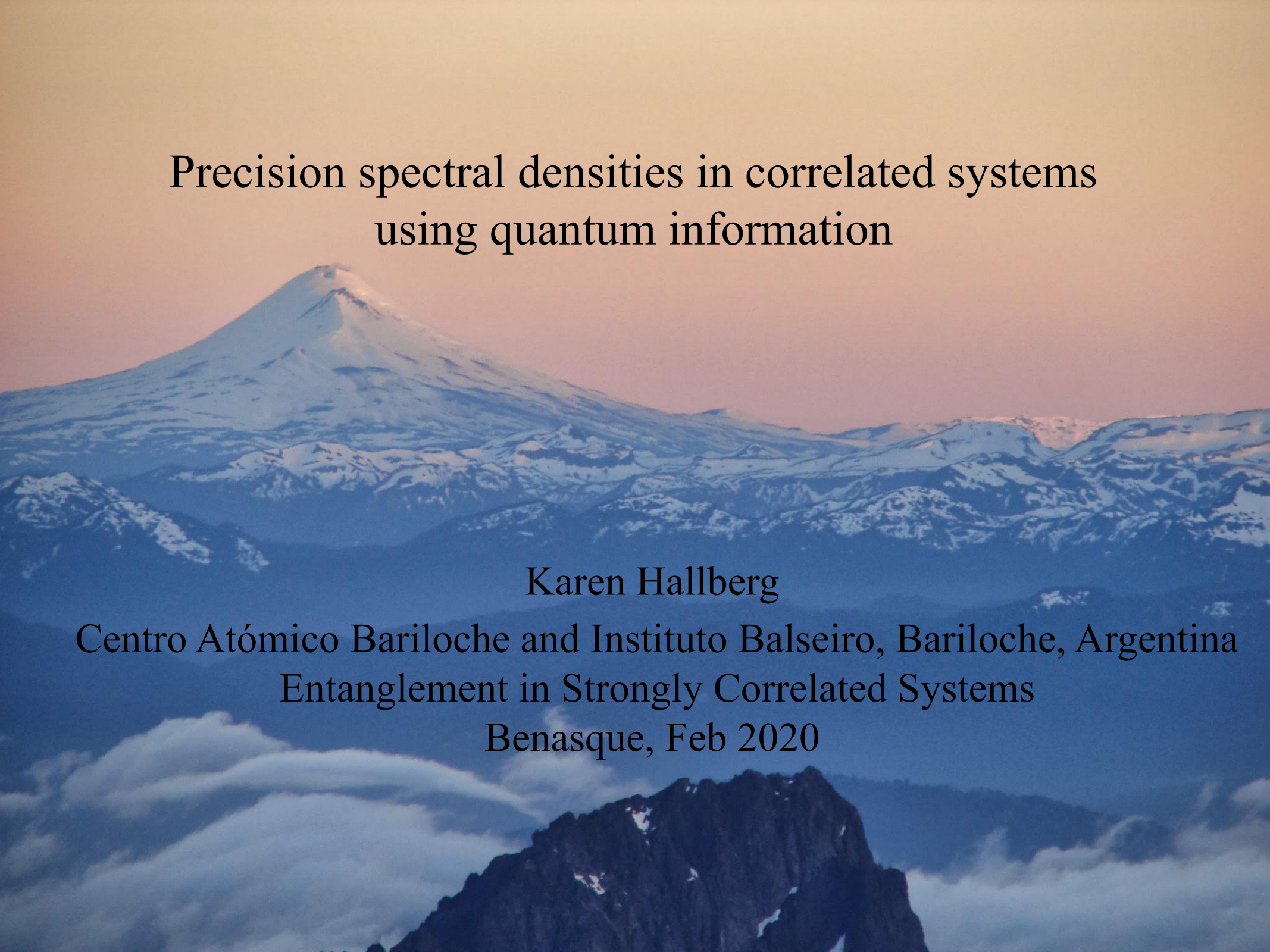
Precision spectral densities in correlated systems using quantum information



Karen Hallberg
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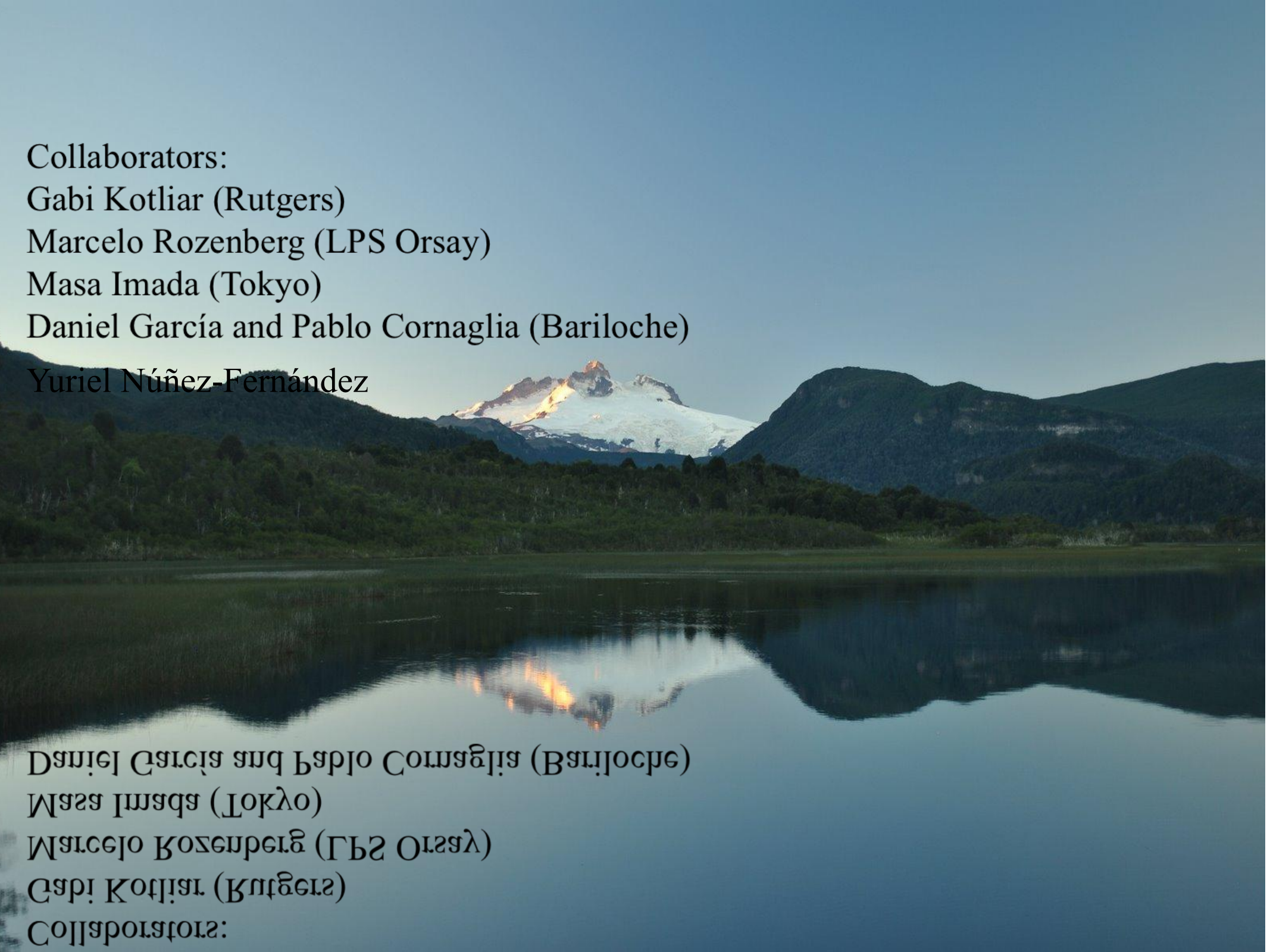
Entanglement in Strongly Correlated Systems
Benasque, Feb 2020

Bariloche, Argentina



Collaborators:
Gabi Kotliar (Rutgers)
Marcelo Rozenberg (LPS Orsay)
Masa Imada (Tokyo)
Daniel García and Pablo Cornaglia (Bariloche)

Yuriel Núñez-Fernández

Motivation:

Great interest in interacting models with several bands.
In particular, where localized and itinerant electrons coexist:
- Iron-based superconductors
- TMO: Ruthenates ($Ca_{2-x}\ Sr_xRuO_4$), Manganites ($La_{1-x}\ Sr_x\ MnO_3$), VO_2
- ^{3}He bilayers
- 4f and 5f rare earth heavy fermion materials $CeRhIn_5$, $CeCu_{6x}\ Au_x$, $YbRh_2Si_2$
- U compounds

... which can give rise to **in-gap states** and an **Orbital Selective Mott Transition (OSMT).**

Causes:
-Orbitals with different bandwidths
-Large crystal field splitting
-Different orbital degeneracy

Two-orbital Kanamori-Hubbard model

$$H = t_p \sum_{i\alpha} a^\dagger_{i\alpha} a_{i\bar{\alpha}} - \mu \sum_i n_i + \sum_{\langle ij\rangle \alpha\beta} t^{\alpha\beta} a^\dagger_{i\alpha} a_{j\beta} + \sum_i \hat{V}_i$$

