Numerical solution of the Dyson equation in the two-times plane: applications to quantum quenches and transport in many-body quantum systems

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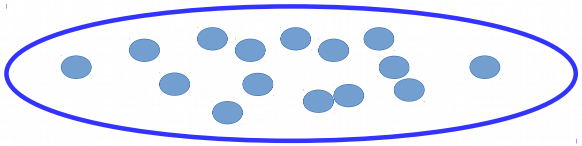
Summary

- Dyson equation
- How to parallelize : “localize” computation
- Applications
- Some ideas to improve performances and/or precision

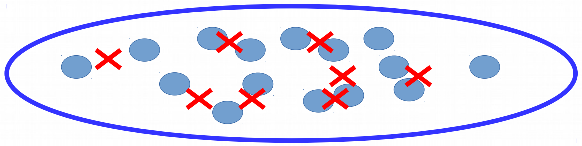
NEGFs approach, MBPT and KB Eqs.

Many-body quantum systems

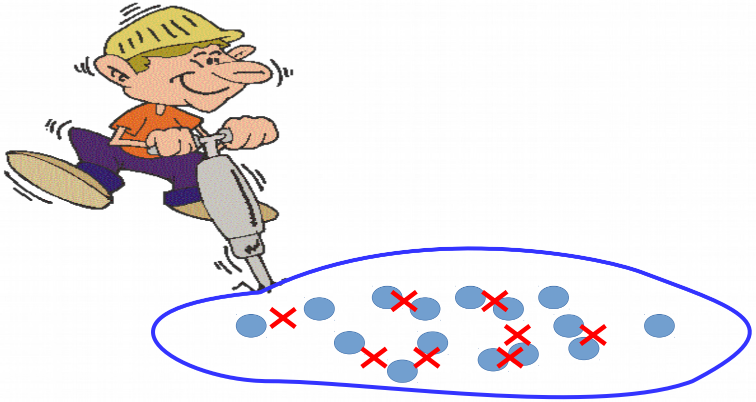


Many-body quantum systems

MB Interactions



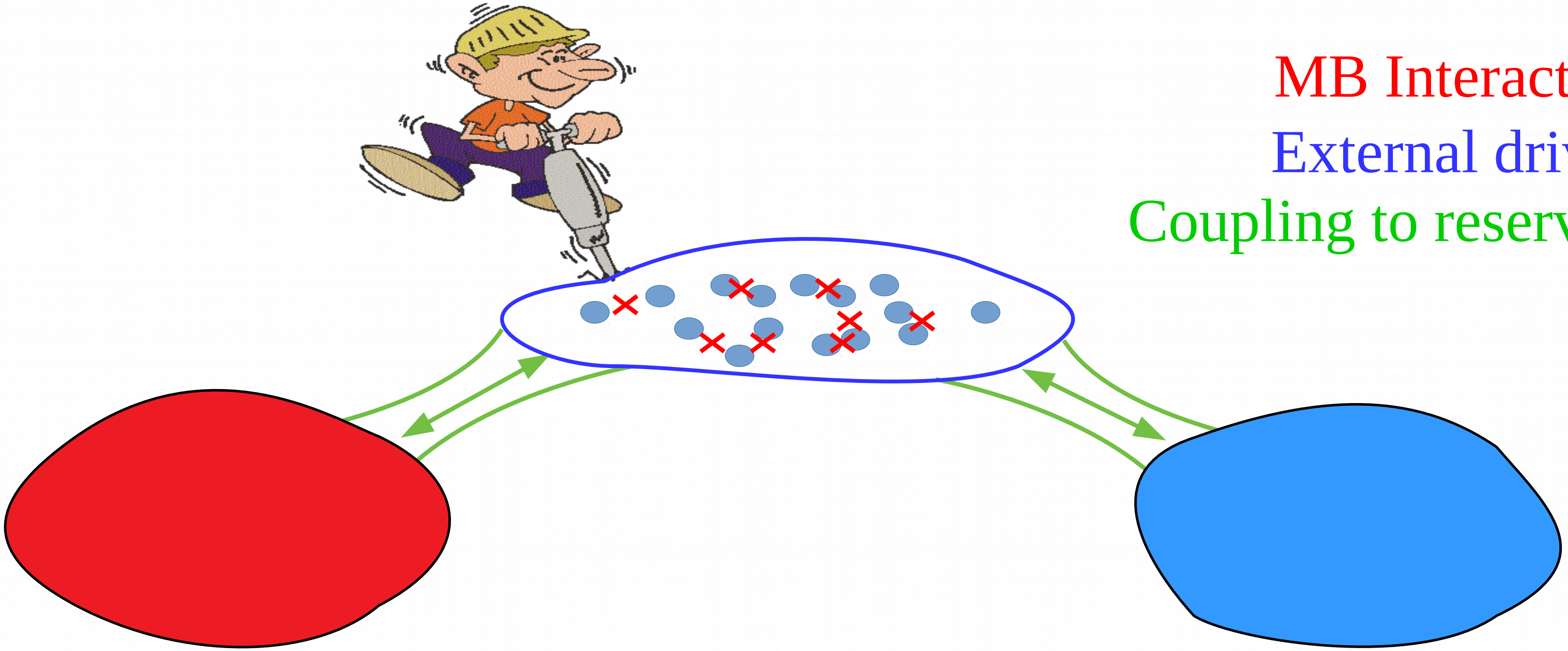
Many-body quantum systems



MB Interactions

External driving

Many-body quantum systems



MB Interactions

External driving

Coupling to reservoirs

Particles on a contour

$$\hat{H} = \hat{H}_0 + \hat{V} + \hat{H}_{SL}$$

$$\hat{H}_0 = \sum_{i,j} h_{ij}\hat{d}_i^\dagger \hat{d}_j$$

Free

$$\hat{V} = \sum_{i,j,i',j'} v_{iji'j'}\hat{d}_i^\dagger \hat{d}_{i'}^\dagger \hat{d}_{j'}\hat{d}_j$$

MB Interactions

$$\hat{H}_{SL} = \sum_{\alpha}\sum_{ki} g_{ki}^{\alpha}\hat{D}_{\alpha,k}^\dagger \hat{d}_i + h.c.$$

Coupling to reservoirs

Particles on a contour

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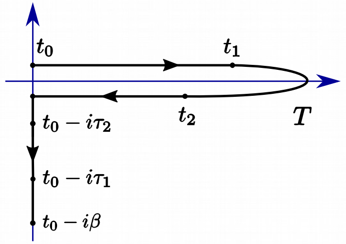
Coupling to reservoirs

Keldysh-Schwinger contour



Single particle Green's function

$$G_{ij}(z;z') = -\imath \langle T_\gamma \hat{d}_i(z) \hat{d}_j(z') \rangle$$

Kadanoff-Baym equations

$$\left[\mathrm{i}\frac{d}{dt} - h(t)\right] G^{\rceil}(t,\tau) = \left[\Sigma^{\mathrm{R}}_{\mathrm{tot}} \cdot G^{\rceil} + \Sigma^{\rceil}_{\mathrm{tot}} \star G^{\mathrm{M}}\right](t,\tau),$$

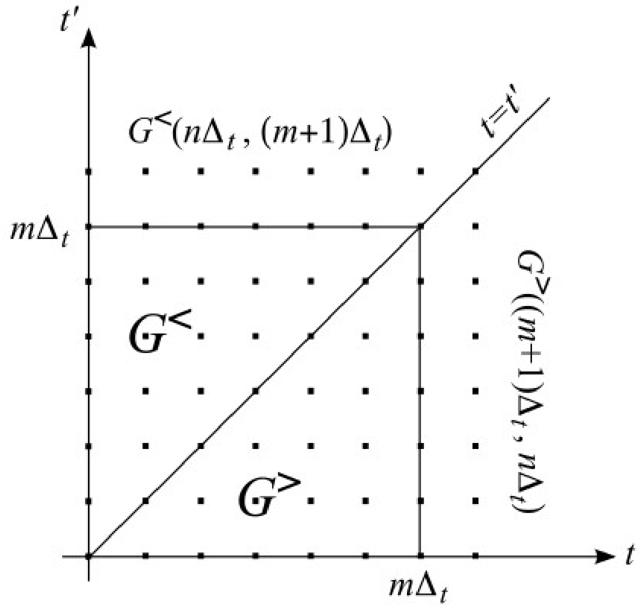
$$\left[\mathrm{i}\frac{d}{dt} - h(t)\right] G^{>}(t,t') = \left[\Sigma^{\mathrm{R}}_{\mathrm{tot}} \cdot G^{>} + \Sigma^{>}_{\mathrm{tot}} \cdot G^{\mathrm{A}} + \Sigma^{\rceil}_{\mathrm{tot}} \star G^{\lceil}\right](t,t')$$

