Cálculo preciso de propiedades electrónicas en sistemas correlacionados usando información cuántica

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XI Workshop Chile-México, Pucón 26/11/19

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 ($La_{1-x}Sr_xMnO_3$), 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

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

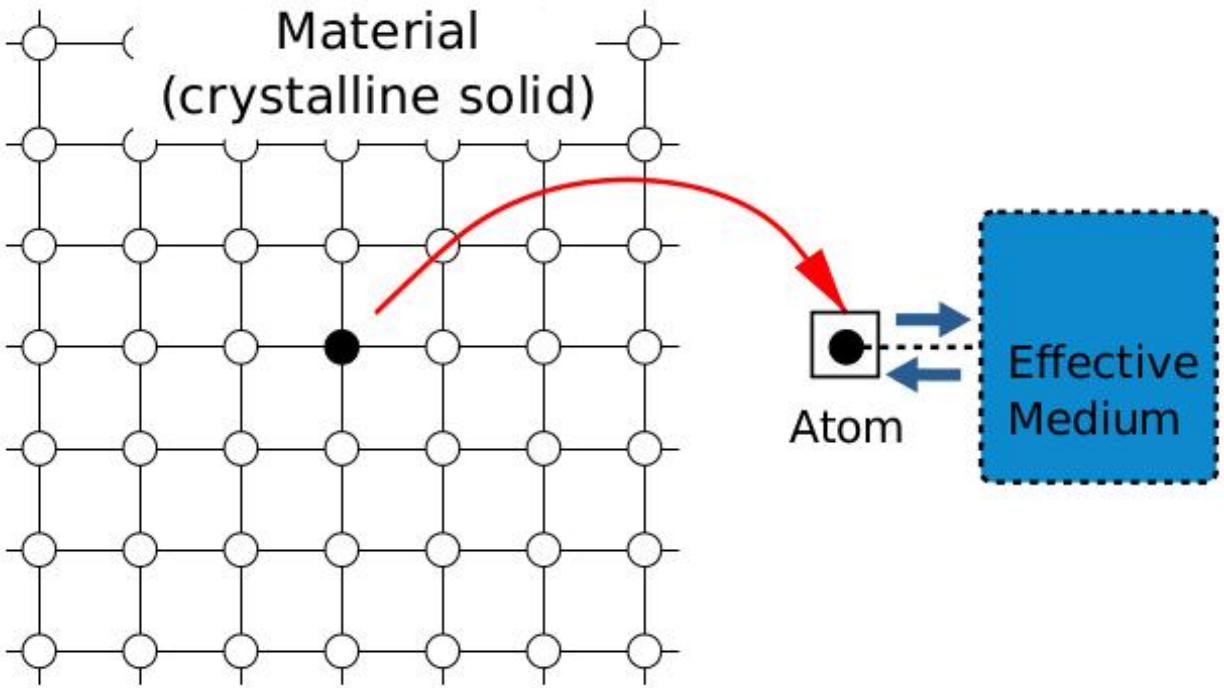
$$T = \left(t^{\alpha\beta}\right) = \begin{pmatrix} t_1 & 0 \\ 0 & t_2 \end{pmatrix}$$

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

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

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)

DMFT Impurity solvers:

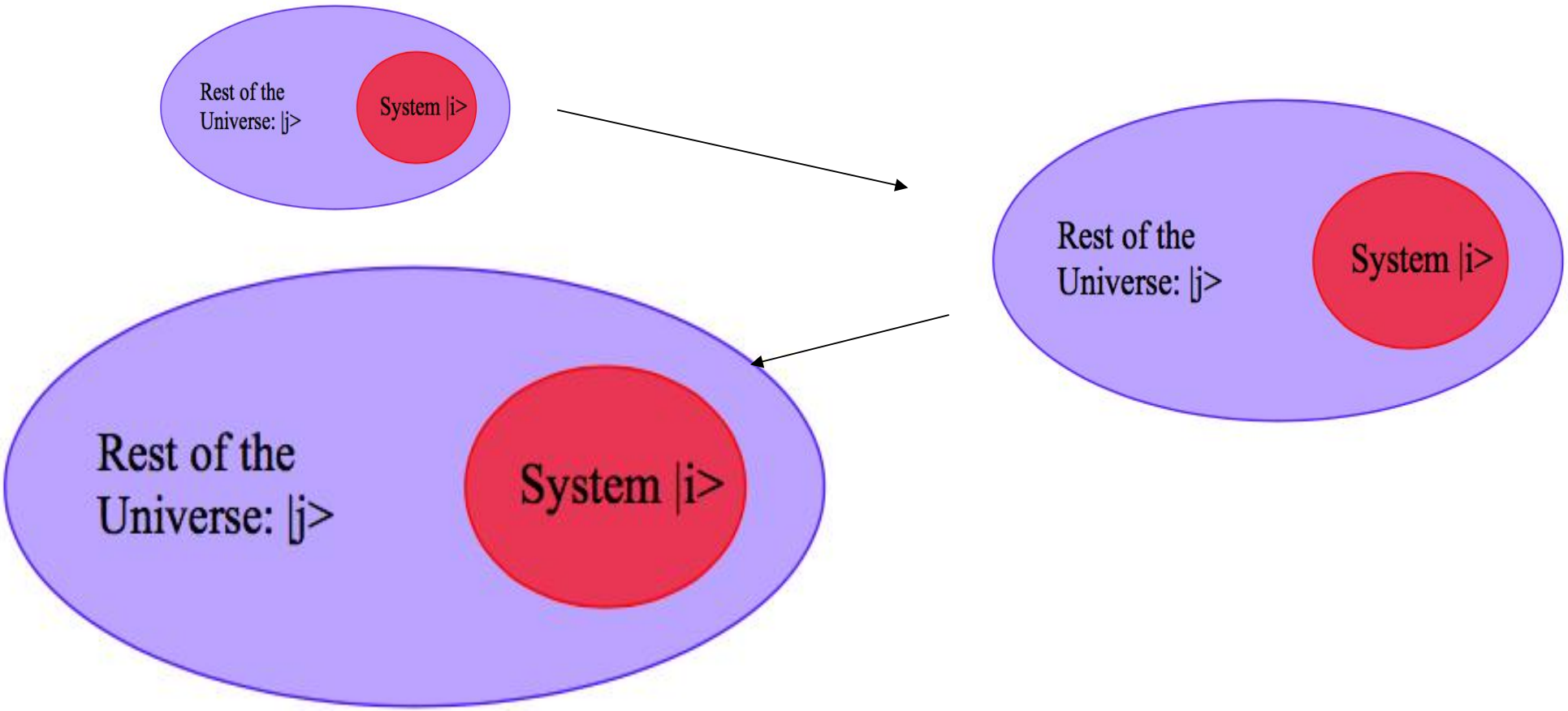
- **IPT** (Georges A. and Kotliar G., Phys. Rev. B 1992)
- **ED** (Caffarel M. and Krauth W., Phys. Rev. Lett. 1994)
- **HFQMC** (Zhang X. Y., Rozenberg M. J., Kotliar G., Phys. Rev. B 1993)
- **NCA** (Pruschke T., Cox D. L. and Jarrell M., Phys. Rev. Lett. 1993)
- **NRG** (Bulla R., Costi T. and Vollhardt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

"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)

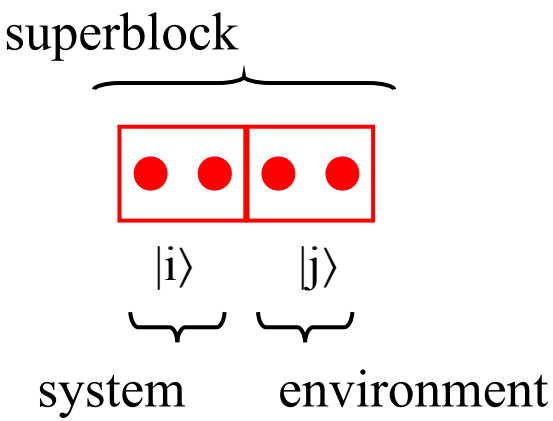
(Gaite 2001, 2003; Latorre et al. 2003, Osborn et al. 2001...)

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)