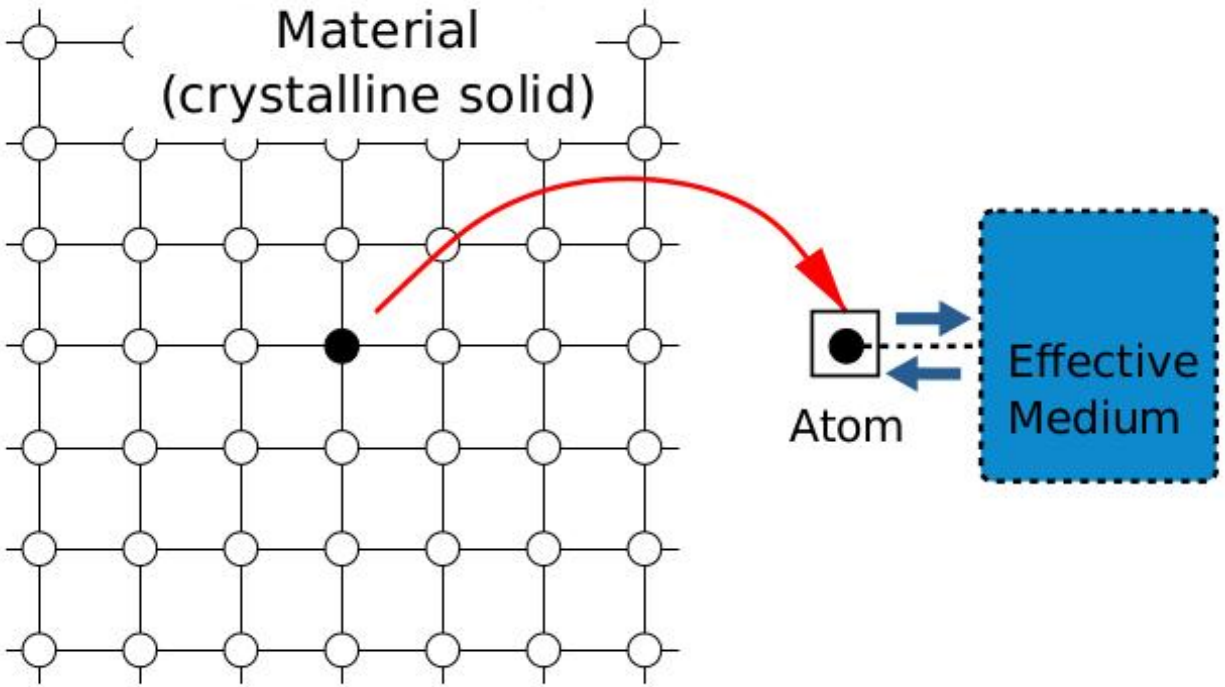
$$T = (t^{\alpha\beta}) = \begin{pmatrix} t_1 & 0 \\ 0 & t_2 \end{pmatrix}$$

$$\hat{V}_i = U \sum_\alpha n_{i\alpha\uparrow} n_{i\alpha\downarrow} + \sum_{\sigma\sigma'} \left(U_2 - J\delta_{\sigma\sigma'}\right) n_{i1\sigma} n_{i2\sigma'} -$$
$$- J \left(a^\dagger_{i1\uparrow} a_{i1\downarrow} a^\dagger_{i2\downarrow} a_{j2\uparrow} + a^\dagger_{i1\uparrow} a_{i1\downarrow} a^\dagger_{i2\downarrow} a_{j2\uparrow} \right)$$
$$- J \left(a^\dagger_{i1\uparrow} a^\dagger_{i1\downarrow} a_{j2\uparrow} a_{i2\downarrow} + a^\dagger_{i2\uparrow} a^\dagger_{i2\downarrow} a_{j1\uparrow} a_{i1\downarrow} \right)$$

rotational invariant case: U_2=U-2J and J>0 (FM)

- Emergent low-energy bound states in the two-orbital Hubbard model,
Y. Núñez- Fernández, G. Kotliar, and K. Hallberg, Phys. Rev. B 97, 121113(R) (2018)
- Renormalized dispersing multiplets in the spectrum of nearly Mott localized systems,
Y. Komijani, K. Hallberg and G Kotliar, PRB (2019)

Dynamical Mean Field Theory (DMFT)



Infinite dimensions

⇓

Local self-energy

⇓

$$\Sigma_{ij}(\omega) \approx \Sigma(\omega)\delta_{ij}$$

Georges, A., Kotliar, G., Krauth, W., Rozenberg, M. Rev. Mod. Phys. 68 , 13125 (1996)

How DMFT works:

i) Set $\Sigma(\omega) = 0$

ii) Obtain $G(\omega) = \frac{1}{N}\sum_{k}\left[\omega - t(\mathbf{k}) - \Sigma(\omega)\right]^{-1} = G_0\left(\omega - \Sigma(\omega)\right)$

iii) Calculate the hybridization $\Gamma(\omega) = \omega + \mu - \Sigma(\omega) - \left[G(\omega)\right]^{-1}$

iv) Fit the hybridization to define a Hamiltonian $\Gamma_d(\omega) = \sum_i \frac{v_i^2}{\omega - \lambda_i}$

v) Calculate $G_{imp}(\omega)$ ← Impurity solver, e.g. DMRG

vi) Obtain $\Sigma(\omega) = \omega + \mu - \left[G_{imp}(\omega)\right]^{-1} - \Gamma_d(\omega)$

vii) Go to ii)

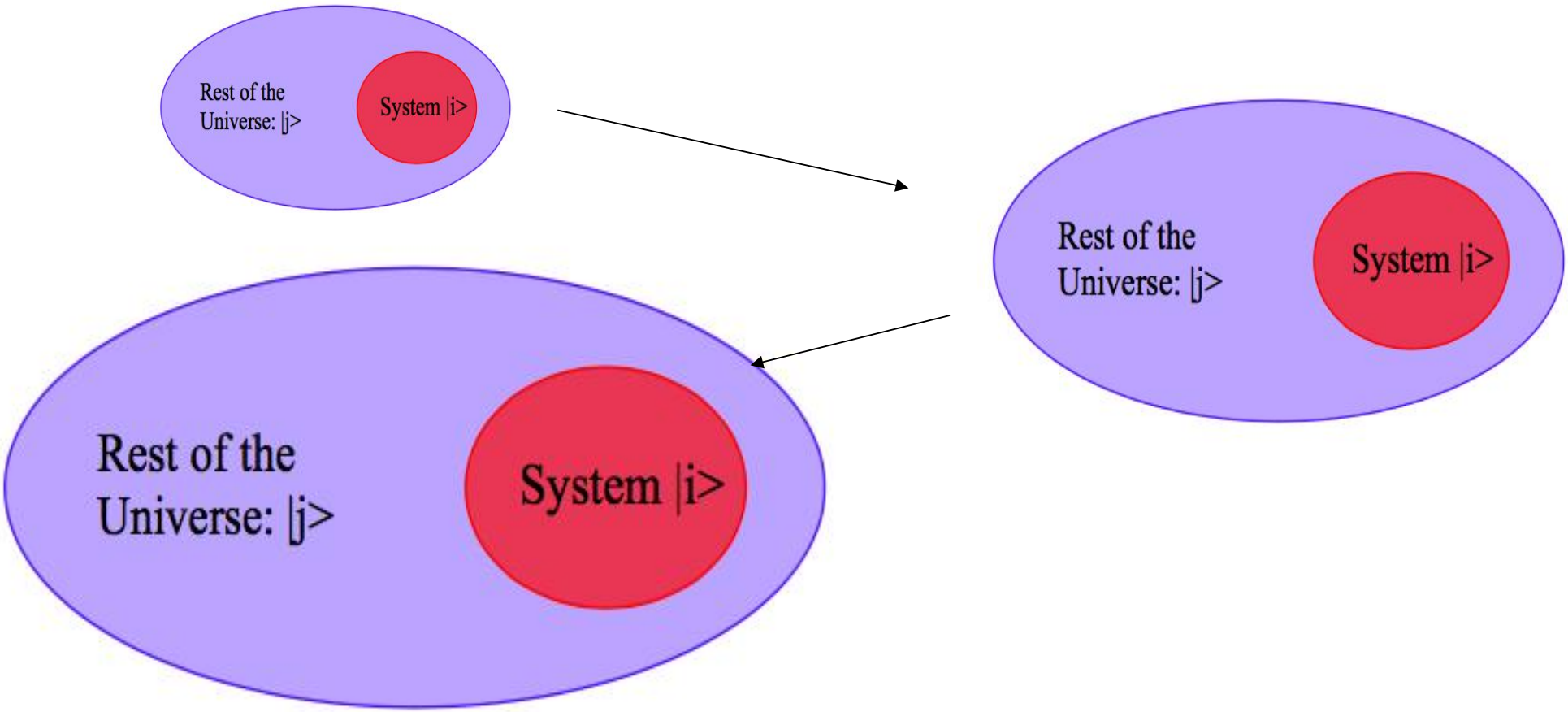
DMFT Impurity solvers:

- **IPT** (Georges A. and Kotliar G., Phys. Rev. B 1992)
- **ED** (Caffarel M. and Krauth W., Phys. Rev. Lett. 1994)
- **HFQMC** (Zhang X. Y., Rozenberg M. J., Kotliar G., Phys. Rev. B 1993)
- **NCA** (Pruschke T., Cox D. L. and Jarrell M., Phys. Rev. Lett. 1993)
- **NRG** (Bulla R., Costi T. and Vollhardt D., Phys. Rev. B, 2001)

More recently:

- **DMRG** (Garcia, Hallberg, Rozenberg, PRL. 2004, PRB(RC) 2005;
Y. Núñez-Fernández and K. Hallberg, Front. Phys. 6:13 (2018);
Karski, Raas, Uhrig, 2005, F. Wolf, I. McCulloch and U. Schollwoeck 2014)
- **CTQMC** (review: Gull E., et al, Rev. Mod. Phys. 2011)
- **FLEX** (Kotliar et al, J. Phys.: Cond. Matt. 2004)
- **TEBD** for dynamics: Verstraete et al, PRB 2014
- **CI** techniques (Zgid et al, 2011, 2012)
- and several other methods...