$$G^{<}(t,t')\left[-\mathrm{i}\frac{\overleftarrow{d}}{dt'} - h(t')\right] = \left[G^{\mathrm{R}} \cdot \Sigma^{<}_{\mathrm{tot}} + G^{<} \cdot \Sigma^{\mathrm{A}}_{\mathrm{tot}} + G^{\rceil} \star \Sigma^{\lceil}_{\mathrm{tot}}\right](t,t')$$

$$\mathrm{i}\frac{d}{dt}G^{<}(t,t) - \left[h(t), G^{<}(t,t)\right]_{-} = -\left[G^{\mathrm{R}} \cdot \Sigma^{<}_{\mathrm{tot}} + G^{<} \cdot \Sigma^{\mathrm{A}}_{\mathrm{tot}} + G^{\rceil} \star \Sigma^{\lceil}_{\mathrm{tot}}\right](t,t) + \mathrm{H.c.}$$

G. Stefanucci, R. Van Leeuwen – *Nonequilibrium many-body theory of quantum systems*

Numerical solutions of the KB Eqs



Integrals have to be performed up to the latest time

All matrices inside the square are needed

Each dot is a matrix

G. Stefanucci, R. Van Leeuwen – *Nonequilibrium many-body theory of quantum systems*

Dyson Equation
and its numerical solution

Why the Dyson equation?

"Mathematics is the language in which God has written the universe"

Galileo Galilei

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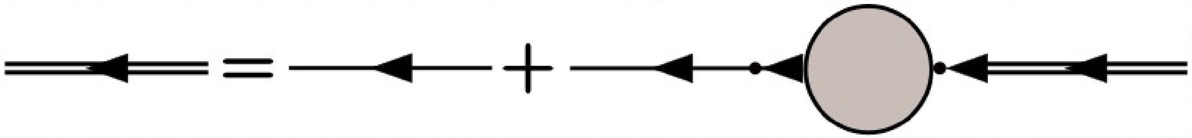
"… and every branch of science has its own dialect"

$$G(1;2) = G_0(1;2) + \int d3\, d4 G_0(1;3)\Sigma(2;4)G(4;2)$$

$G(1;2) =$ 

The Dyson equation

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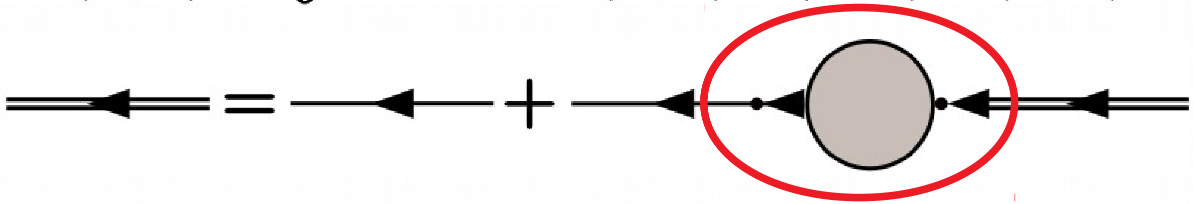
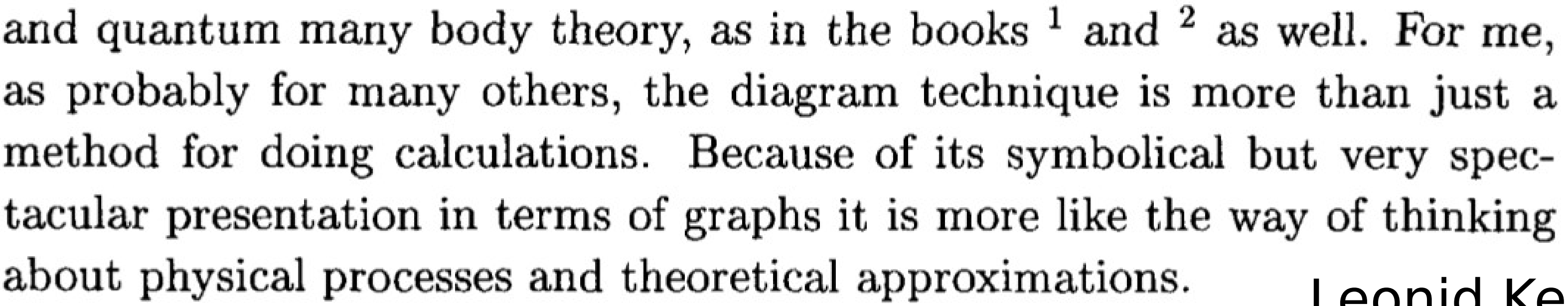
$G(1;2) =$ 

From drawings to physical processes


and quantum many body theory, as in the books [1] and [2] as well. For me, as probably for many others, the diagram technique is more than just a method for doing calculations. Because of its symbolical but very spectacular presentation in terms of graphs it is more like the way of thinking about physical processes and theoretical approximations.

Leonid Keldysh

From drawings to physical processes

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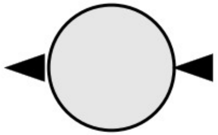
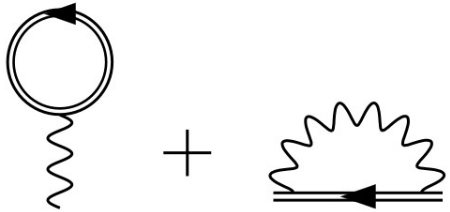
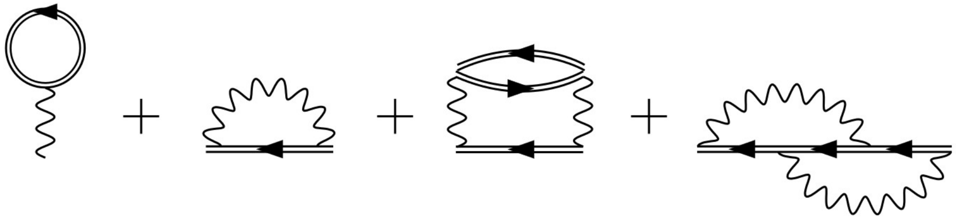
The menu of Self-energies



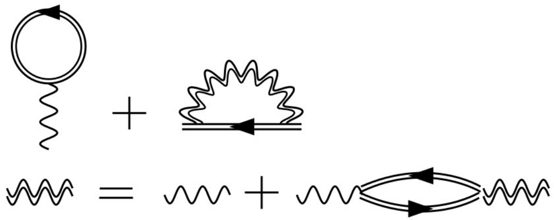
Hartree - Fock



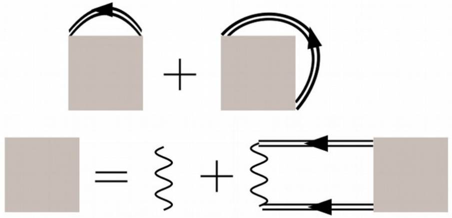
Second Born



GW (RPA)

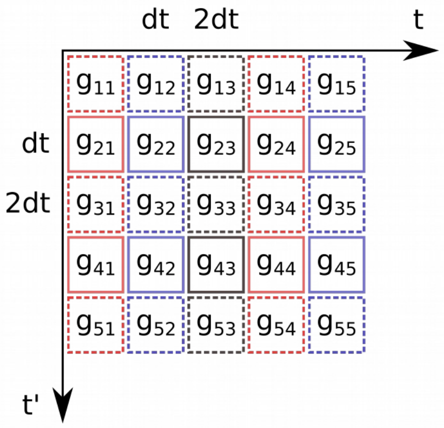


Ladder/T-Matrix



2D block cyclic distribution

$$G(1;2) = G_0(1;2) + \int d3\, d4 G_0(1;3)\Sigma(2;4)G(4;2)$$



N. Lo Gullo and L. Dell'Anna, PRB **94**, 184308 (2016); W. Talarico et al., arxiv:1809.10111

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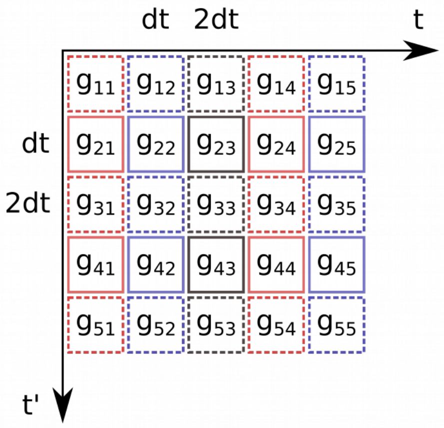

