plasmon bosonic oscillations** (this will lead to the inclusion of plasmon satellites in the model)

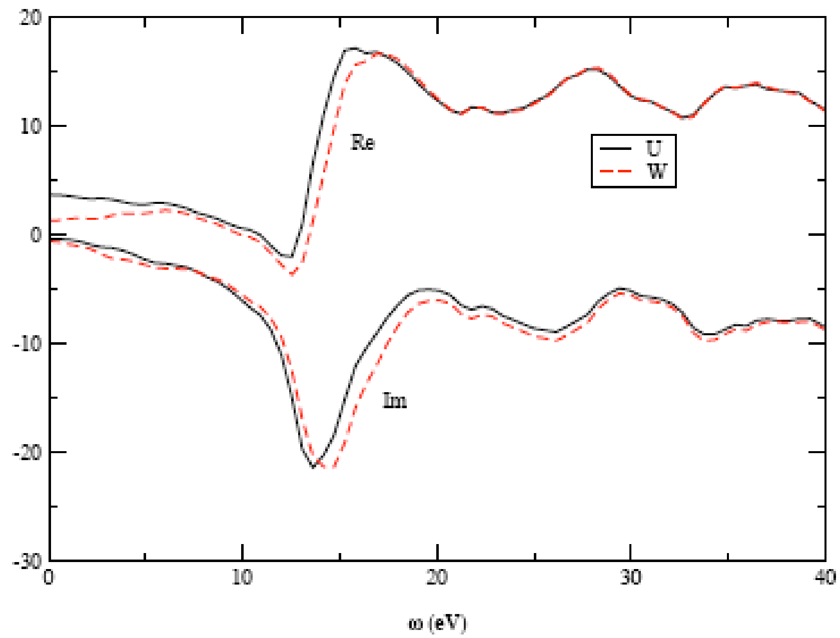
Frequency dependent U

Screening effects lead to an on-site retarded (frequency dependent) interaction in the modelization of strongly correlated systems



cRPA in the maximally localized Wannier functions for paramagnetic Nickel

Miyake and Aryasetiawan (2008)



cRPA in the LMTO functions for SrVO3

Aryasetiawan et al. (2008)

Hubbard-Holstein model

Retardation effects due to screening can be described by a set of bosonic bath of plasmons (Langreth 1970 to describe core-electron photoemission)

Density fluctuations responsible for screening described as bosonic modes

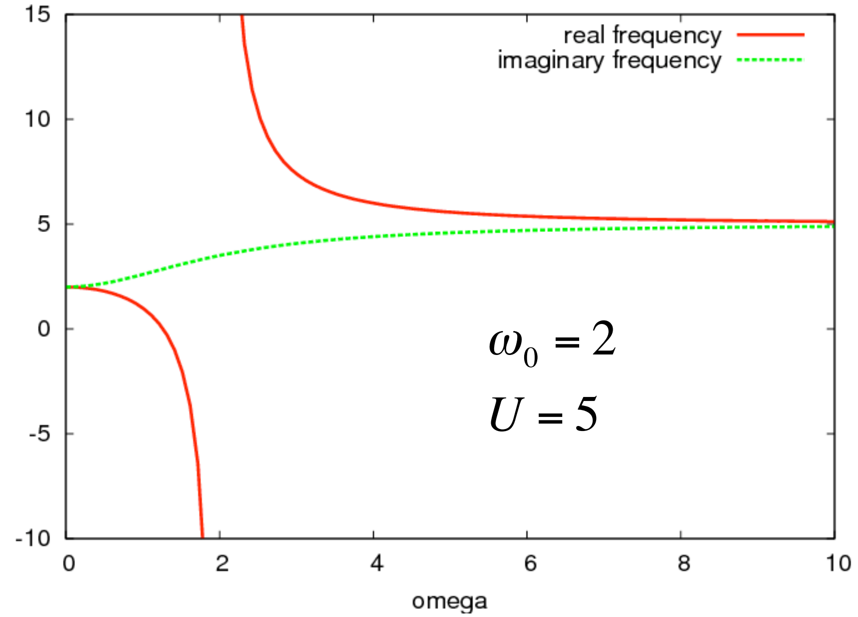
Simplest model: single mode approximation (Holstein model)

$$H = \sum_{\vec{k}\sigma} \epsilon(\vec{k}) c^{\dagger}_{\vec{k}\sigma} c_{\vec{k}\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \omega_0 \sum_i b_i^{\dagger} b_i$$