We use the Density Matrix Renormalisation Group (S. White 1992):
- it uses **quantum information** to keep the **most relevant quantum states**



- Text book: I. Peschel, X. Wang, M. Kaulke, and K. Hallberg (Eds.), *Density-Matrix Renormalization: A New Numerical Method in Physics*, in the Serie *Lecture Notes in Physics* , Springer, Berlin, 1999.
- K. Hallberg, Advances in Physics **55**, pp 477 (2006).
- U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005)

"The most challenging and interesting problems in quantum dynamics involve understanding the behaviour of strongly-coupled many-body systems… Better ways of characterizing the features of many particle entanglement may lead to new and more effective methods for understanding the dynamical behaviour of complex quantum systems." John Preskill (2000)

(Gaite 2001, 2003; Latorre et al. 2003, Osborn et al. 2001...)

Recalling how DMFT works:

i) Set $\Sigma(\omega) = 0$

ii) Obtain $G(\omega) = \frac{1}{N}\sum_{k}[\omega - t(\mathbf{k}) - \Sigma(G(\omega) = G_0\,(\omega - \Sigma(\omega))$

iii) Calculate the hybridization $\Gamma(\omega) = \omega + \mu - \Sigma(\omega) - [G(\omega)]^{-1}$

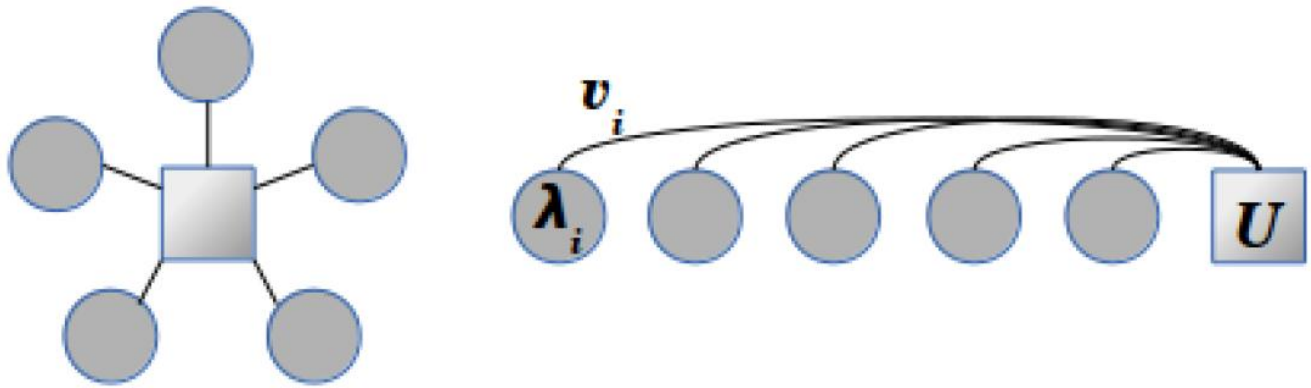
iv) Fit the hybridization to define a Hamiltonian $\Gamma_d(\omega) = \sum_i \frac{v_i^2}{\omega - \lambda_i}$

v) Calculate $G_{imp}(\omega)$ ← Impurity solver, e.g. DMRG

vi) Obtain $\Sigma(\omega) = \omega + \mu - [G_{imp}(\omega)]^{-1} - \Gamma_d(\omega)$

vii) Go to ii)

Cluster DMFT+DMRG in the star geometry

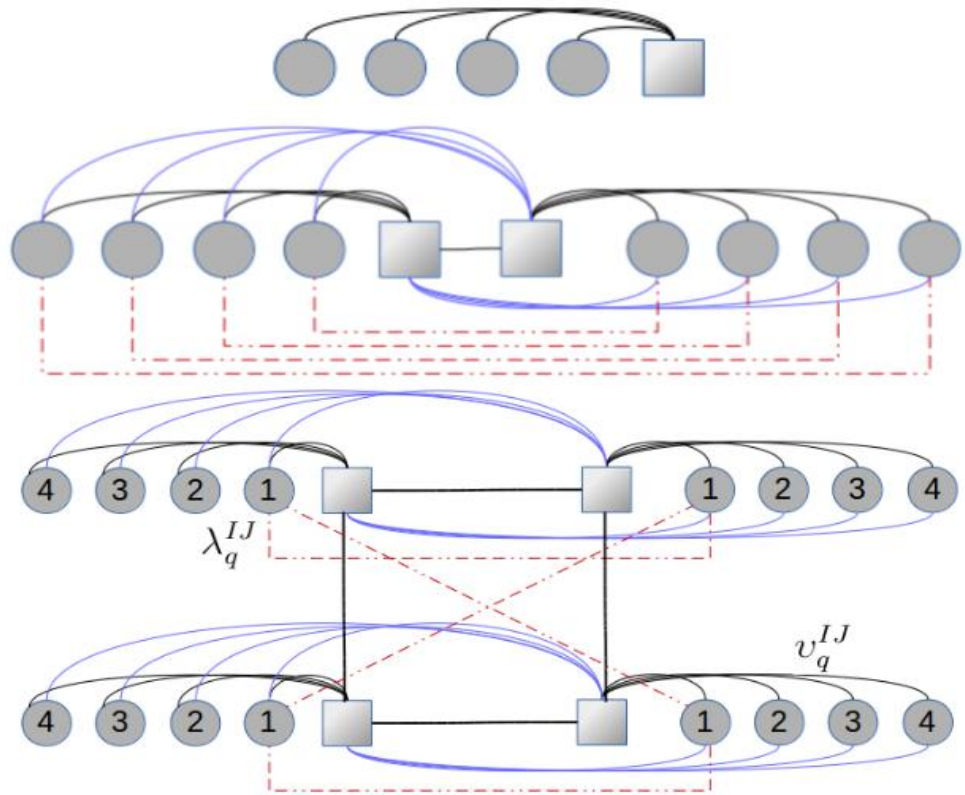


$$H_{imp} = H_{loc} + H_b$$

$$H_b = \sum_{i\sigma} \lambda_i b^\dagger_{i\sigma} b_{i\sigma} + \sum_{i\sigma} v_i \left[b^\dagger_{i\sigma} c_{0\sigma} + H.c. \right]$$

$$\Gamma_d(\omega) = \sum_i \frac{v_i^2}{\omega - \lambda_i}$$

Complex “impurity” (multi-site, multi-band)



$$H_{imp} = \hat{h}_0^0 + \hat{V}_0 + H_b$$

$$H_b = \sum_{IJq\sigma} \lambda_q^{IJ} b_{Iq\sigma}^\dagger b_{Jq\sigma} + \sum_{IJq} v_q^{IJ} \left[b_{Iq\sigma}^\dagger c_{0J\sigma} + H.c. \right]$$

We want to calculate the following dynamical correlation function:

$$C_A(t\text{-}t') = \langle \psi_0 | A^\dagger(t) A(t') | \psi_0 \rangle$$

Fourier transforming:

$$C_A(\omega) = \sum_n |\langle \psi_n | A | \psi_0 \rangle|^2 \, \delta(\omega - (E_n - E_0))$$

$$G_A(\omega + i\,\eta) = \langle 0 | A^\dagger \frac{1}{E_0 + \omega + i\,\eta - H} A | 0 \rangle \qquad C_A(\omega) = -\frac{1}{\pi} \lim_{\eta \to 0^+} \mathcal{Im}\; G_A(\omega + i\,\eta)$$

Obtained either with:

- Lanczos dynamics (K. Hallberg, PRB 52, 9827, 1995)
- Correction vector dynamics (Ramasesha et al., 1989 & succ.; Kühner and White, 1999; Jeckelmann, 2002)

Advantages of using DMRG as the impurity solver:

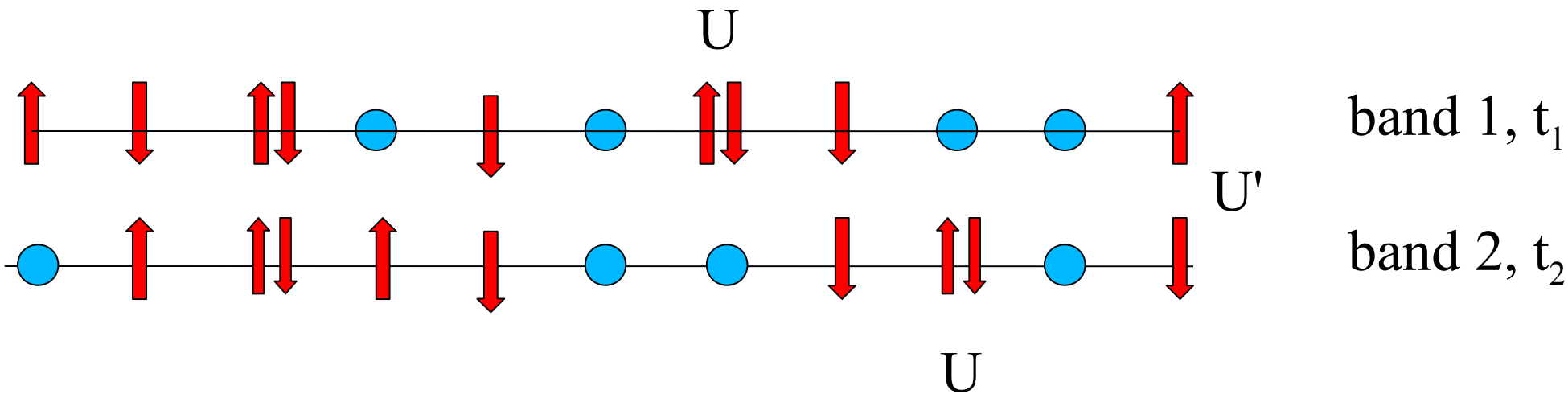
Real ω axis
All ω scales
Arbitrary interactions
No sign problem
Large baths
Several orbitals
Several sites (k-dependence)
Finite T (?)