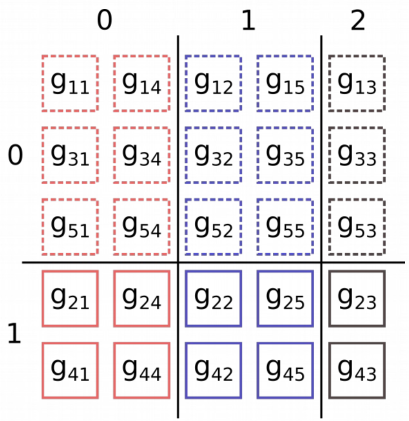

- Processes are elements in a process grid
- Each process receives chunk which contain a whole (t;t') point
- Each computation should minimize (avoid if possible) communication

N. Lo Gullo and L. Dell'Anna, PRB **94**, 184308 (2016); W. Talarico et al., arxiv:1809.10111

General scheme

General approach

$$G^{R/A}(t_n, t'_n) = [G_0^{R/A} + G_0^{R/A} \circ \Sigma^{R/A} \circ G^{R/A}](t_n, t'_n)$$

$$G^{\lessgtr}(t_n, t'_n) = [G_0^{\lessgtr} + G_0^{R} \circ \Sigma^{\lessgtr} \circ G^{A} + G_0^{\lessgtr} \circ \Sigma^{A} \circ G^{A} + G_0^{R} \circ \Sigma^{R} \circ G^{\lessgtr}](t_n, t'_n)$$

General approach

- Initialization $g_0(1;1')$

- Calculation of the self-energy $\Sigma(1;1')$
- Solution of the Dyson Equation

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Until convergence

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Until convergence

Checks: Symmetries, particle current due to MB SE

$$G^{\lessgtr}(1;1') = -[G^{\lessgtr}(1';1)]^*$$

$$G^R - G^A = G^> - G^<$$

$$I_{MB}(t) = 2\mathrm{Re}\{\mathrm{Tr}[\Sigma^<_{MB} \cdot G^A + \Sigma^R_{MB} \cdot G^<](t;t)\}$$

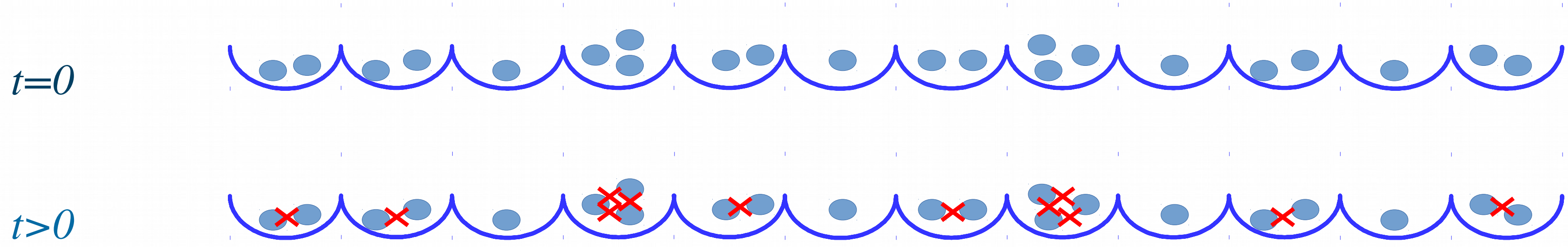
Quenches in bosonic systems

Interacting bosons

$$\hat{H} = \hat{H}_0 + \hat{V}(t)$$

$$\hat{H}_0 = \sum_i \epsilon_i \, \hat{b}_i^\dagger \hat{b}_i - \sum_{\langle i,j \rangle} \frac{J}{2} (\hat{b}_i^\dagger \hat{b}_j + \text{H.c.})$$

$$\hat{V}(t) = \frac{U(t)}{2} \sum_i \hat{b}_i^\dagger \hat{b}_i^\dagger \hat{b}_i \hat{b}_i$$