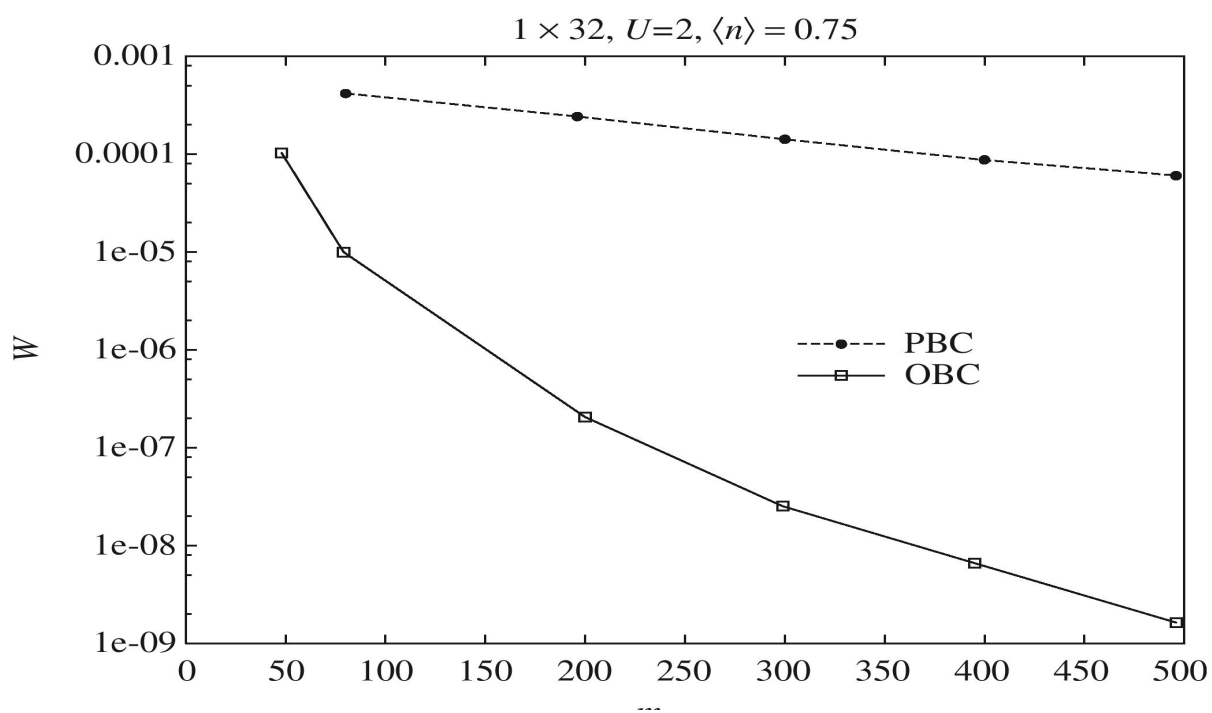
Quantum information and the DMRG



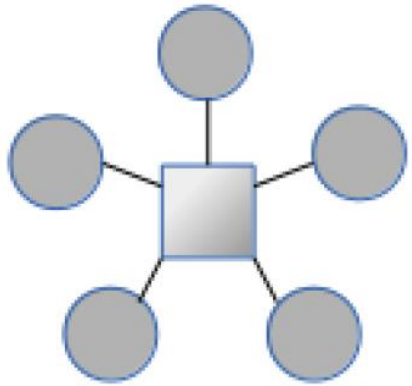
$$|\psi_0\rangle = \sum_{i,j=1}^{M} \psi_{ij}|i\rangle|j\rangle$$

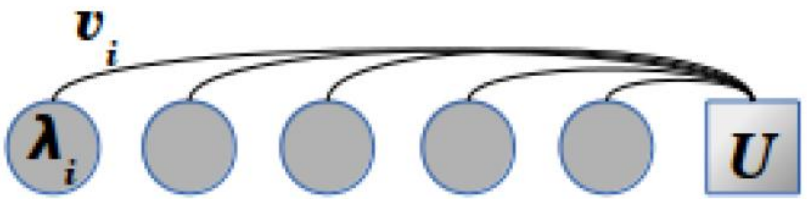
$$\rho_{ii'} = \sum_j \rho_{ij,i'j} = \sum_j \langle j|\langle i|\psi_0\rangle\langle\psi_0|i'\rangle|j\rangle = \sum_j \psi_{ij}\psi_{i'j}$$

Von Neumann entropy (T=0!): $S_S = -\mathrm{Tr}\rho_S \log_2 \rho_S = -\sum_\alpha \omega_\alpha^S \log_2 \omega_\alpha^S$



