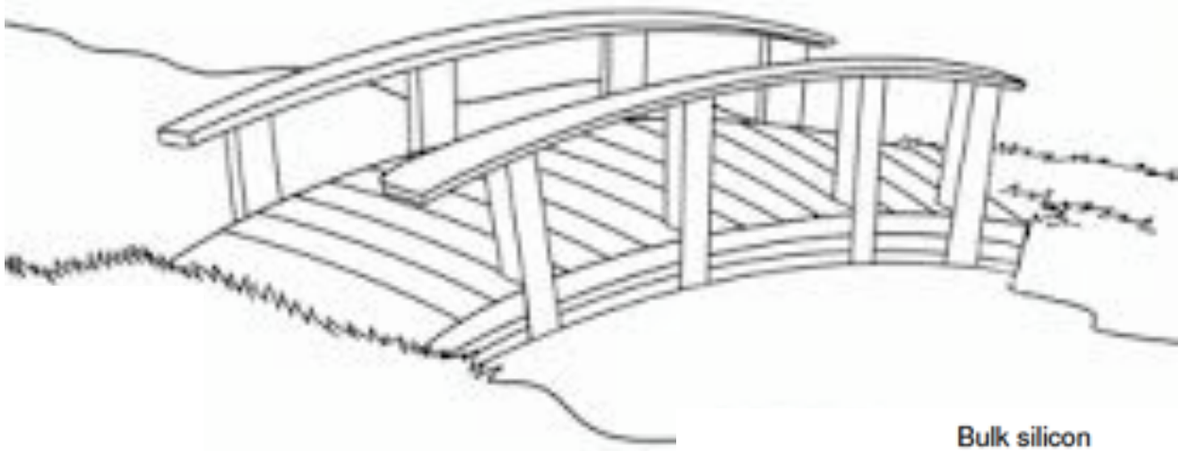
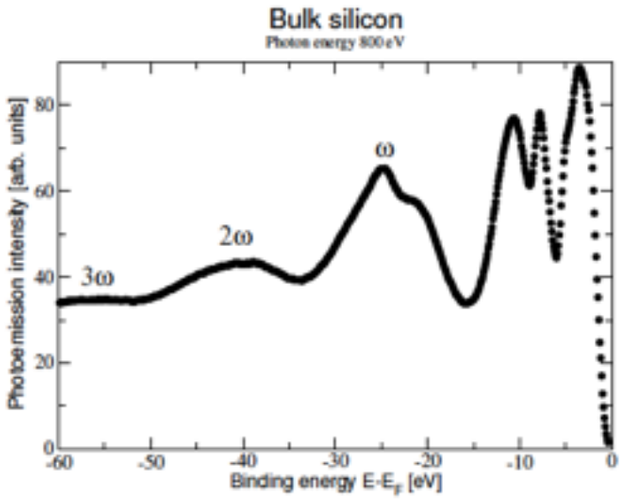
How to accurately get the polarisability from an impurity model?

Sophie Chauvin[1,2,3], Lucia Reining [1,3], Silke Biermann [2,3]

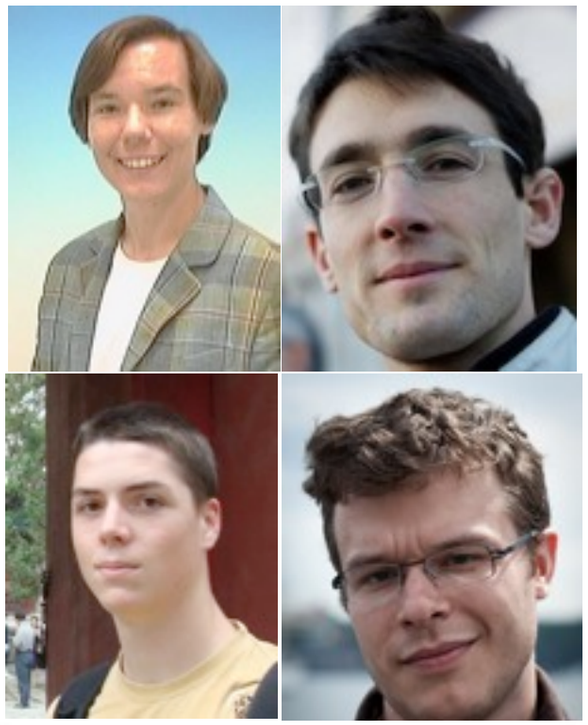
[1]Laboratoire des Solides Irradiés, Ecole polytechnique, France
[2]Centre de Physique Théorique, Ecole polytechnique, France
[3]European Theoretical Spectroscopy Facility (ETSF)