- García, Hallberg, Rozenberg, PRL 2004
- García, Miranda, Hallberg, Rozenberg, PRB(RC) 2007
- F. Wolf, I. McCulloch and U. Schollwoeck, Phys. Rev. B 2014
- Hallberg, García, Cornaglia, Facio, Núñez Fernández, EPL Perspectives 2015
- Y. Núñez-Fernández and K. Hallberg, *Front. Phys. 6:13 (2018): Solving the multi-site and multi-orbital Dynamical Mean Field Theory using DMRG*

Two band Hubbard model (finite U_{12}, even with J=0):

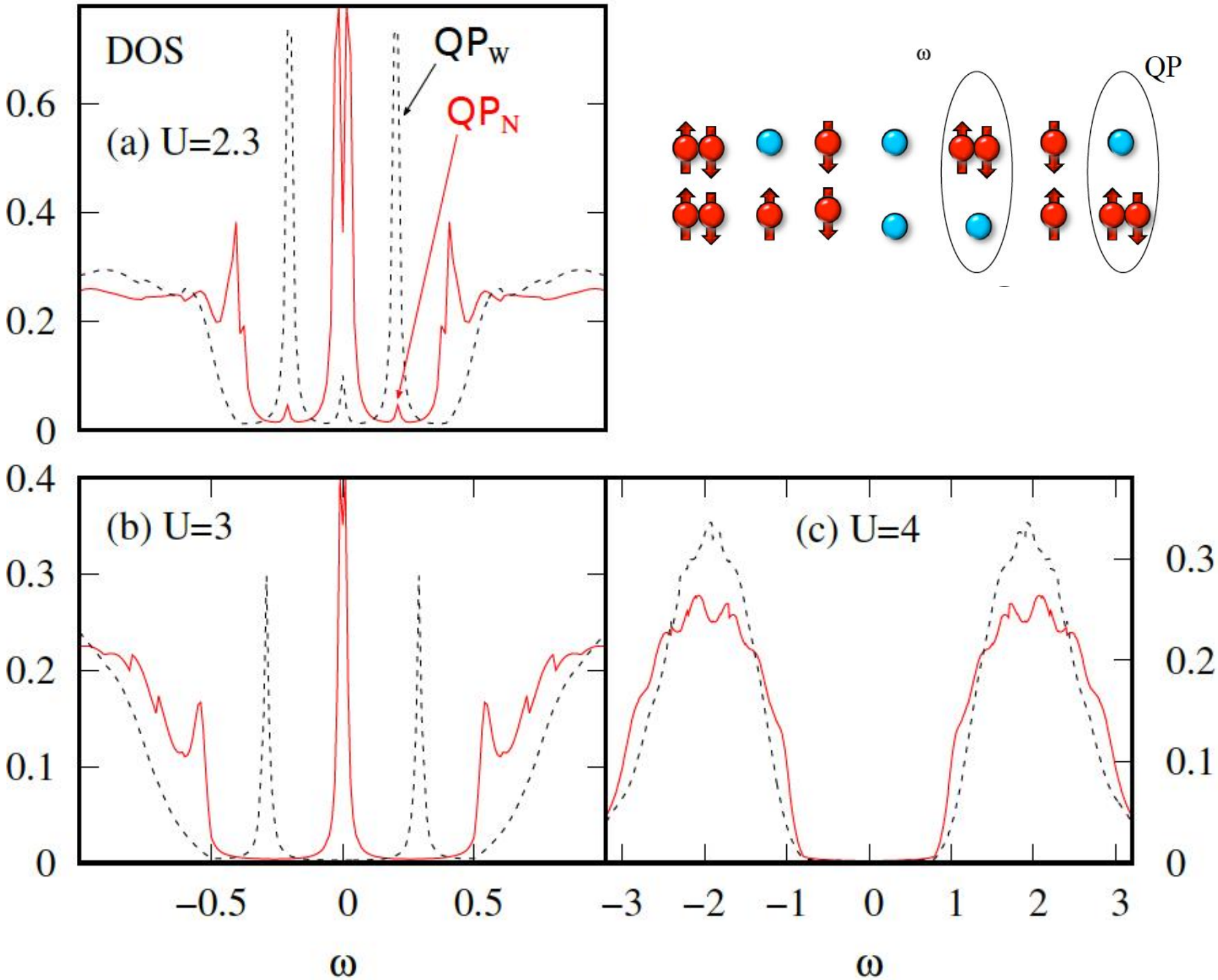
$$H = \sum_{\langle ij\rangle\alpha\sigma} t_\alpha c^\dagger_{i\alpha\sigma} c_{j\alpha\sigma} +$$

$$+ U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + \sum_{i\sigma\sigma'} \text{U'}\, n_{i1\sigma} n_{i2\sigma'}$$



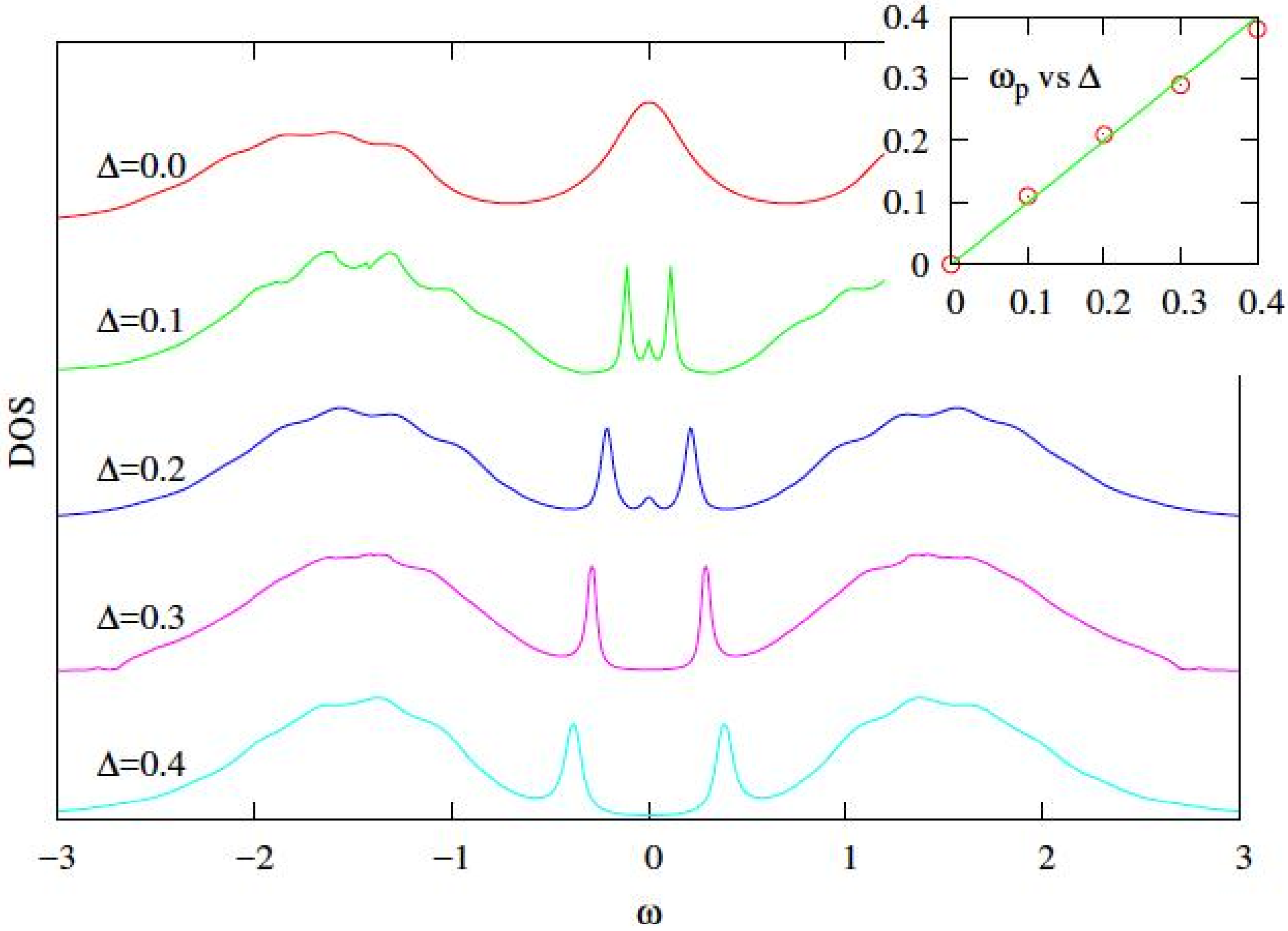
Half-filled and doped T=0 t'=0 $t_1 \geq t_2$ $U' \leq U$ $\Delta = U - U'$