$$+ g \sum_i (b_i^{\dagger} + b_i)(n_{i\uparrow} + n_{i\downarrow} - 1).$$

Retarded interaction after integration of bosons

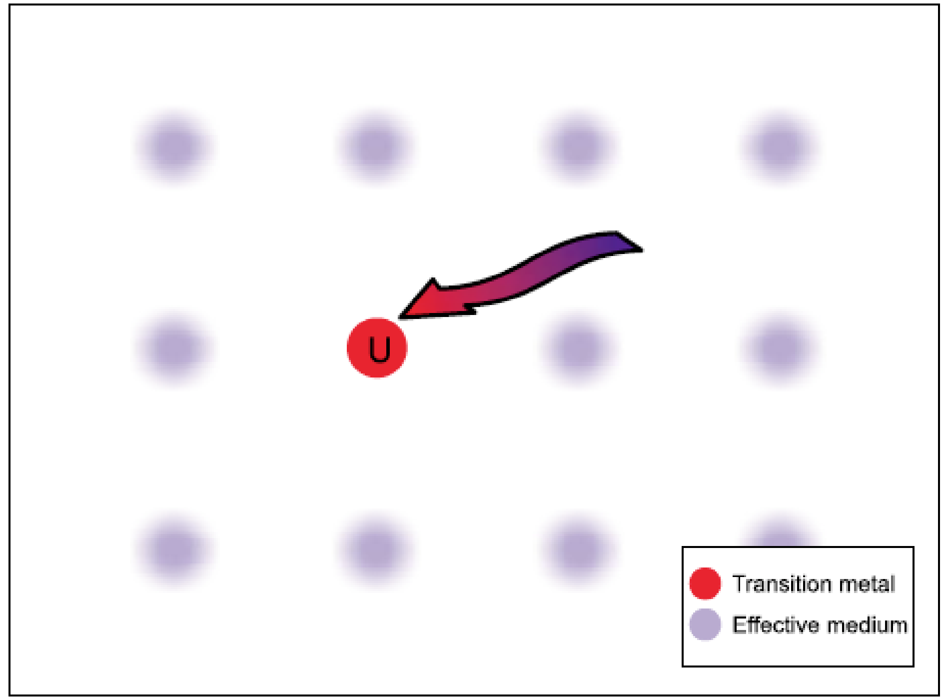
$$U_{\rm eff}(\omega) = U + \frac{2\, g^2\, \omega_0}{\omega^2 - \omega_0^2}.$$



Dynamical mean field approach

DMFT maps the full lattice problem into a single site hamiltonian hybridized with a self-consistent bath

Quantum effects from non locality in imaginary time!
The method could include screening as dynamical effect



Hubbard-Holstein mapped into
an *Anderson-Holstein impurity model*:
How to solve such an impurity problem? (quite difficult task)

Impurity atomic limit (hybridization Δ=0) ansatz

$$S = \int_0^\beta d\tau \int_0^\beta d\tau' \sum_l c_l^+ \tilde{G}_0^{-1}(\tau'-\tau) c_l + \frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau' U(\tau'-\tau) \sum_l n_l(\tau) \sum_{l'} n_{l'}(\tau')$$

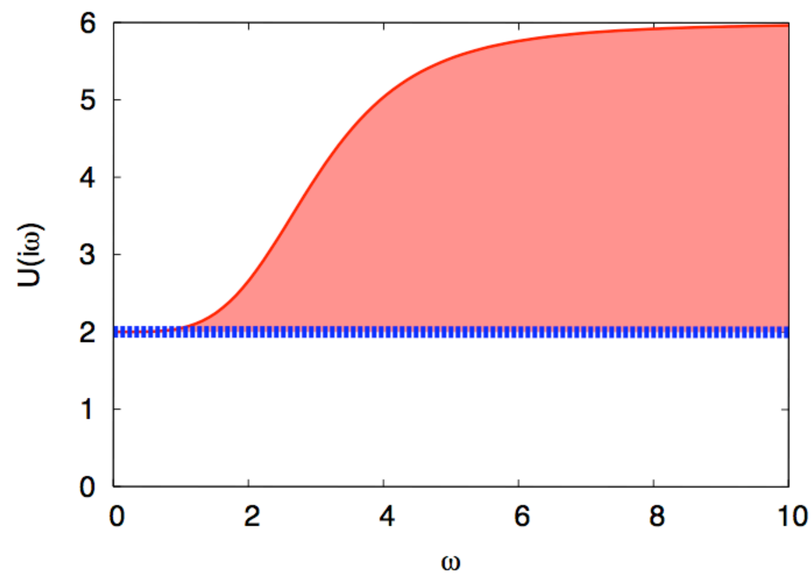
In the atomic limit the action can be worked out analytically (Florens PhD thesis):

$$G_{\mathrm{at}}(\tau) = \underbrace{G_0(\tau)}_{\text{Static part}} \underbrace{e^{F(\tau)}}_{\text{Dynamic part}},$$