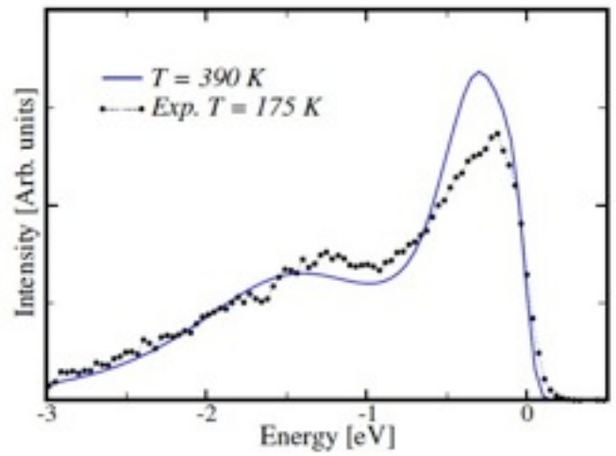


Many-body perturbation theory



Dynamical mean field theory





Overview

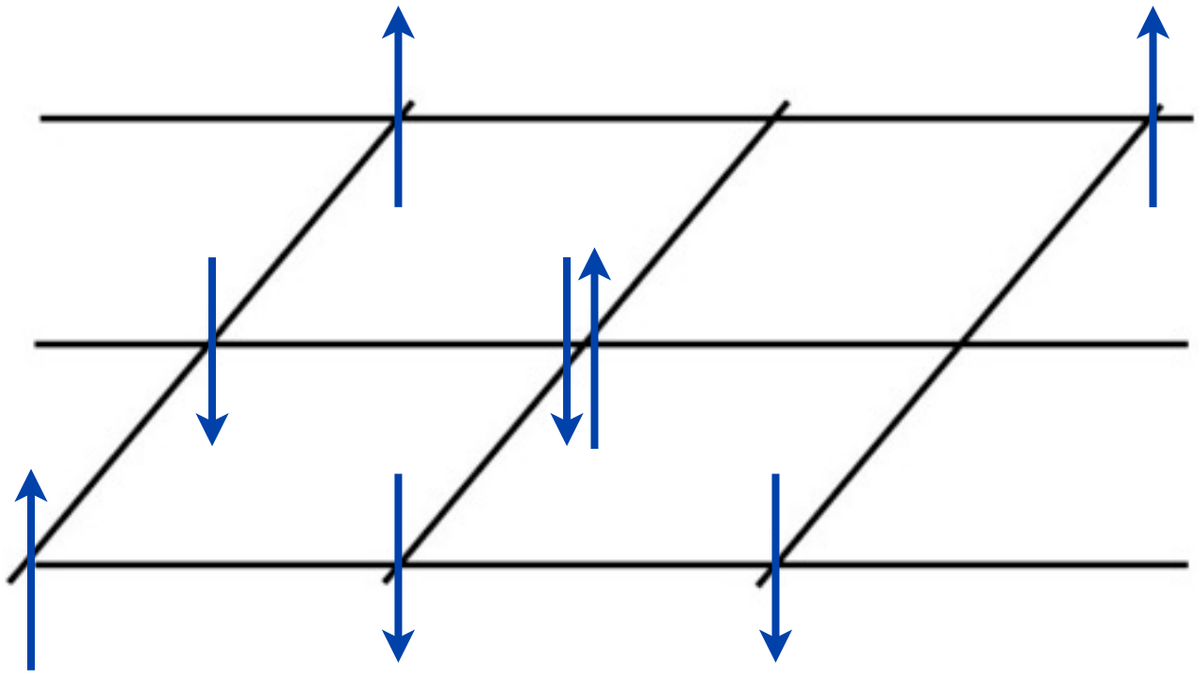
1. Introduction to correlated materials: the Mott transition
2. Dynamical Mean Field theory (DMFT)
3. Extended DMFT (EDMFT)
4. EDMFT and the Hubbard dimer

Correlated materials

- Localised orbitals: *3d*, *4f*, ...