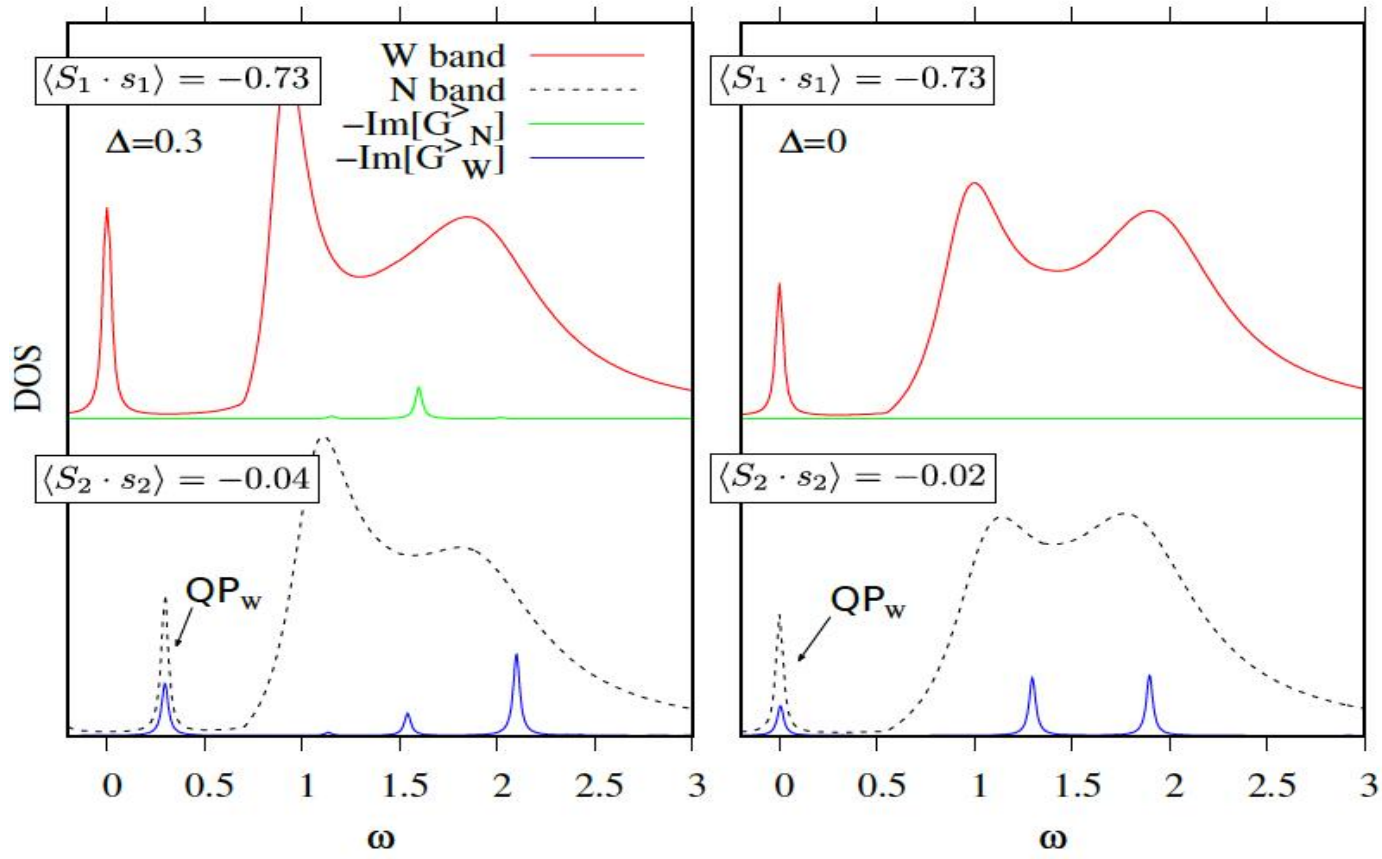
square lattice (2D)


DOS
(a) U=2.3
QP_W
QP_N
0.6
0.4
0.2
0
ω
QP
(b) U=3
(c) U=4
0.4
0.3
0.2
0.1
0
0.3
0.2
0.1
0
−0.5
0
0.5
−3
−2
−1
0
1
2
3
ω
ω

Δ=U-U'

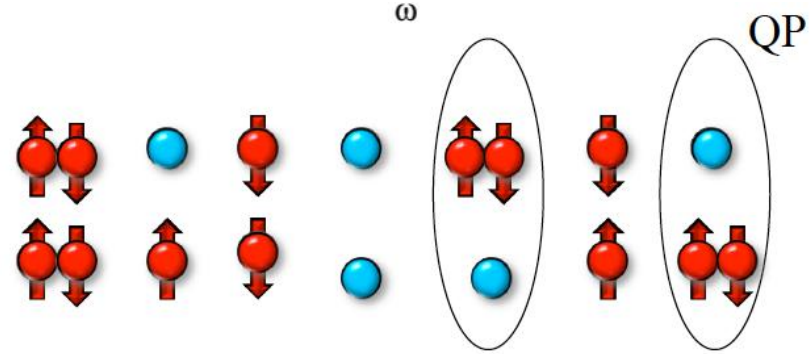
Band 2





$$a_W^\dagger = (1 - n_{1\uparrow})(1 - n_{1\downarrow}) n_{2\downarrow} c_{2\uparrow}^\dagger$$

We found new quasiparticles!



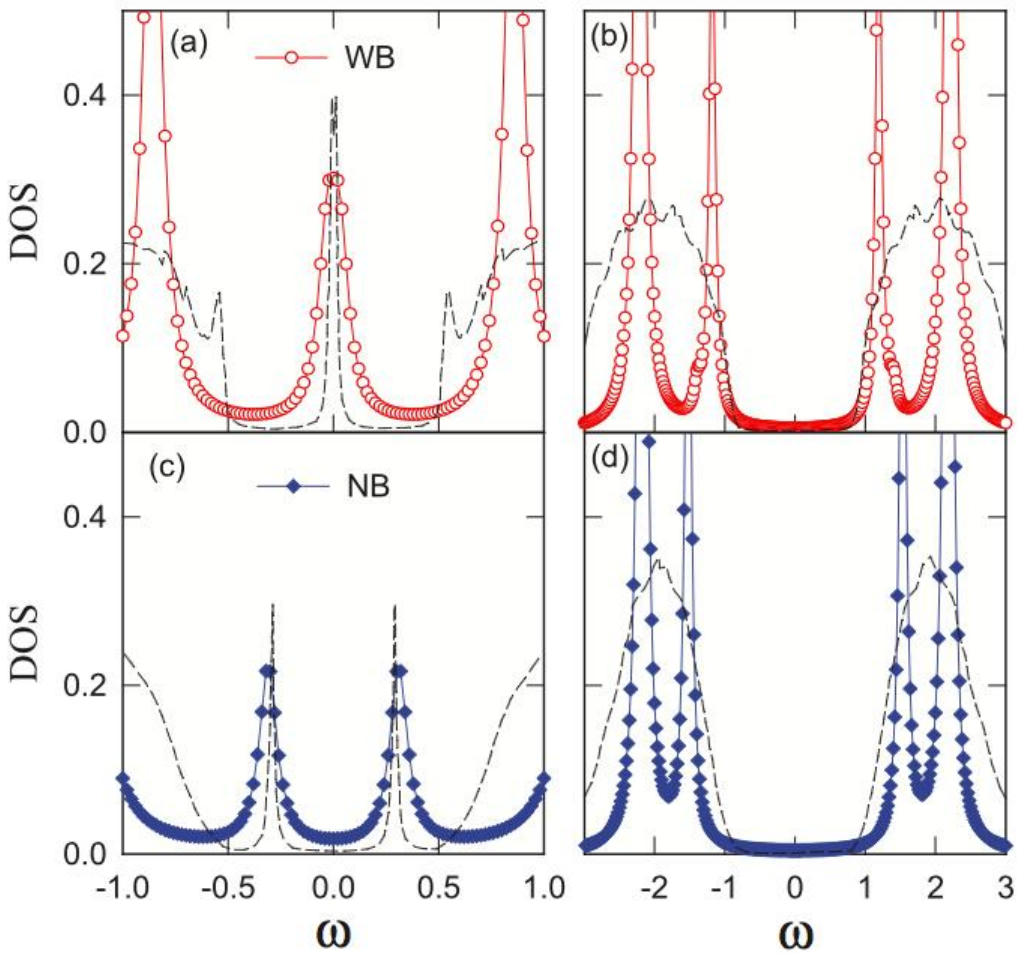
Núñez-Fernández, Kotliar, Hallberg, PRB(R) 2018