Cluster DMFT+DMRG in the star geometry



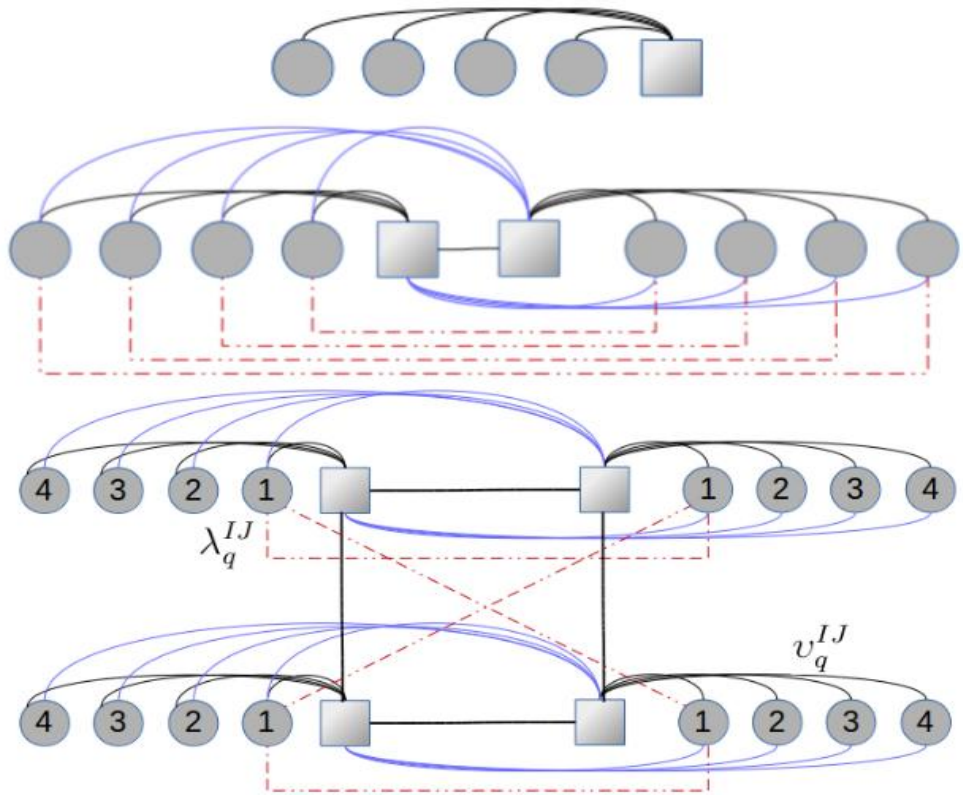


$$H_{imp} = H_{loc} + H_b$$

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

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

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:

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

Fourier transforming:

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

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

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)

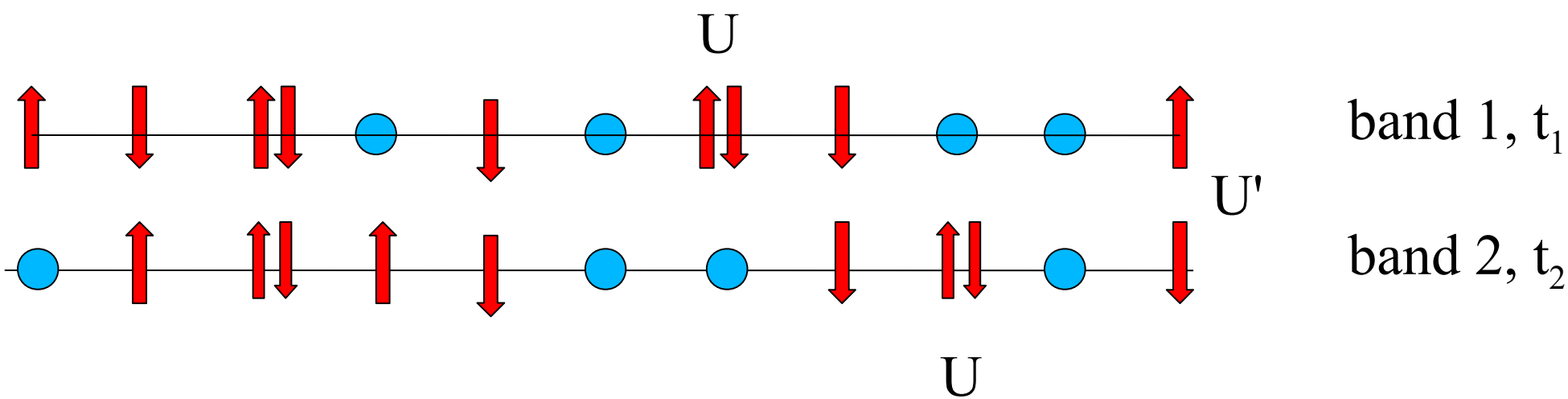
Advantages of using DMRG as the impurity solver:

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*

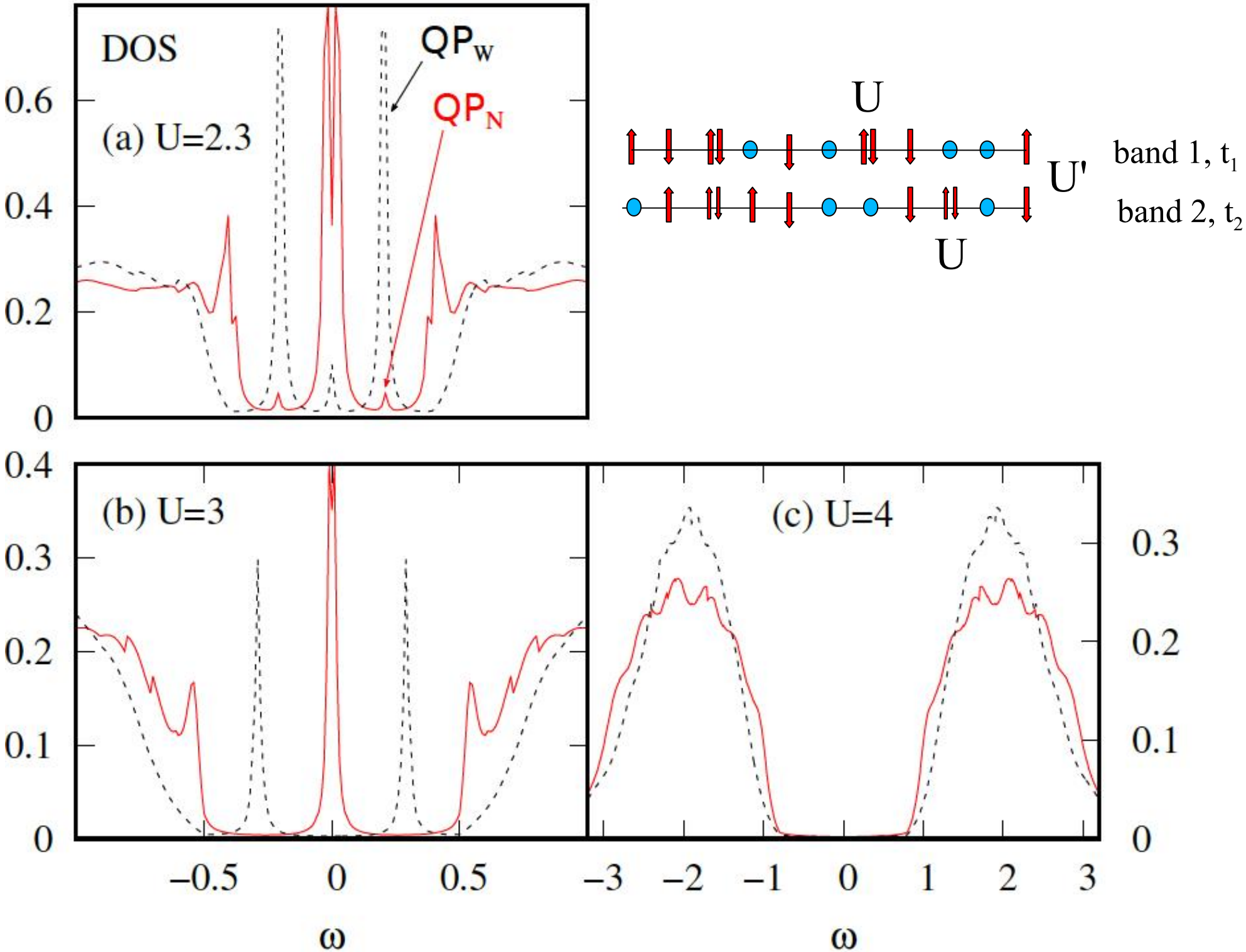
Two band Hubbard model (finite U_{12}, even with J=0):

$$H = \sum_{\langle ij\rangle\alpha\sigma} t_\alpha c^\dagger_{i\alpha\sigma} c_{j\alpha\sigma} + \\ + U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + \sum_{i\sigma\sigma'} U' \, n_{i1\sigma} n_{i2\sigma'}$$