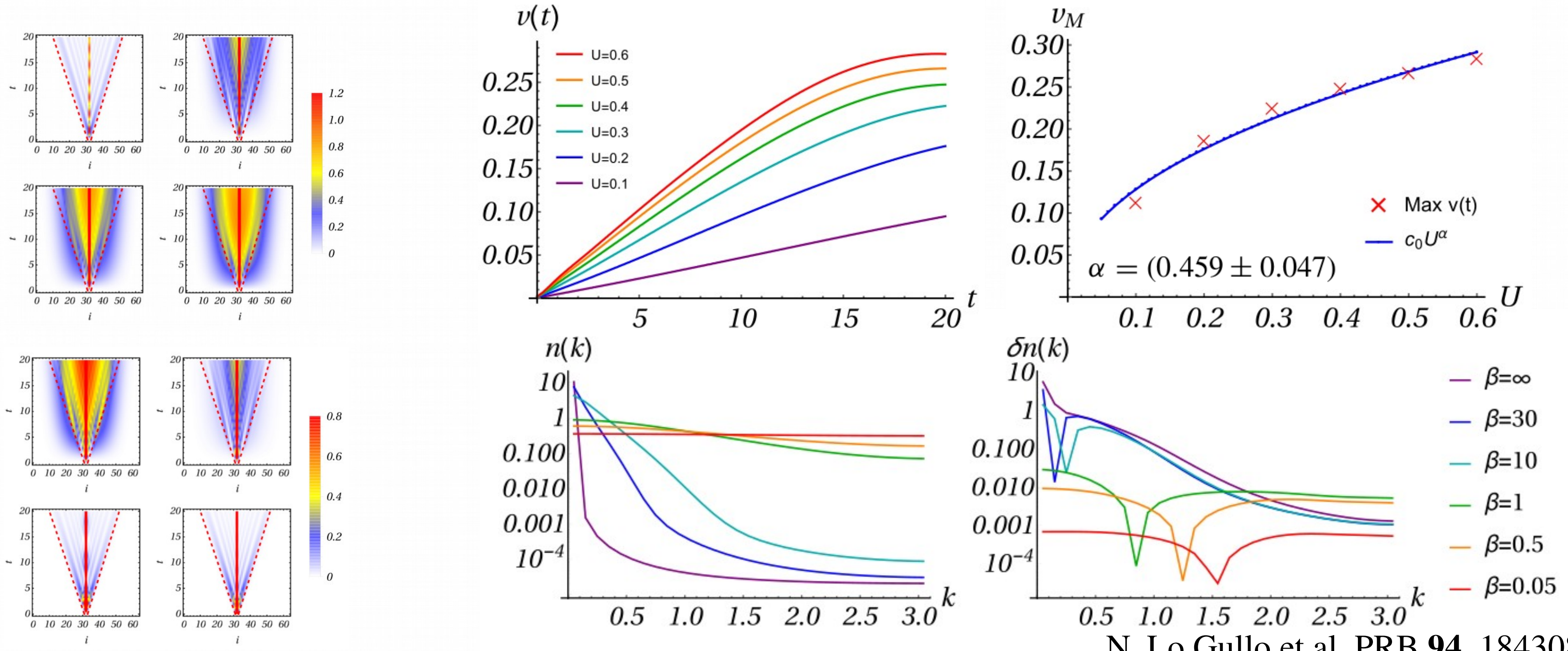


N. Lo Gullo et al, PRB **94**, 184308 (2016)

Propagation of correlations in 1D

$T=0$

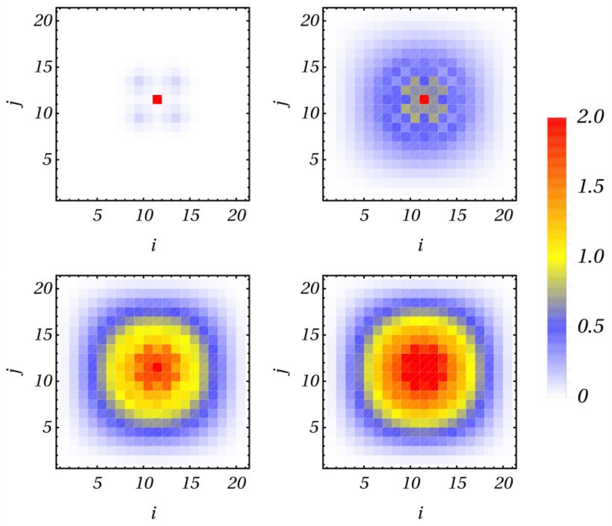
$T\neq0$



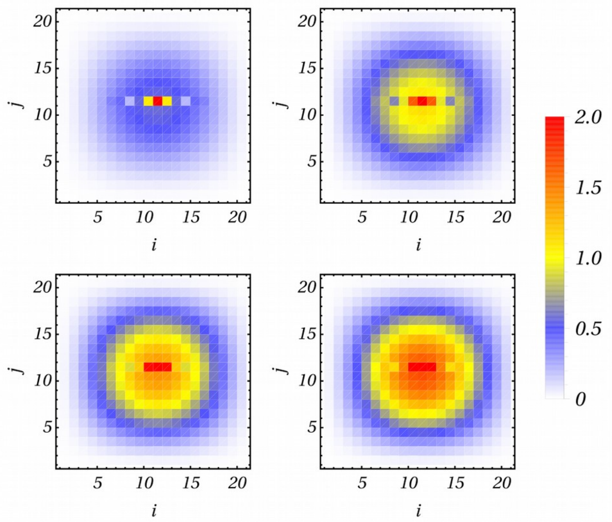
N. Lo Gullo et al, PRB **94**, 184308 (2016)

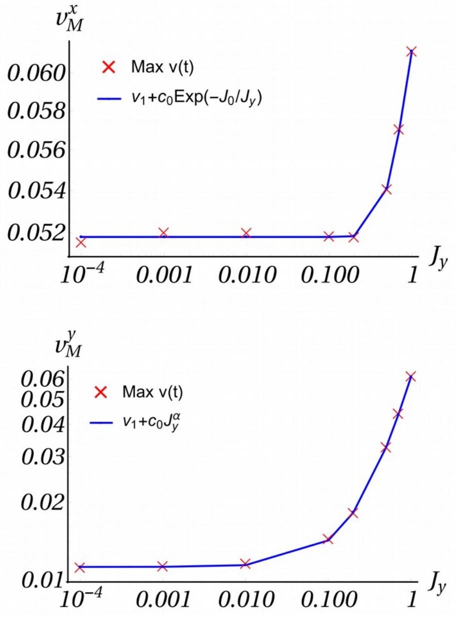
Propagation of correlations in 2D

Isotropic



Anisotropic





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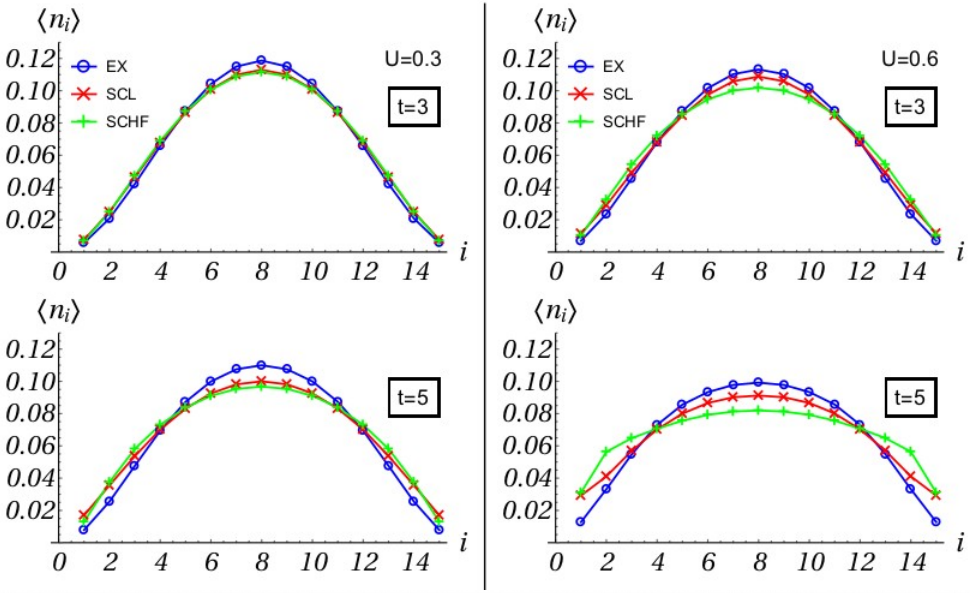
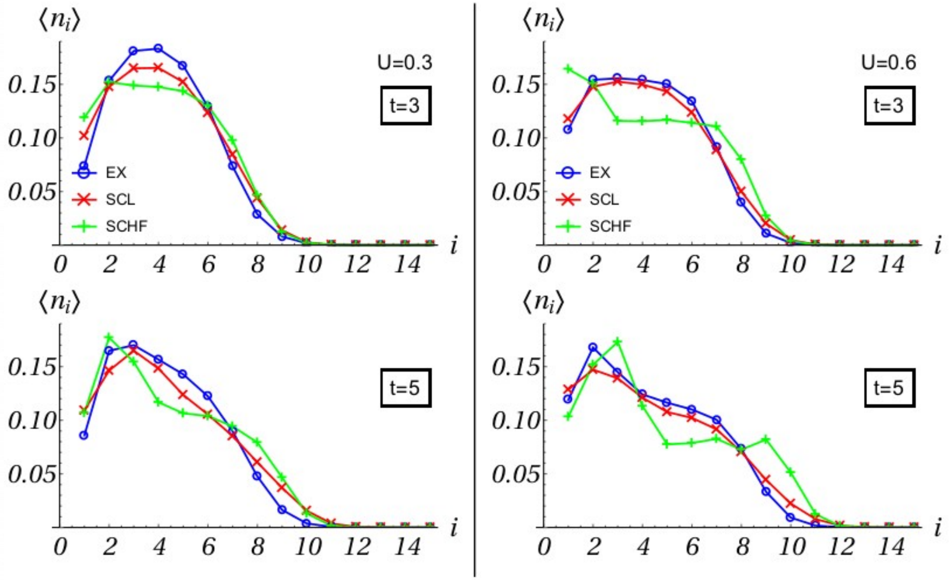
Comparison with ED

Homogeneous



Harmonic potential at i=2



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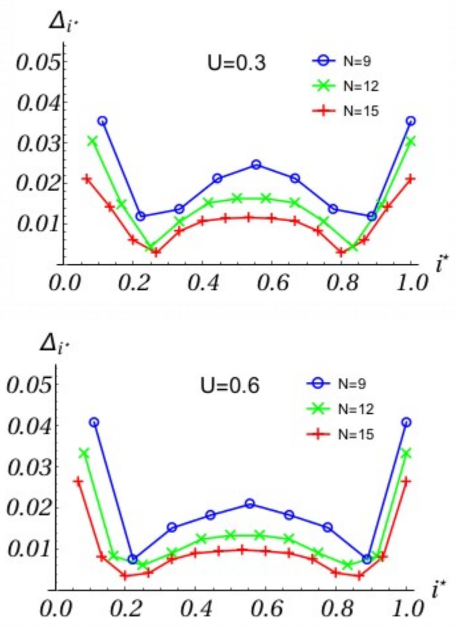

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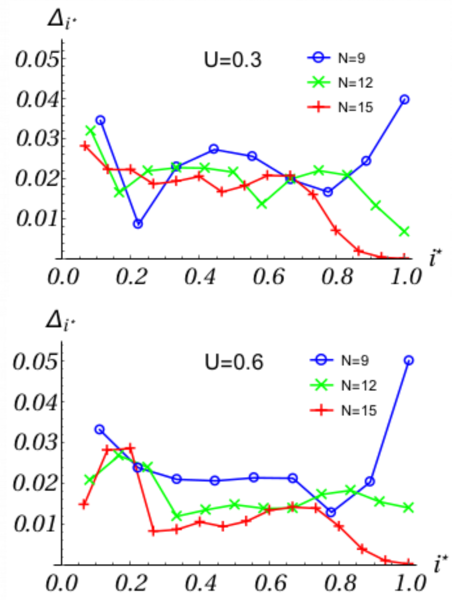