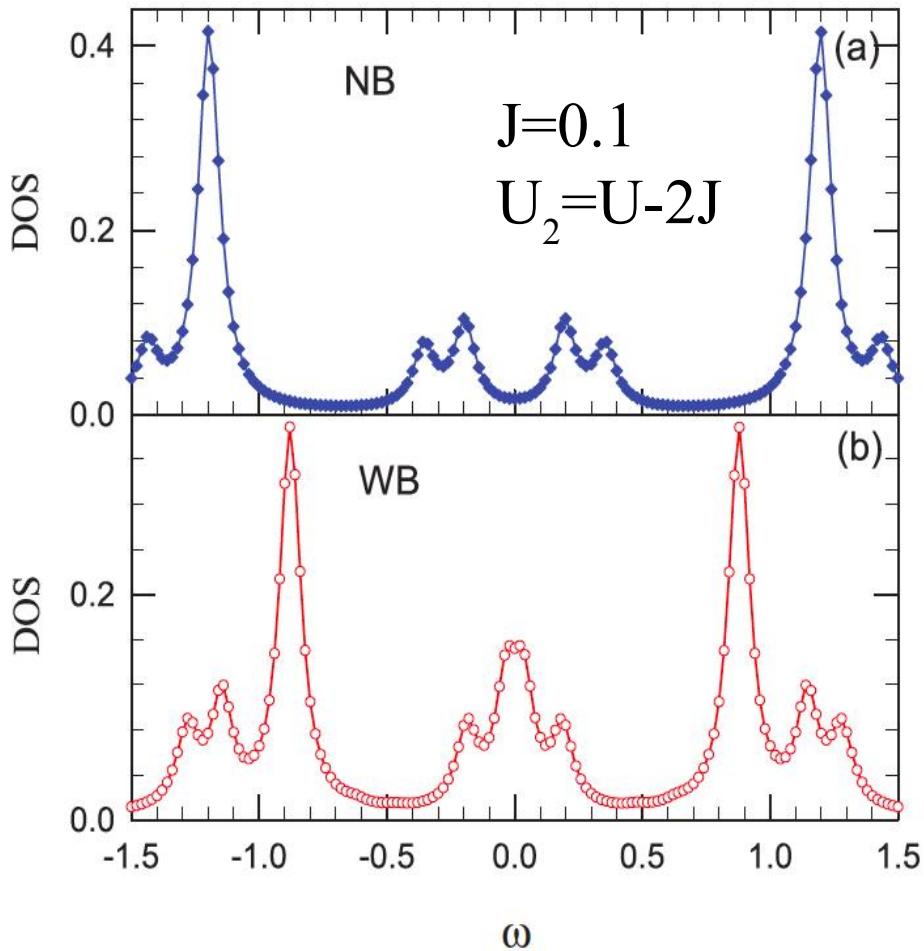
Doublon-holon excitations split by Hund's rule coupling within the orbital-selective Mott phase

Yuekun Niu,[1] Jian Sun,[2] Yu Ni,[1] Jingyi Liu,[1] Yun Song,[1,*] and Shiping Feng[1]

[1]*Department of Physics, Beijing Normal University, Beijing 100875, China*

[2]*Beijing National Laboratory for Condensed Matter Physics,Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*





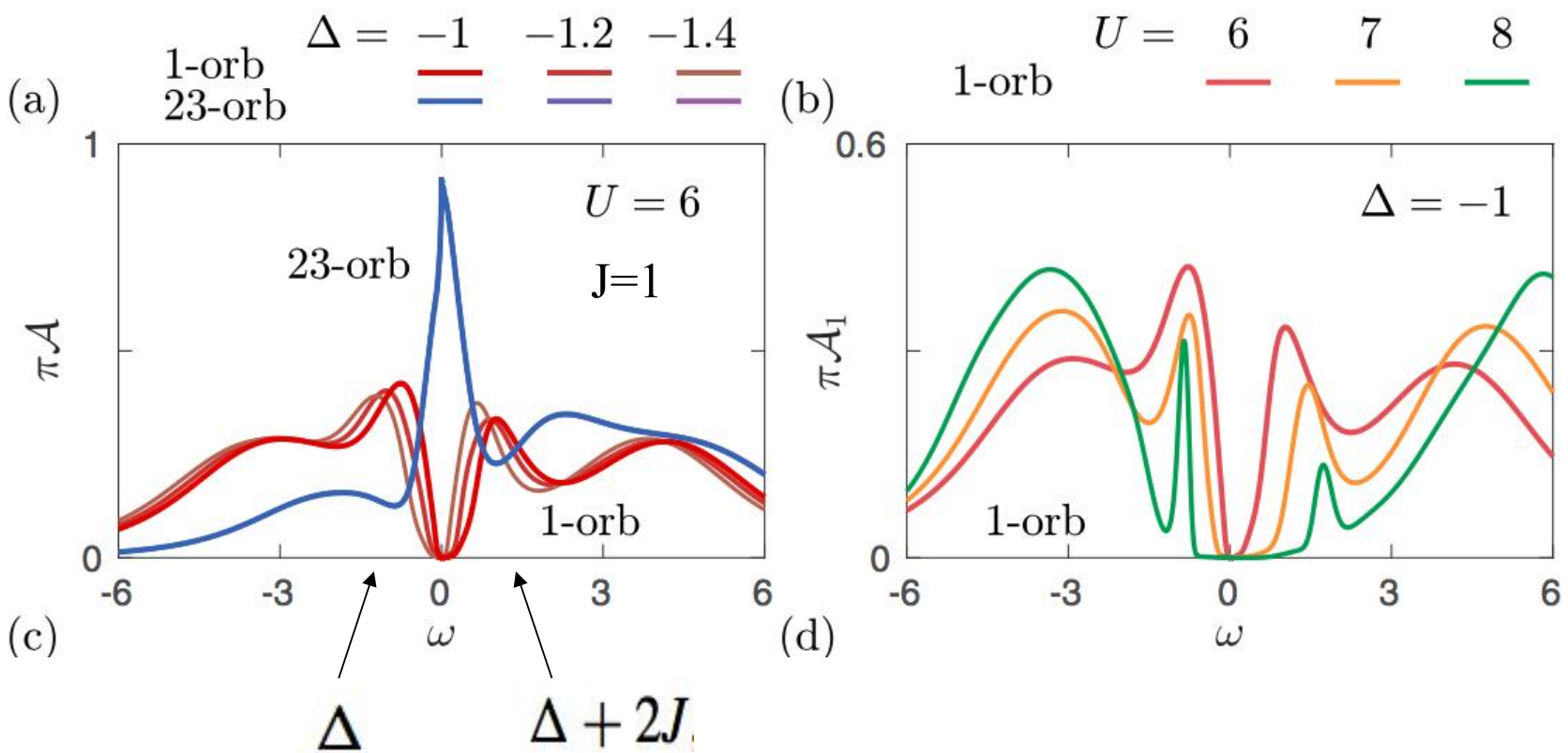
Orbital differentiation in Hund metals

Fabian B. Kugler,[1] Seung-Sup B. Lee,[1] Andreas Weichselbaum,[2,1] Gabriel Kotliar,[2,3] and Jan von Delft[1]

[1]*Arnold Sommerfeld Center for Theoretical Physics, Center for NanoScience, and Munich Center for Quantum Science and Technology, Ludwig-Maximilians-Universität München, 80333 Munich, Germany*

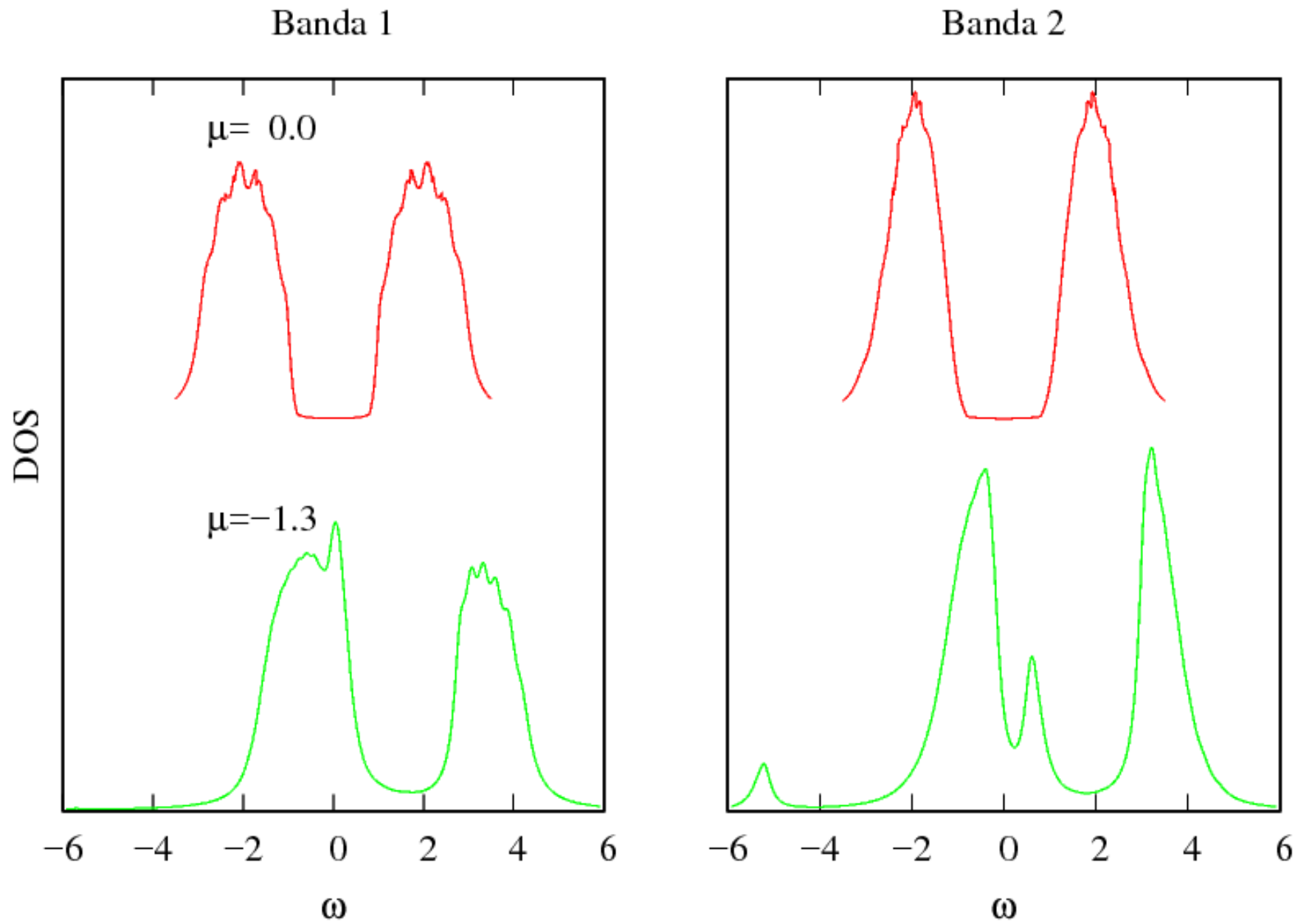
[2]*Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA*