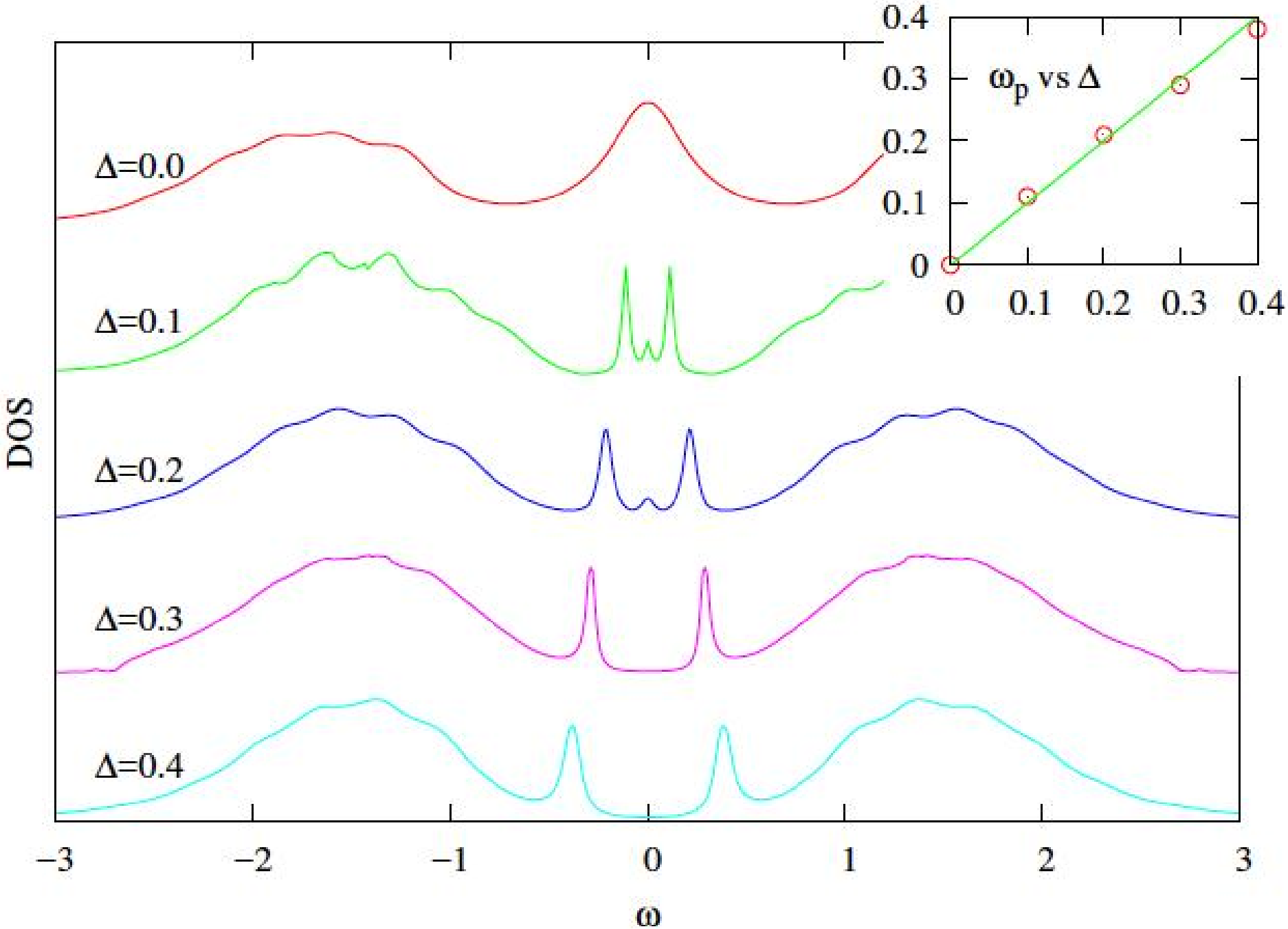
Half-filled and doped T=0 t'=0 $t_1 \geq t_2$ $U' \leq U$ $\Delta = U - U'$