N. Lo Gullo et al, PRB **94**, 184308 (2016)

Anomalous diffusion in aperiodic geometries

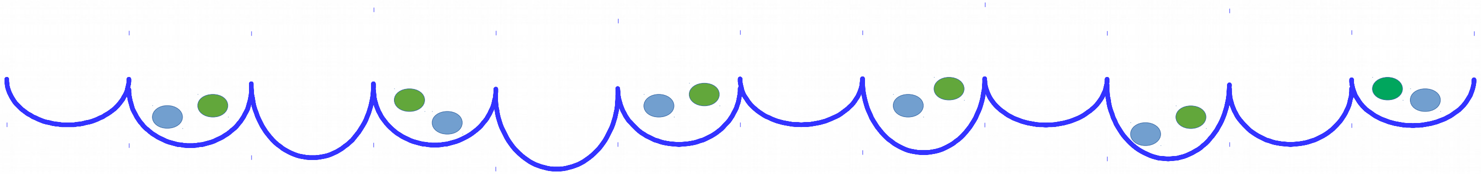
The model

$$\hat{H} = \hat{H}_0 + \hat{V}$$

$$\hat{H}_0 = \sum_{i\sigma} \epsilon_i \, \hat{n}_{i\sigma} - \frac{J}{2} \sum_{i\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{i+1\sigma} + \text{h.c.}$$

$$\hat{V} = U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

t=0



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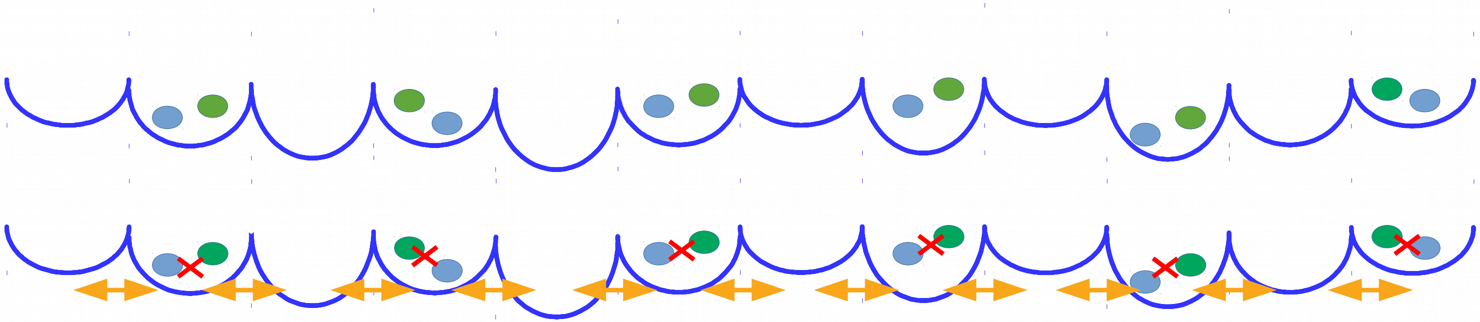
t=0

t>0



Non-interacting case

Aubry–André Model

$$\epsilon_i = \lambda \cos(2\pi\tau i)$$

Metal-to-insulator transition

Non-interacting case

Aubry–André Model

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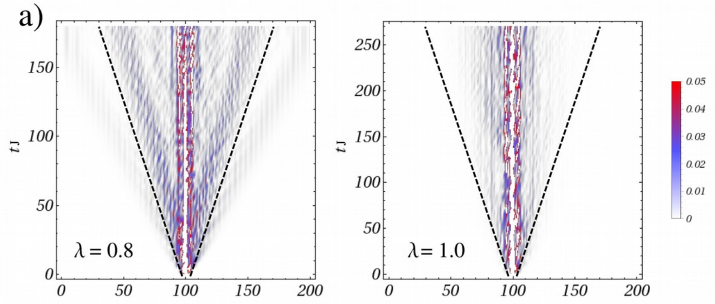

Spreading of correlations

$$P_i(t) = \left|G^<_{i_0 i}(0;t)\right|^2$$

A. Suto J. Stat. Phys. **56**, 525 (1989)

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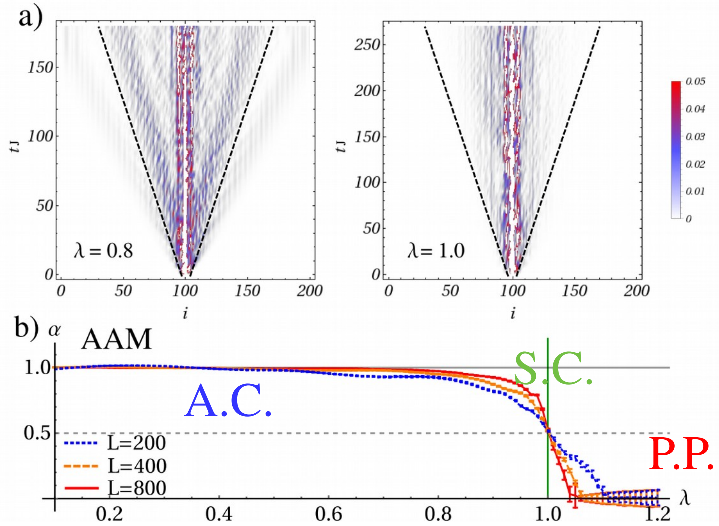
$$\sigma(t) \propto t^\alpha$$



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Non-interacting case

Aubry–André Model

$$\epsilon_i = \lambda \cos(2\pi\tau i)$$

Onsite Fibonacci Model

$$\epsilon_i = \lambda \left(\lfloor (i+1)/\tau \rfloor - \lfloor i/\tau \rfloor \right)$$

Spreading of correlations

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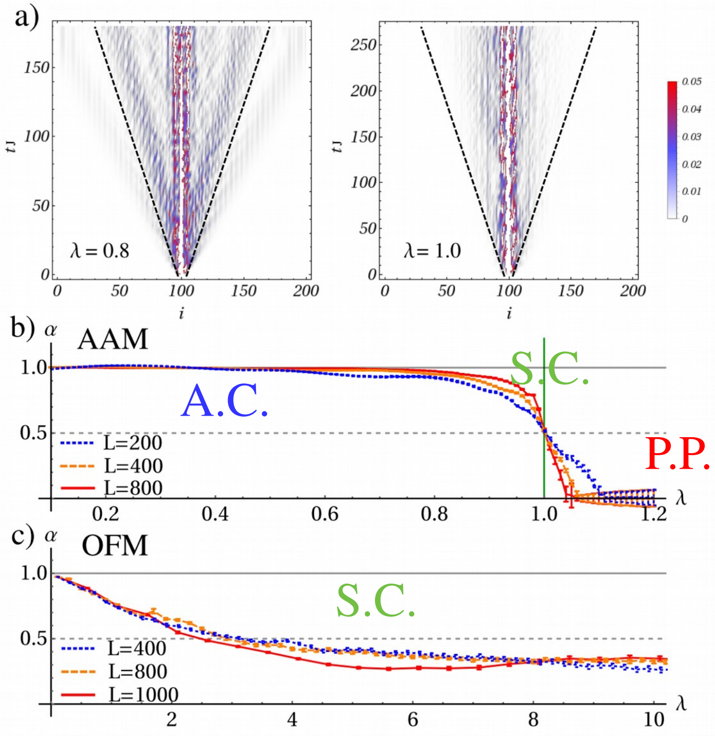

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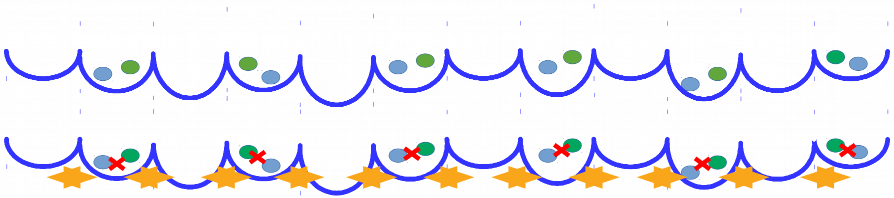
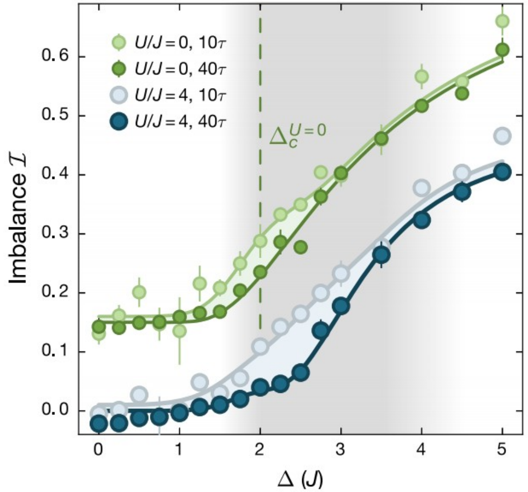
A.D. in interacting systems

t=0

t>0



$$\Delta N(t) = \frac{(N_e(t) - N_o(t))}{N_{tot}}$$



H.P. Luschen et al., Phys. Rev. Lett. **119**, 260401 (2017)