[3]*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*



using NRG as the impurity solver in DMFT

Doping the insulator



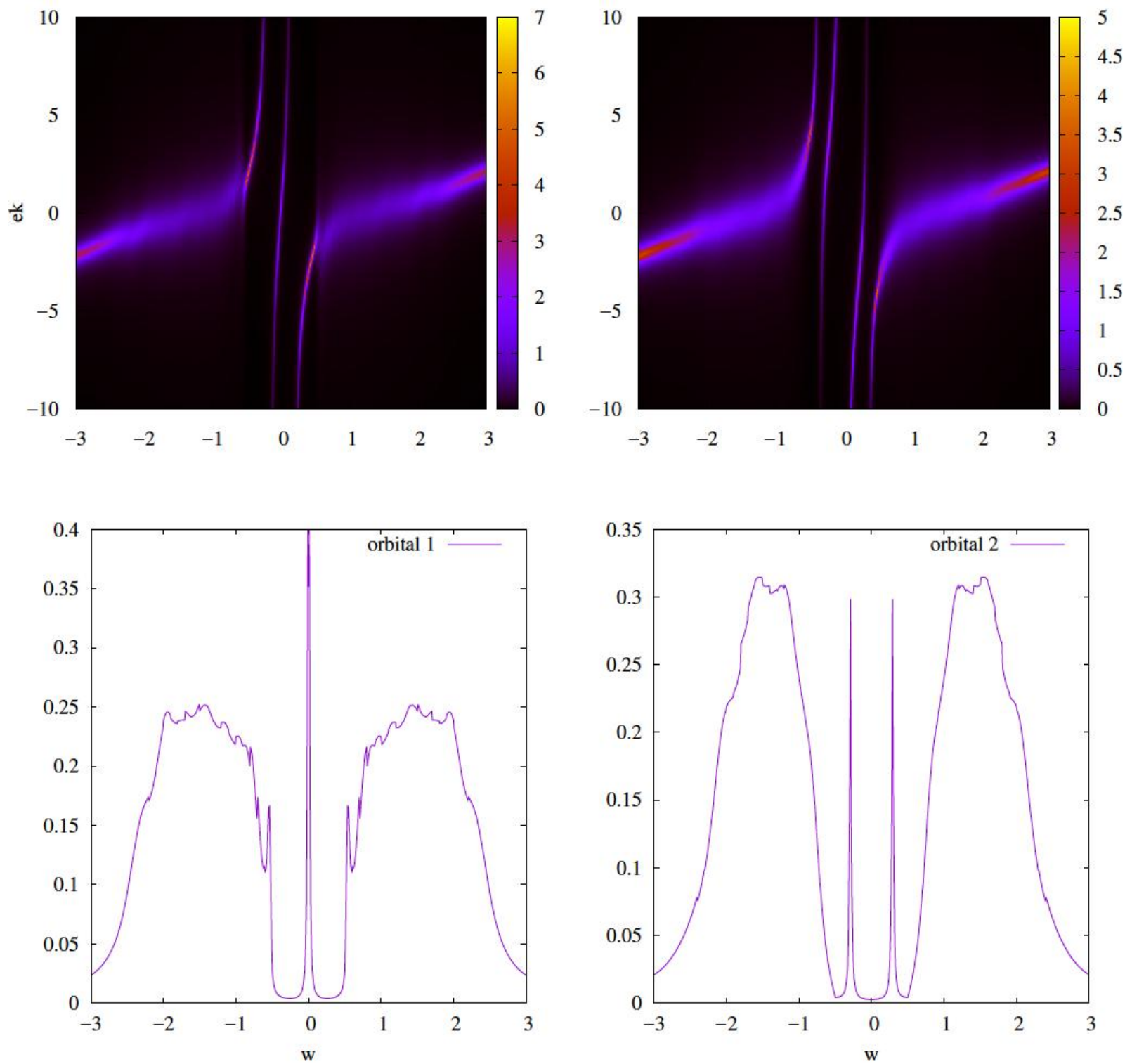
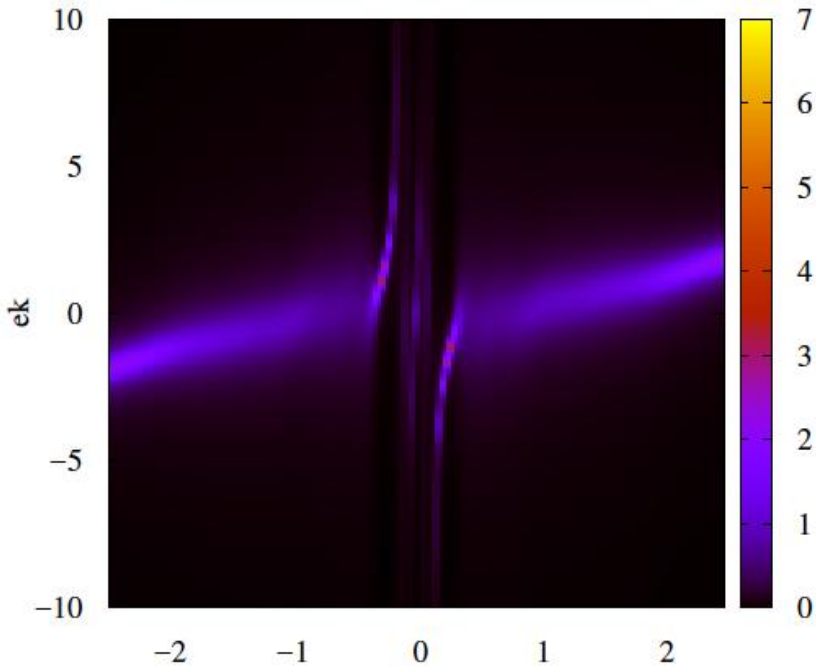
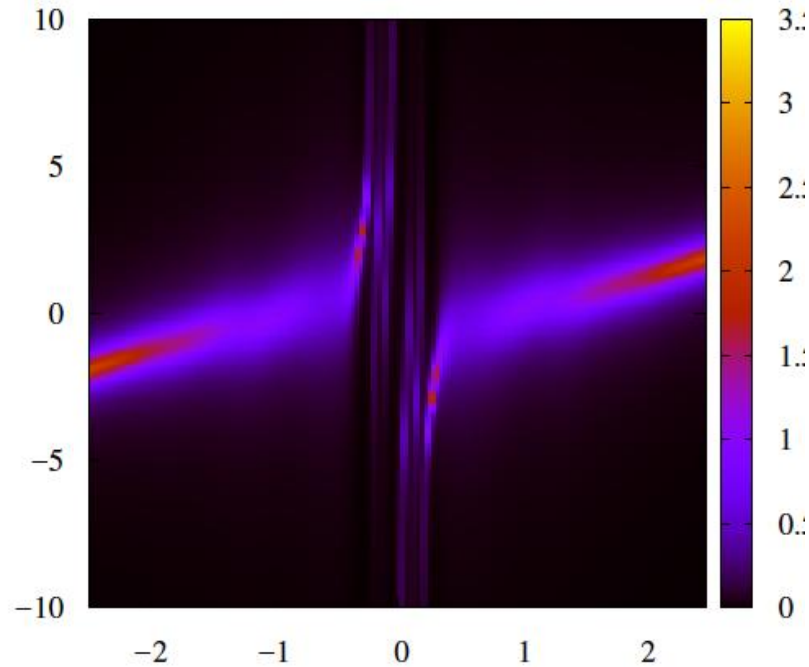
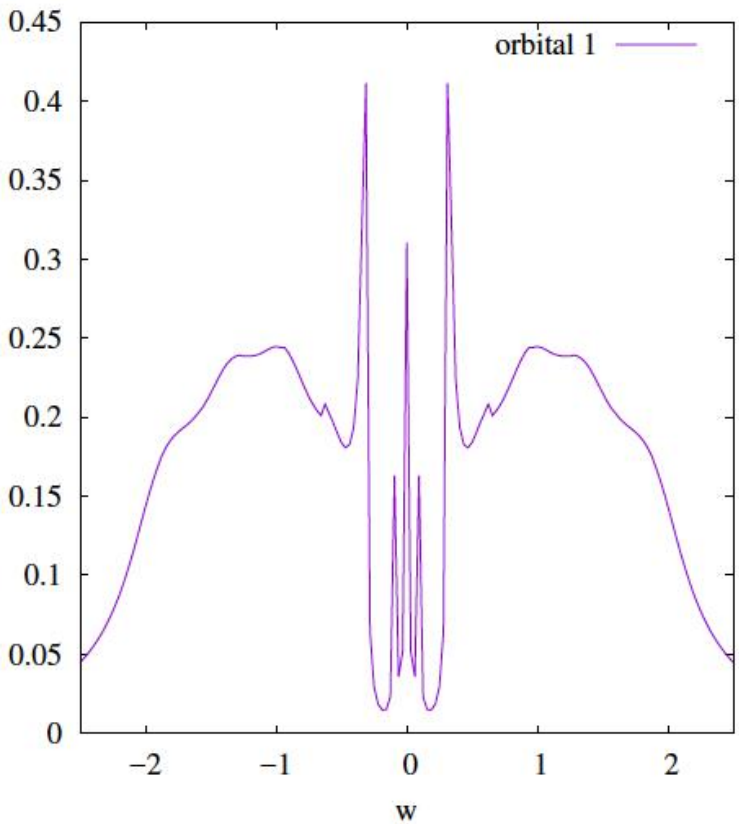
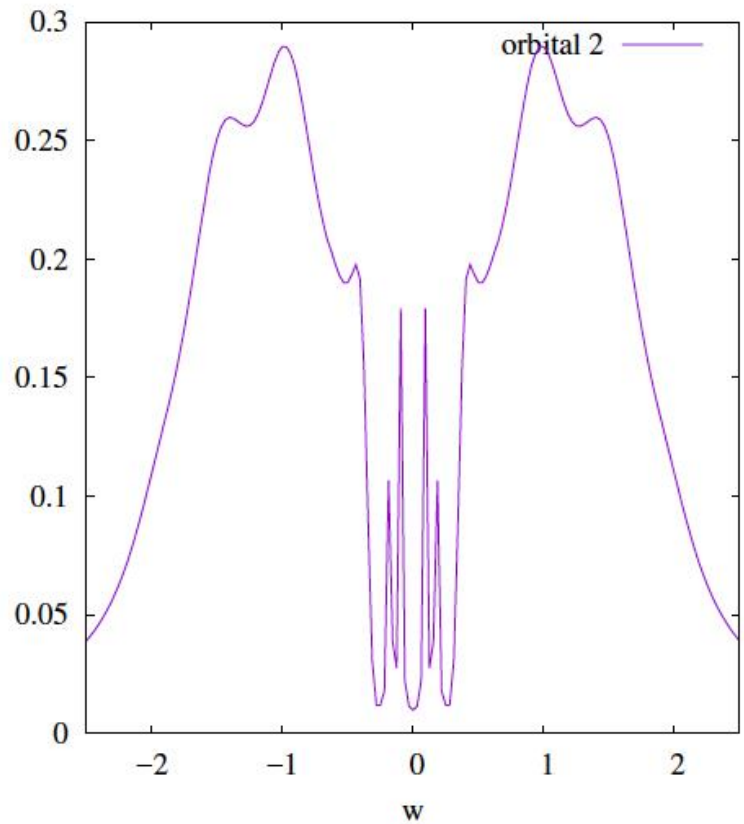