Static part depends only on U(0)

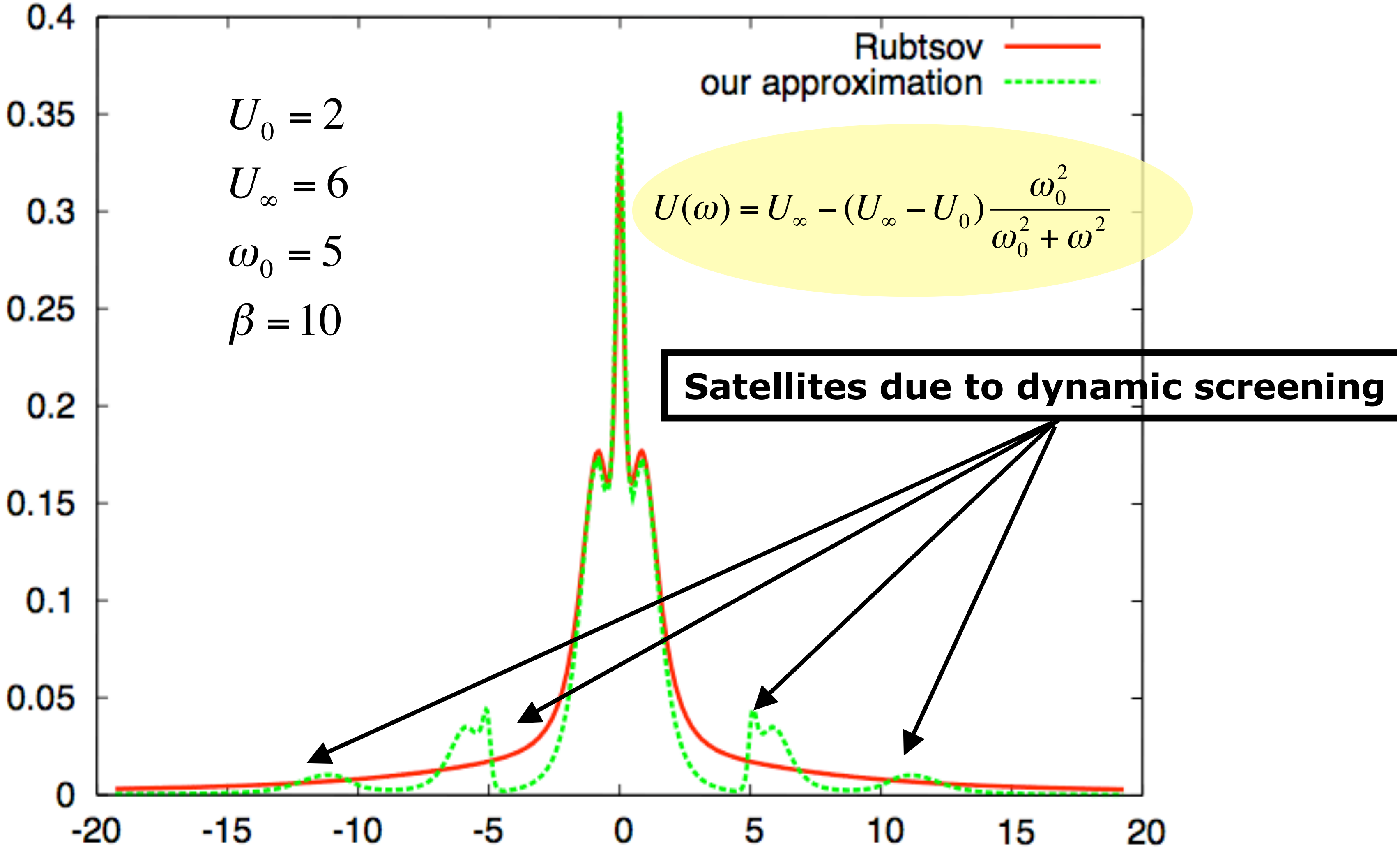
Dynamic part depends on U(i omega)-U(0)

$$F(\tau) = \frac{1}{\beta}\sum_n \frac{U(i\nu_n) - U_0}{\nu_n^2}\left(e^{i\nu_n \tau} - 1\right)$$