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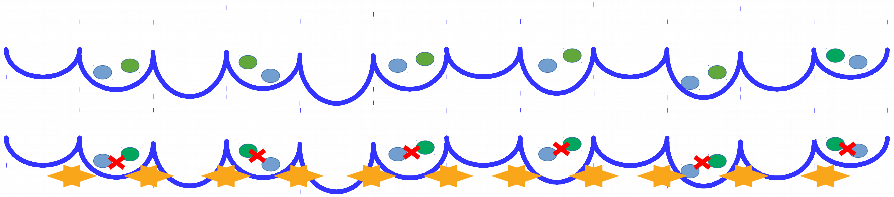

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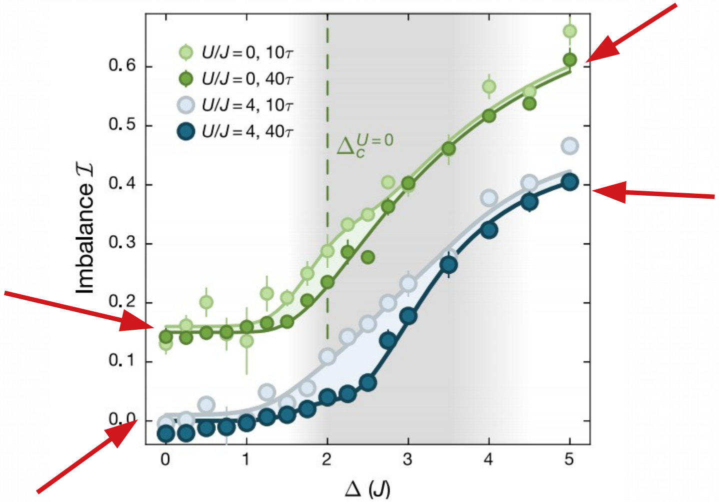

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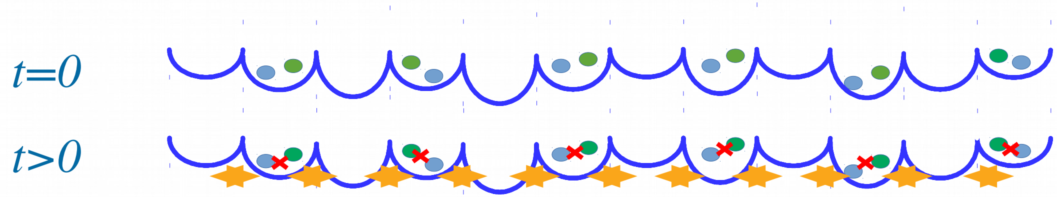

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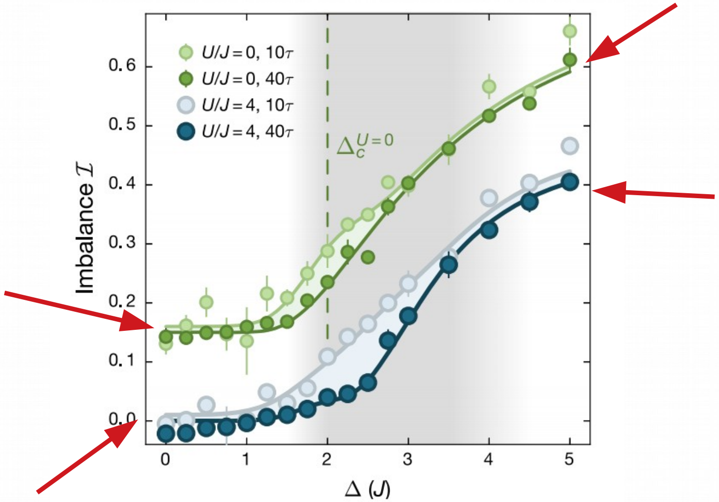

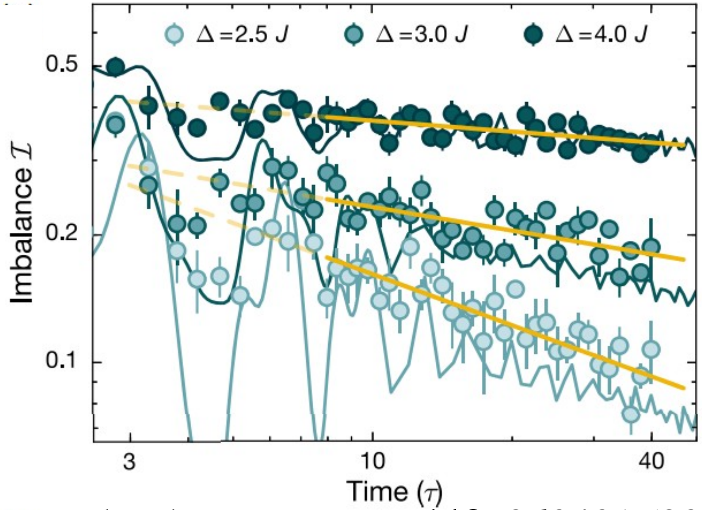

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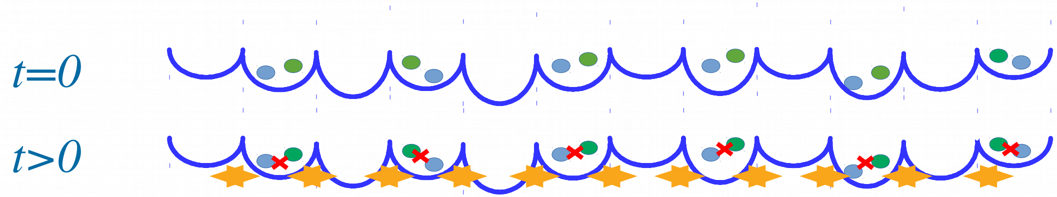

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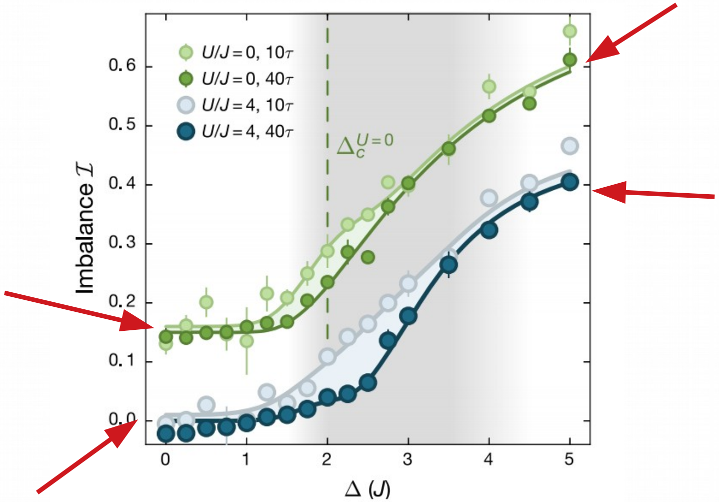