Figure 2: Relación de dispersión de la QP sin J, $U = 3$, $U_{12} = 2.7$, $J = 0$, $t_2 = t_1/2$.


ek
10
5
0
−5
−10
−2
−1
0
1
2
7
6
5
4
3
2
1
0


10
5
0
−5
−10
−2
−1
0
1
2
3
2
1
0


orbital 1
w
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
−2
−1
0
1
2


orbital 2
w
0.3
0.25
0.2
0.15
0.1
0.05
0
−2
−1
0
1
2

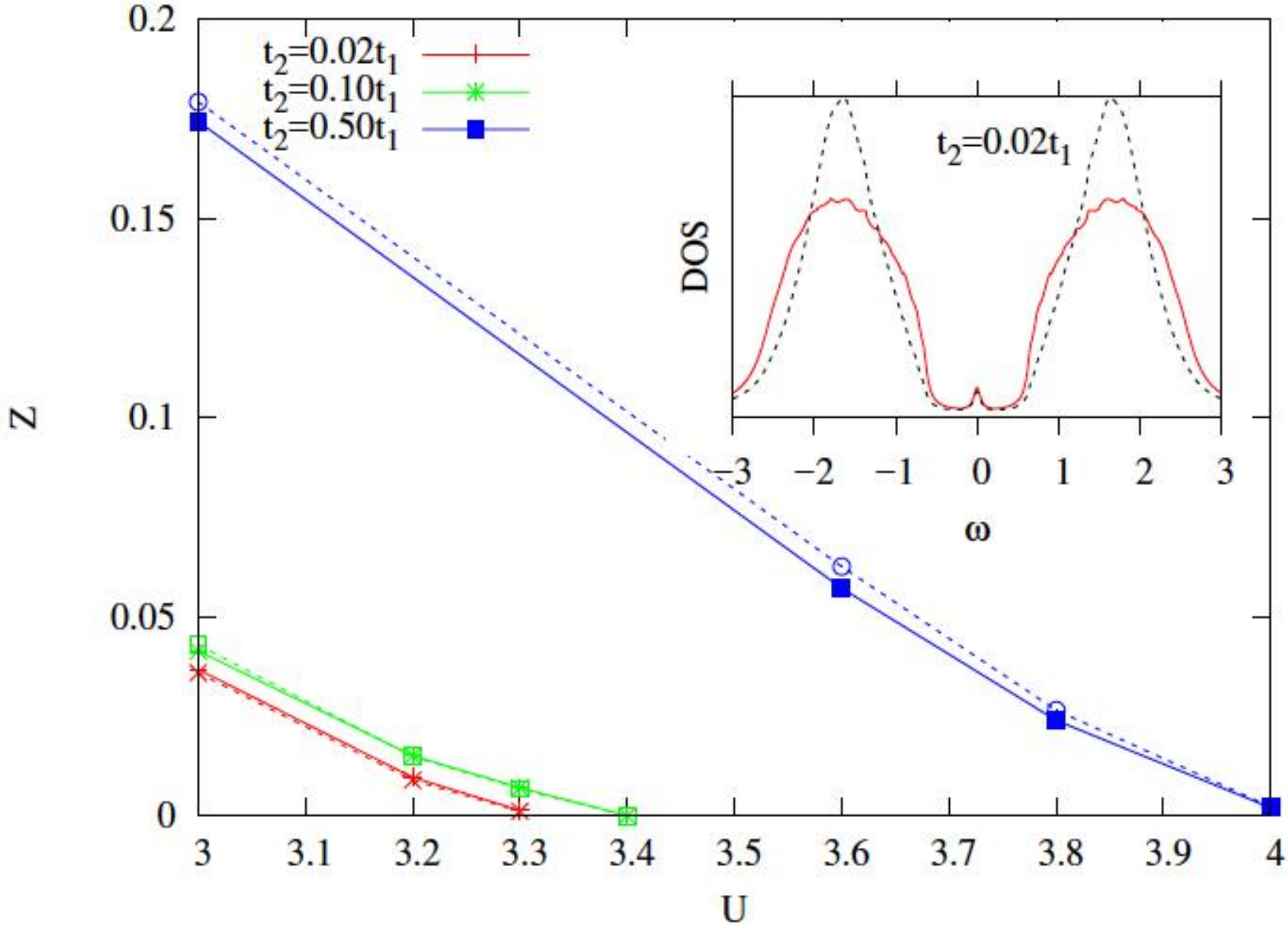
Is there an OSMT when $U=U'$ ($\Delta=0$)?

Previous contradicting results:

Yes: E. A. Winograd and L. de' Medici, PRB (2014)
M. Ferrero, F. Becca, M. Fabrizio, and M. Capone, PRB (2005)
L. de' Medici, A. Georges, and S. Biermann, PRB (2005)

No: A. Liebsch, Europhys. Lett. 63, 97 (2003)
A. Koga, N. Kawakami, T. M. Rice, and M. Sigrist, PRL (2004)
(2014)

For $\Delta=0$:


0.2
0.15
0.1
0.05
0
Z
3
3.1
3.2
3.3
3.4
3.5
3.6
3.7
3.8
3.9
4
U
t2=0.02t1
t2=0.10t1
t2=0.50t1
DOS
t2=0.02t1
−3
−2
−1
0
1
2
3
ω

Holon-doublon excitons:

- Robust with J, interband t', doping, crystal field splitting

Open questions:

- Loss of OSMP by proximity when U'~U (NFL to FL)?

- Features in optical conductivity, ARPES? Auger spectroscopy?

- Other models? Materials?

- Cold atoms?

CONCLUSIONS AND OUTLOOK

- Correlated materials comprise one of the most interesting and challenging systems presenting still not understood emergent phenomena

- Complexity requires sophisticated and precise computational methods

- We have developed a precise method to calculate electronic structure based on the DMRG (QI) as impurity solver of the DMFT

- This led us to analyse the structure in electonic spectra and to find stable interband holon-doublon bound states (Hubbard excitons).


Thank you for your attention!