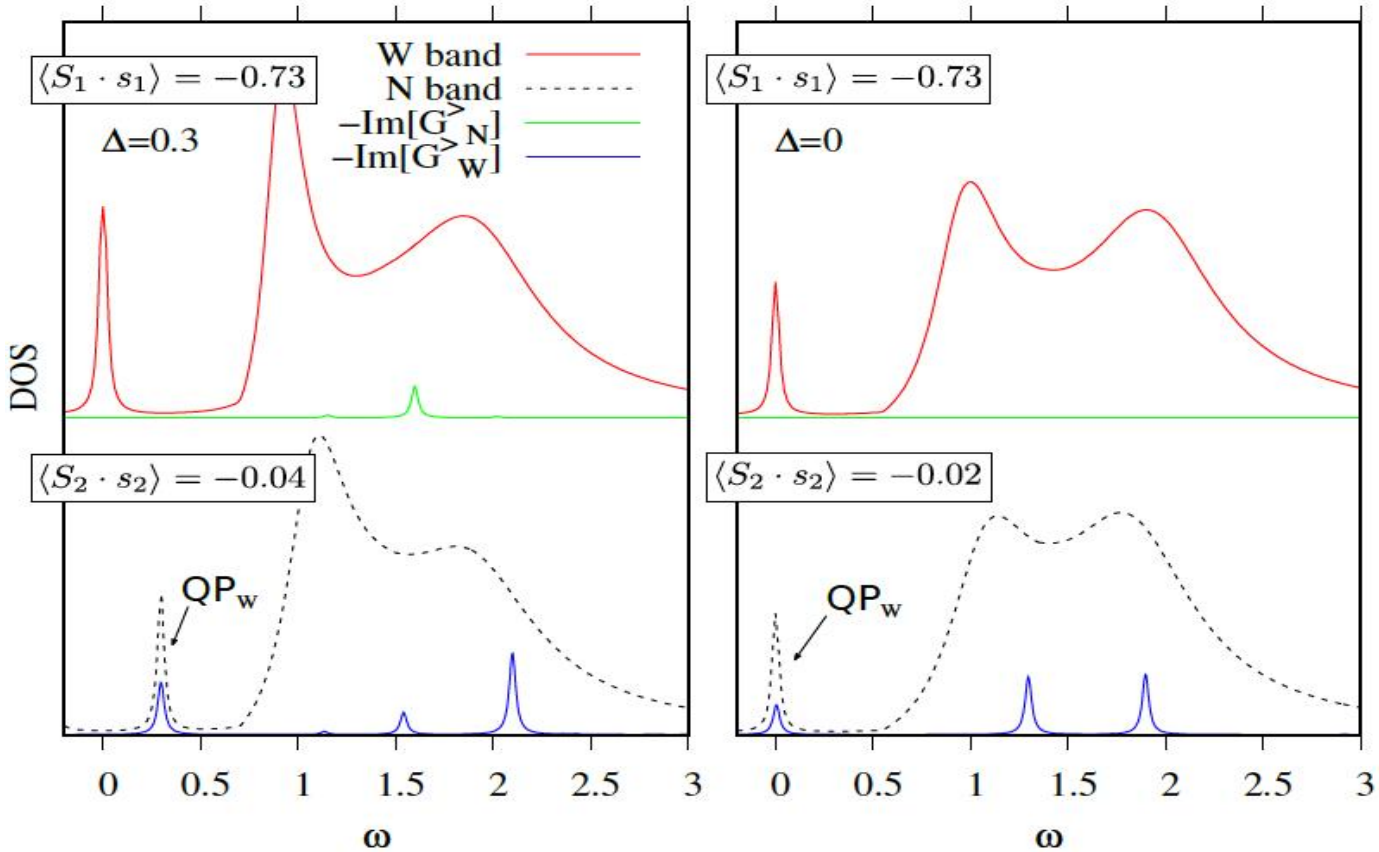
square lattice (2D)


DOS
(a) U=2.3
QP$_W$
QP$_N$
(b) U=3
(c) U=4
0.6
0.4
0.2
0
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
U
U'
U
band 1, t_1
band 2, t_2

Δ=U-U'

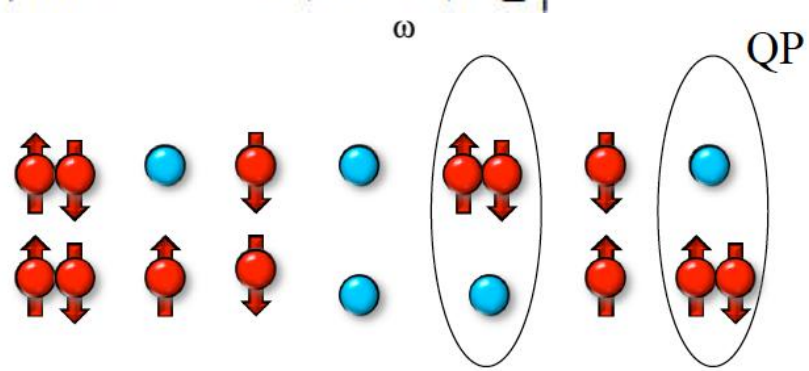
Band 2





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

We found new quasiparticles!



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

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?