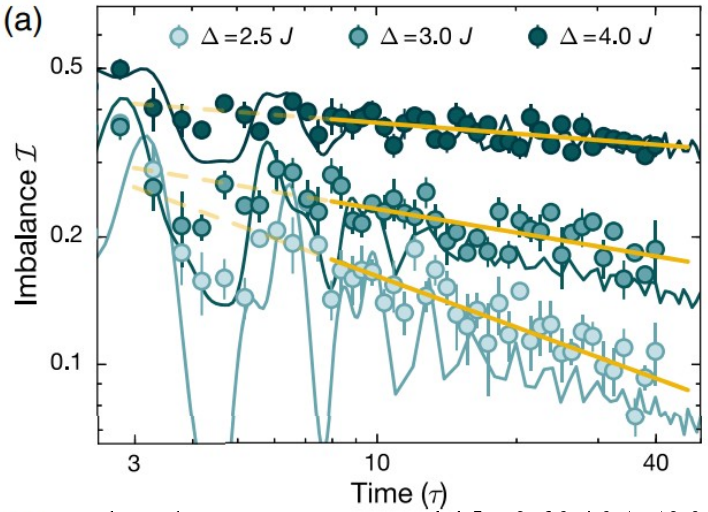

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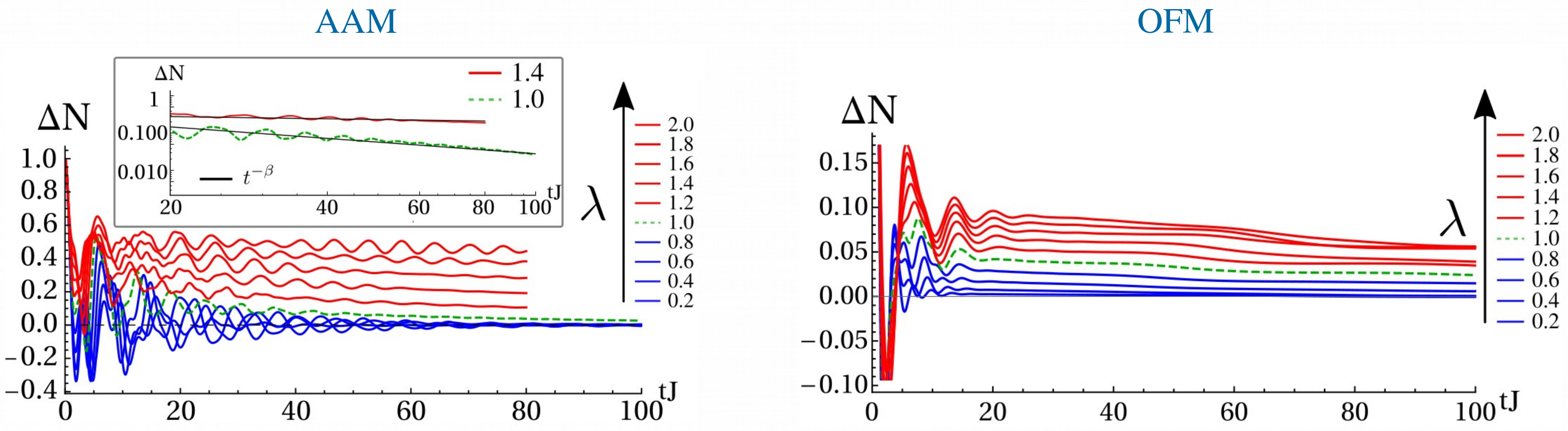
Geometry – interaction interplay (AAM)

Particle imbalance $\Delta N(t) = \frac{(N_e(t) - N_o(t))}{N_{tot}}$

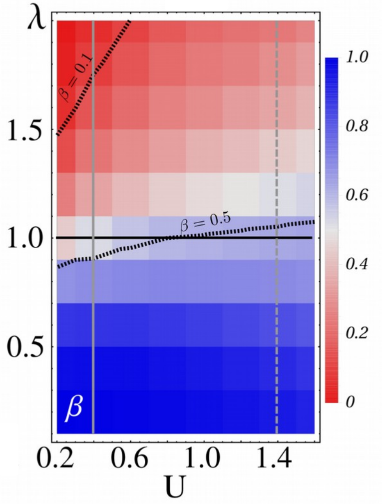


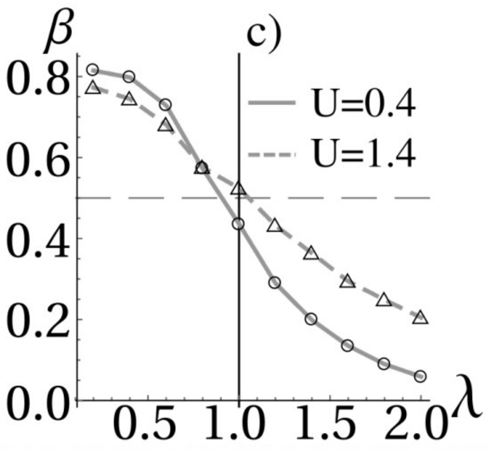
J. Settino et all, arxiv:1809.10524

Power law behavior

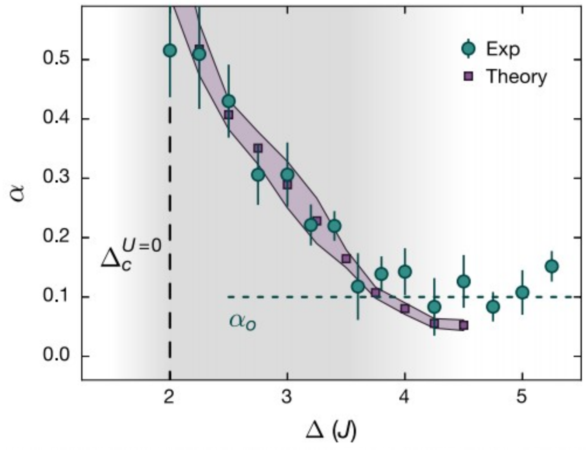
$$\Delta N(t) \approx a t^{-\beta} \quad t\, J \gg 1$$

Theory (NEGF)





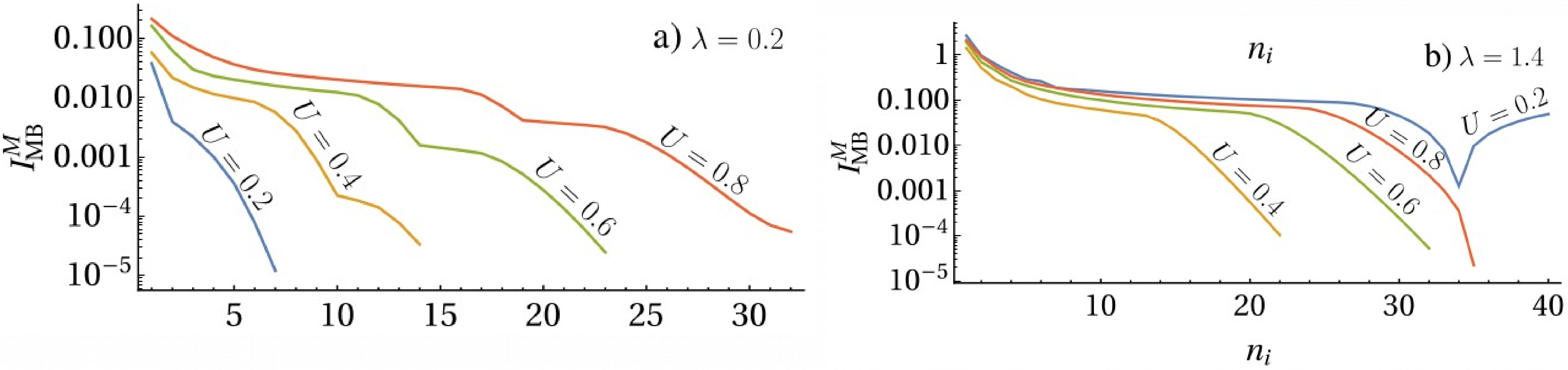
Experiment



J. Settino et all, arxiv:1809.10524

Convergency check

$$I_{MB}(t) = 2\mathrm{Re}\{\mathrm{Tr}[\Sigma^<_{MB} \cdot G^A + \Sigma^R_{MB} \cdot G^<](t;t)\}$$