Transition metals, transition metal oxides, f-electrons (rare earths, actinides, their compounds)

- Hubbard model $\mathcal{H} = -t \sum_{<i,j>,\sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$



1 electron per site

$t \gg U$: kinetic energy dominates

$U \gg t$: repulsion dominates

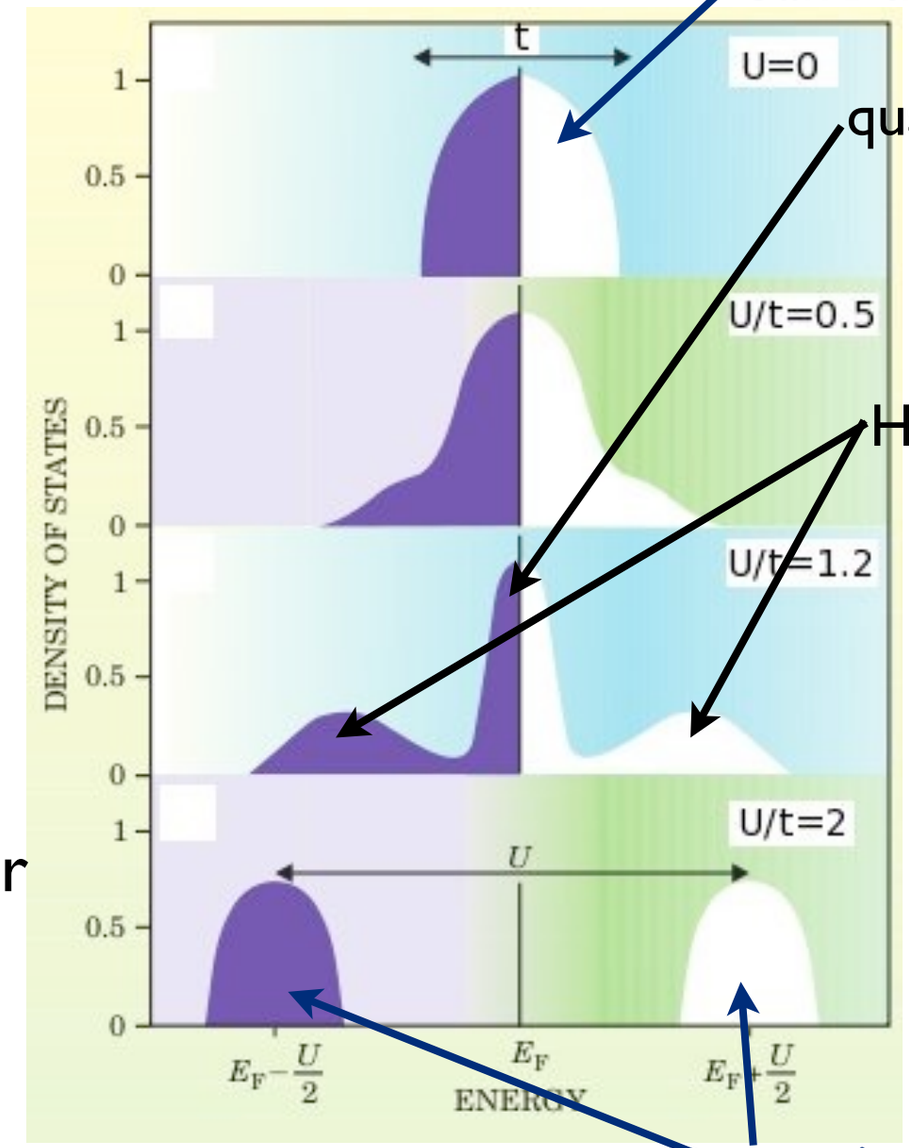
Correlated materials

- The Mott transition: a metal-insulator transition

Metal

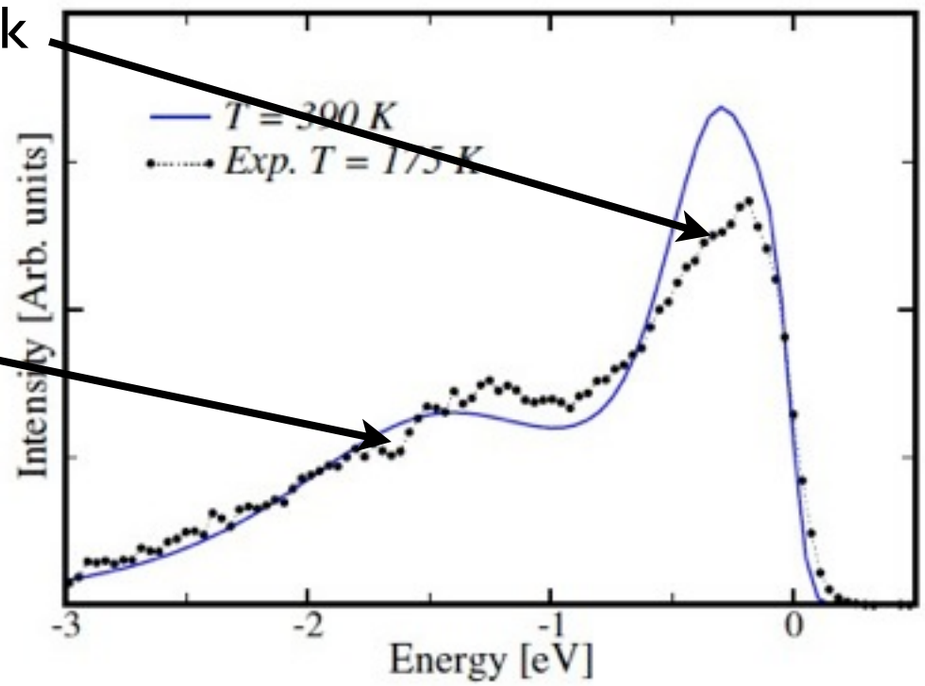
U/t

Insulator



from Kotliar and Vollhardt, *Physics Today* (2004).

- Band theory not suited for these spectra



Photoemission spectrum of metallic V_2O_3 near the Mott transition

from Poteryaev et al., cond-mat/0701263,
adapted from Mo et al., *Phys. Rev. Lett.* 90, 186403 (2003).

Our motto

- The many-body Hamiltonian: $\mathcal{H} = \sum_{i=1}^{N} \left(-\frac{\hbar^2 \nabla_i^2}{2m} - Ze^2 \sum_{\mathbf{R}} \frac{1}{|\mathbf{r}_i - \mathbf{R}|} \right) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$

  10^{23} interacting particles!

- The many-body wave function: $\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$
  we cannot even store the information!