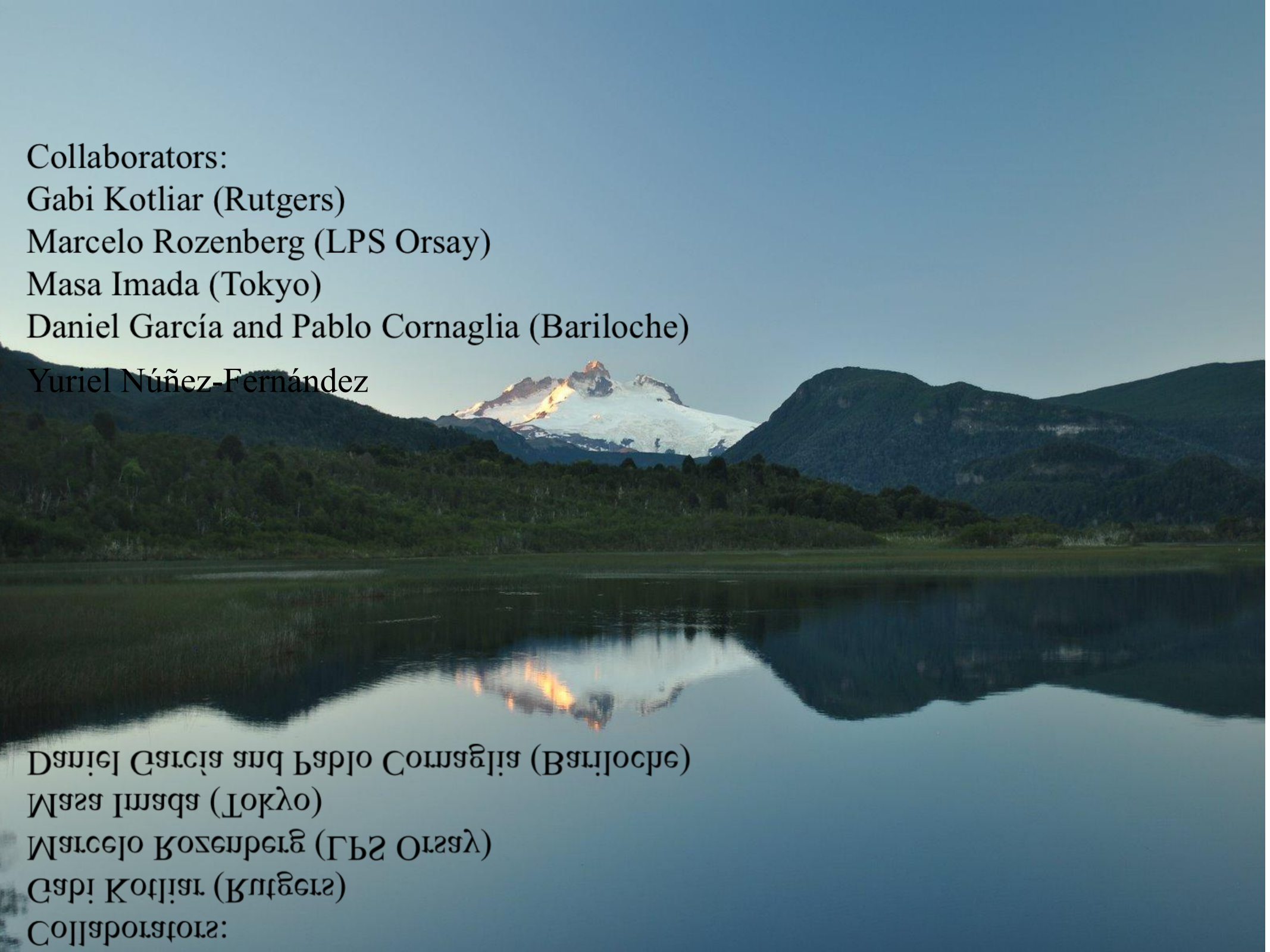
Conclusiones y perspectivas

- Los materiales correlacionados presentan desafíos muy interesantes, entre ellos, fenómenos emergentes aún no entendidos.

- La complejidad de estos sistemas requiere el desarrollo de métodos computacionales sofisticados y precisos.

- Hemos desarrollado un método numérico muy preciso para el cálculo de estructura electrónica basado en el DMRG con conceptos de QI, como resolvedor de impureza efectiva del DMFT.

- Esto nos permitió observar la existencia de cuasipartículas excitónicas en un modelo paradigmático.



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Yuriel Núñez-Fernández


¡Muchas gracias!