This factorizations is **exact** in the atomic limit even **away from half filling** and in the **multiband case**, provided the interaction is a density-density coupling

Benchmark against Rubtsov method



One band symmetric dynamic model

$$U(\omega) = U_\infty - (U_\infty - U_0)\frac{\omega_0^2}{\omega_0^2 + \omega^2}$$

$\beta = 40$ static $U_{c2} \approx 2.5$

=paramagnetic metal

=Mott insulator

$U_0 = 0$

U_∞ \ ω_0	2	5	10	20
5				
10				
20				

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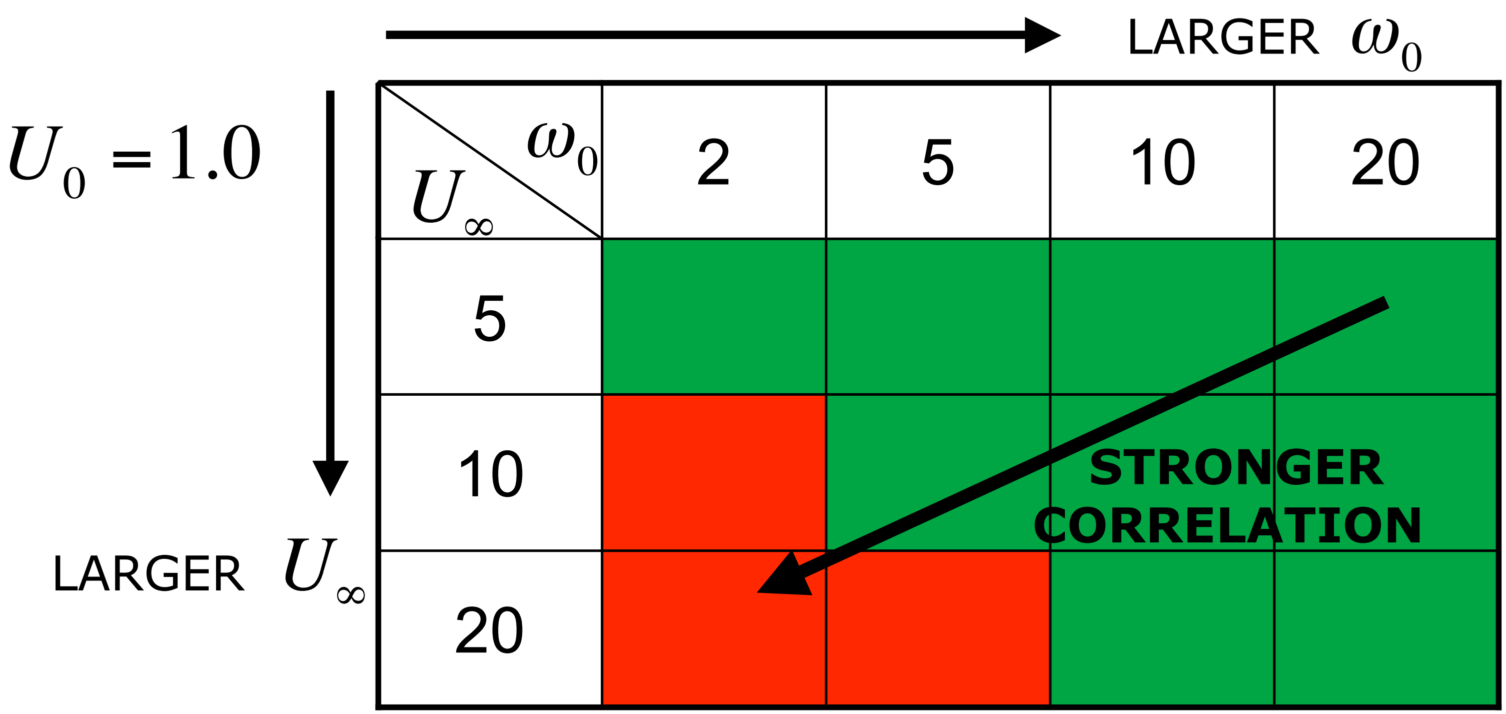
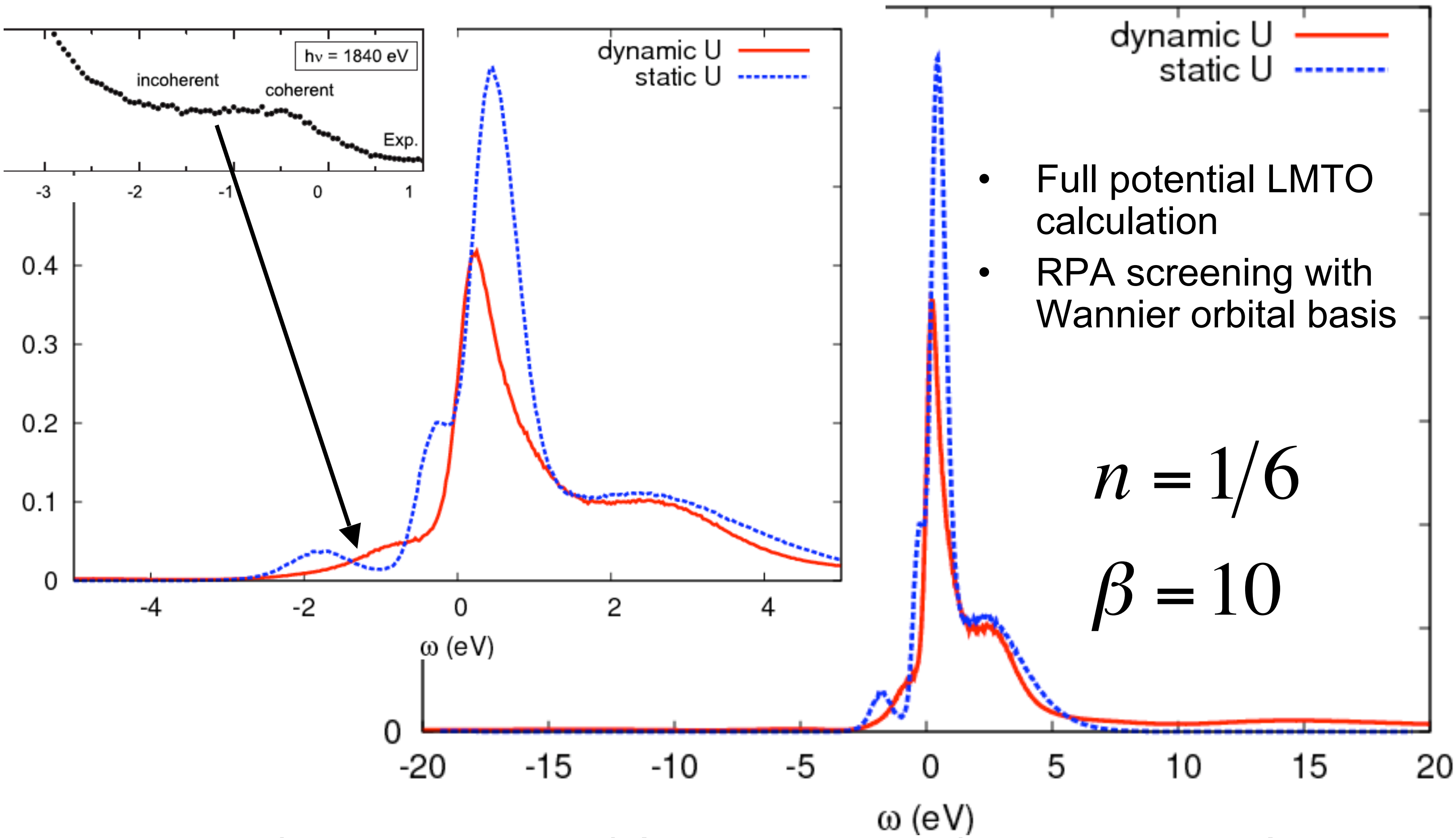


SrVO3 spectral function



- Full potential LMTO calculation
- RPA screening with Wannier orbital basis

$$n = 1/6$$

$$\beta = 10$$

Static model less correlated (static Z=0.64, dynamic Z=0.35)
Broader lower « hubbard » band, due to Oxygen 2p screening
Broad spectral way transfer to higher energies (small satellites)

Conclusions and perspectives

• We developed an approximate solver:

It allows to deal with a generic retarded interaction

Satellites due to screening are described accurately in the spectral function

The approximation is better in the regime interesting for electronic structure calculations (quite high frequency of plasmons, large unscreened interaction)

• **Importance of the dynamic effects on the low energy properties**

• Possible applications beyond the LDA+DMFT framework (in fact it is an essential step toward GW+DMFT)

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