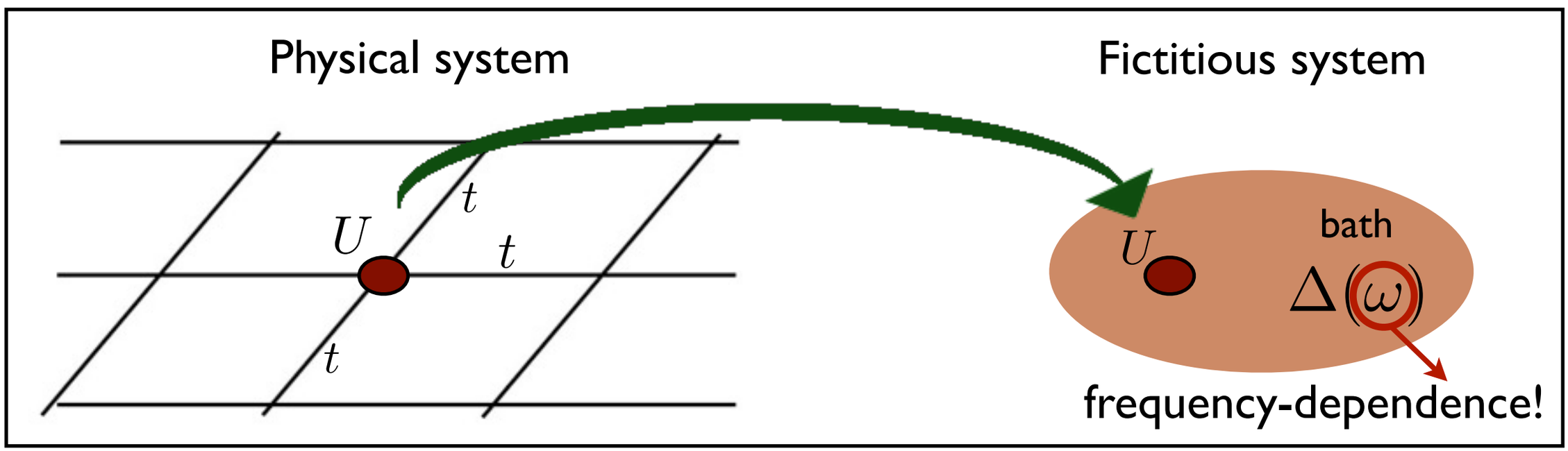
- Focus on reduced quantities

Green's function: propagation of an electron

	DFT	Green's function approaches	Impurity Green's function
Physical system	Interacting electrons	Interacting electrons	Interacting electrons
Physical quantity	Local density $n(\boldsymbol{r})$	Green's function $G(\boldsymbol{r}, \boldsymbol{r}'; t, t')$	Local Green's function $G_{ii}(t, t')$
Experiment	Structural properties, phonons	Angle-resolved photoemission	Direct and inverse photoemission

Dynamical Mean-Field Theory

- Introduce a *dynamical* mean field



Non-locality ⟷ Frequency-dependence

- Self-consistency: $G_{ii} = -i < \mathcal{T} c_i^\dagger(t) c_i(0) > = G_{imp}$

Need approximation

see M. Gatti et al., *Phys. Rev. Lett.* (2007)

see A. Georges, *Exact functionals, effective actions and (Dynamical) Mean-Field Theories: Some Remarks*
or Kotliar and Vollhardt, *Physics Today* (2004)

Extended Dynamical Mean-Field Theory

- Not included in DMFT:
  - long-range interactions v_{ij} ,
  - effects from other bands
- Describe dynamical screening $\epsilon(\omega)$, could affect Mott transition
- Effective, dynamical (screened) Coulomb interaction

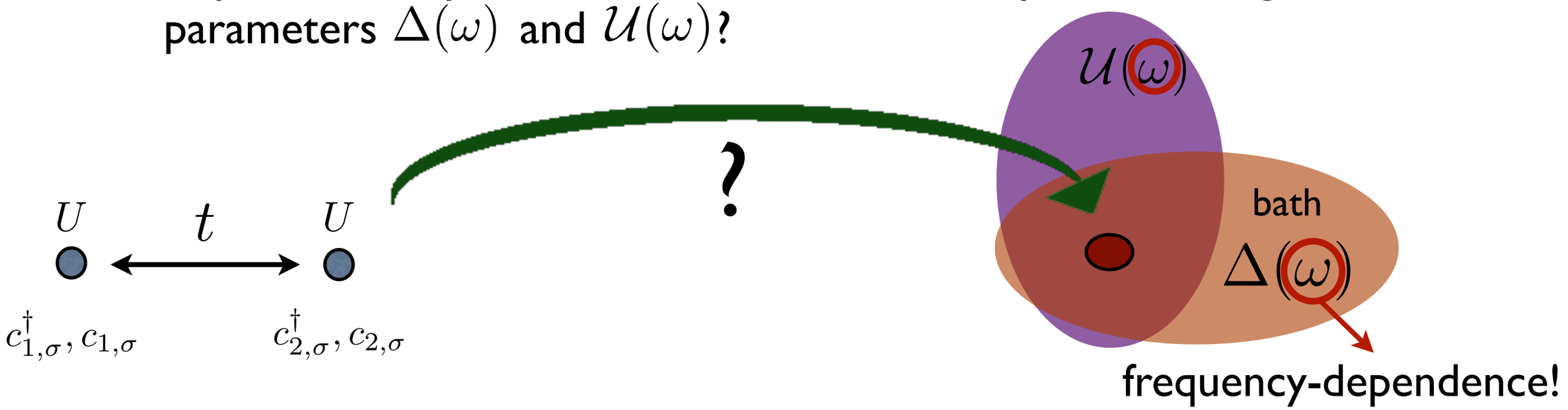
$$U n_i n_i \longrightarrow \mathcal{U}(\tau - \tau') n_i(\tau) n_i(\tau')$$

- Basic variables: electron propagation AND screening (G and W)
- Local point of view

H. Kajueter, PhD (1996). For a pedagogical introduction, see
S. Florens PhD (2003), and Th. Ayral, *Phys. Rev. B* (2013)

Example: the Hubbard dimer

- Can we make EDMFT construction more apparent?
- Representability issue of EDMFT: can we always find the right parameters $\Delta(\omega)$ and $\mathcal{U}(\omega)$?



$$\mathcal{H}_{\text{dimer}} = -t \sum_{\sigma} \left(c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma} \right) + U \sum_{i=1,2} n_{i\uparrow} n_{i\downarrow}$$

- Integrate out degrees of freedom on site 2

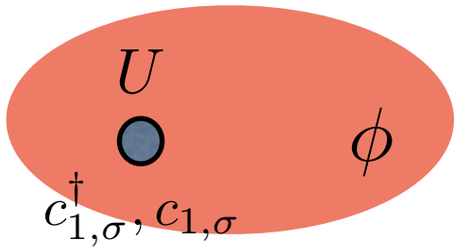
The Hubbard dimer
Intermediate results

$$Z \sim \int \left(\prod_{\sigma} \mathcal{D}[c^*_{1\sigma}, c_{1\sigma}] \right) \int \mathcal{D}[\phi] e^{-S_1} e^{-S_\phi} I$$

$$S_1 = \int_0^\beta d\tau \Big[\sum_\sigma c^*_{1,\sigma}(\tau) \partial_\tau c_{1,\sigma}(\tau) + \frac{U}{2} \sum_{\sigma,\sigma'} \left(c^*_{1,\sigma}(\tau) c_{1,\sigma}(\tau) - \frac{1}{2} \right) \left(c^*_{1,\sigma'}(\tau) c_{1,\sigma'}(\tau) - \frac{1}{2} \right) \Big]$$

$$S_\phi = \int_0^\beta d\tau \left[\frac{1}{2} \frac{1}{U} \phi(\tau)\phi(\tau) - i\phi(\tau) \right]$$

$$I = (\det \mathcal{G})^2 \exp \left(-t^2 \sum_\sigma \iint d\tau d\tau' c^*_{1\sigma}(\tau) \mathcal{G}(\tau, \tau') c_{1\sigma}(\tau') \right)$$



- Interpretation:
  - Site 1 in effective bosonic medium
  - Elementary process:

$$t \sim G^{-1}_{12} \sim G^{-1}_{21}; \quad \mathcal{G} = G_{22}$$

Perspective: Integrate out boson...

Conclusions

- DMFT: an effective single-site problem (or «effective atom») to reproduce the local part G_{ii} (electron propagation)
- EDMFT: transforms long-range interactions into effective local dynamical interaction to reproduce the local quantities G_{ii} and W_{ii} (electron propagation and screening)
- Explicit construction on Hubbard dimer: work in progress