W.N. Talarico et all, arxiv:1809.19111

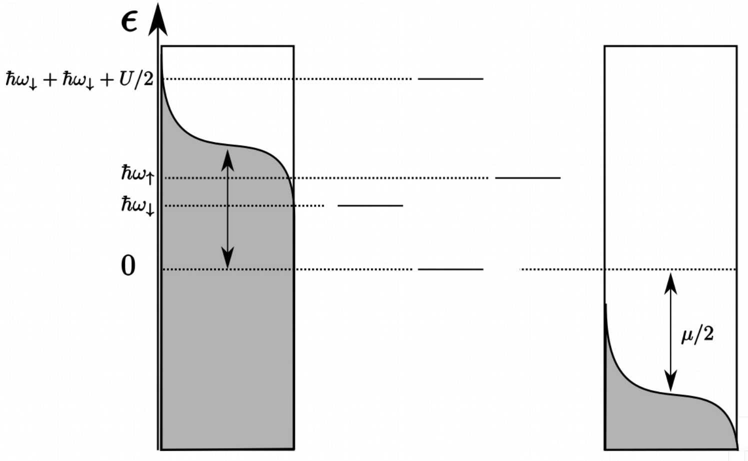
SIAM

The model

$$\hat{H} = \hat{H}_0 + \hat{V} + \hat{H}_{SL}$$

$$\hat{H}_0 = \sum_n \epsilon\ \hat{n}_\sigma$$

$$\hat{V} = U\hat{n}_\uparrow \hat{n}_\downarrow$$



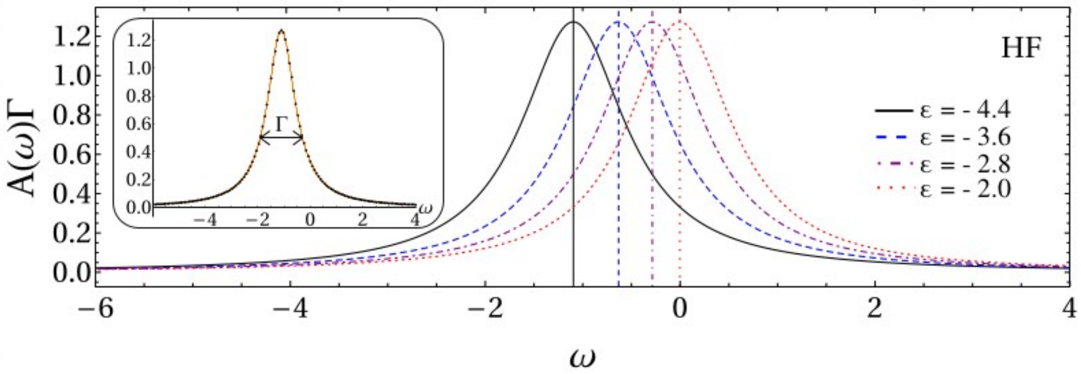
$$\hat{H}_{LS} = \sum_\alpha \sum_{k_\alpha \sigma} T_{k_\alpha \sigma,\alpha} \left[\hat{d}^\dagger_\sigma \hat{c}_{k_\alpha \sigma,\alpha} + \hat{c}^\dagger_{k_\alpha \sigma,\alpha} \hat{d}_\sigma\right]$$

Strong coupling
low temperature

Kondo regime

W.N. Talarico et all, arxiv:1809.19111

A signature of the Kondo regime



W.N. Talarico et all, arxiv:1809.19111

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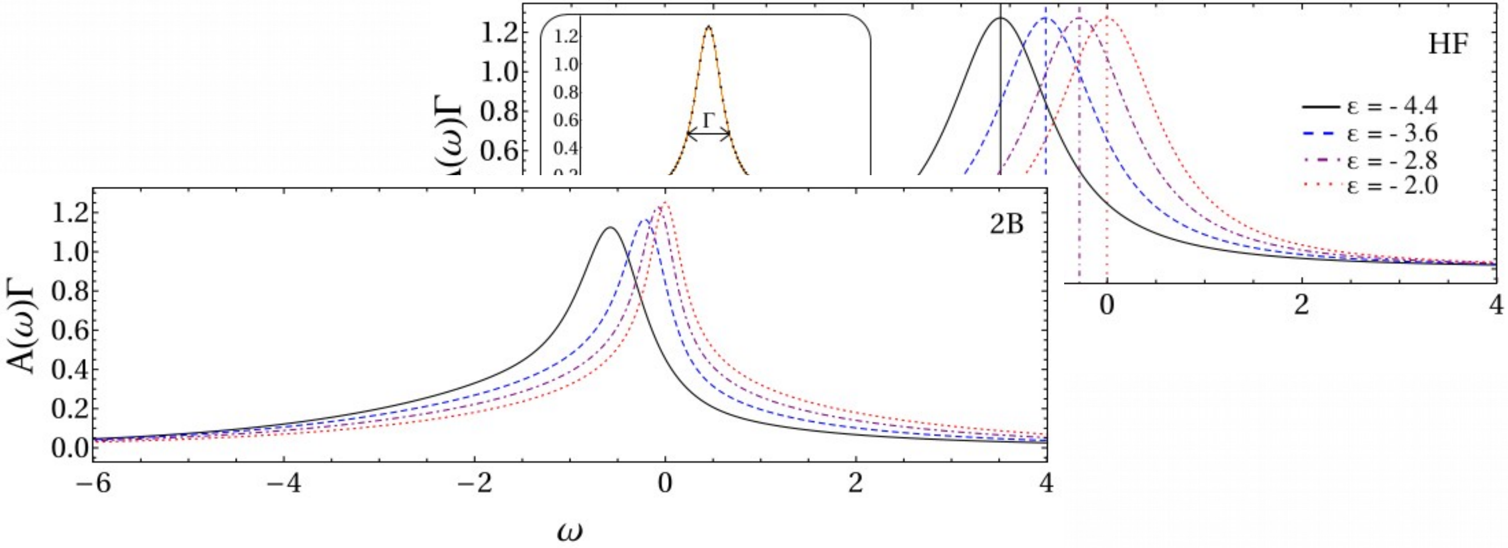

W.N. Talarico et all, arxiv:1809.19111

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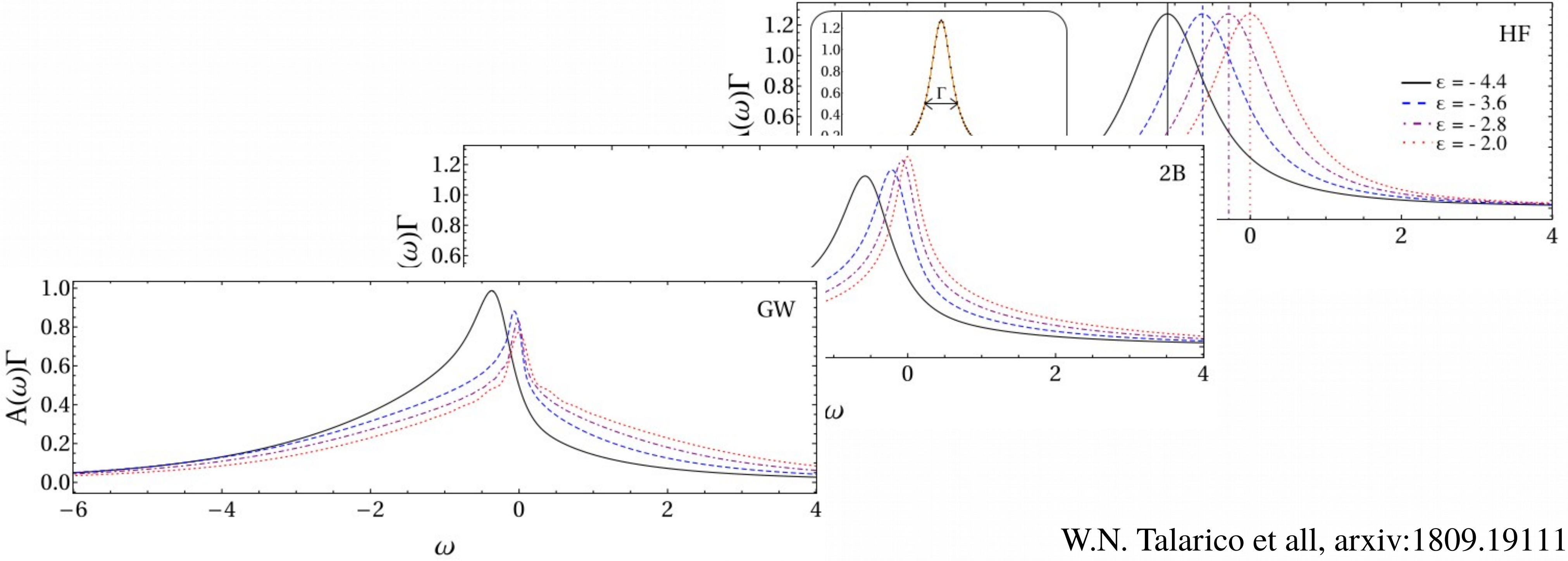
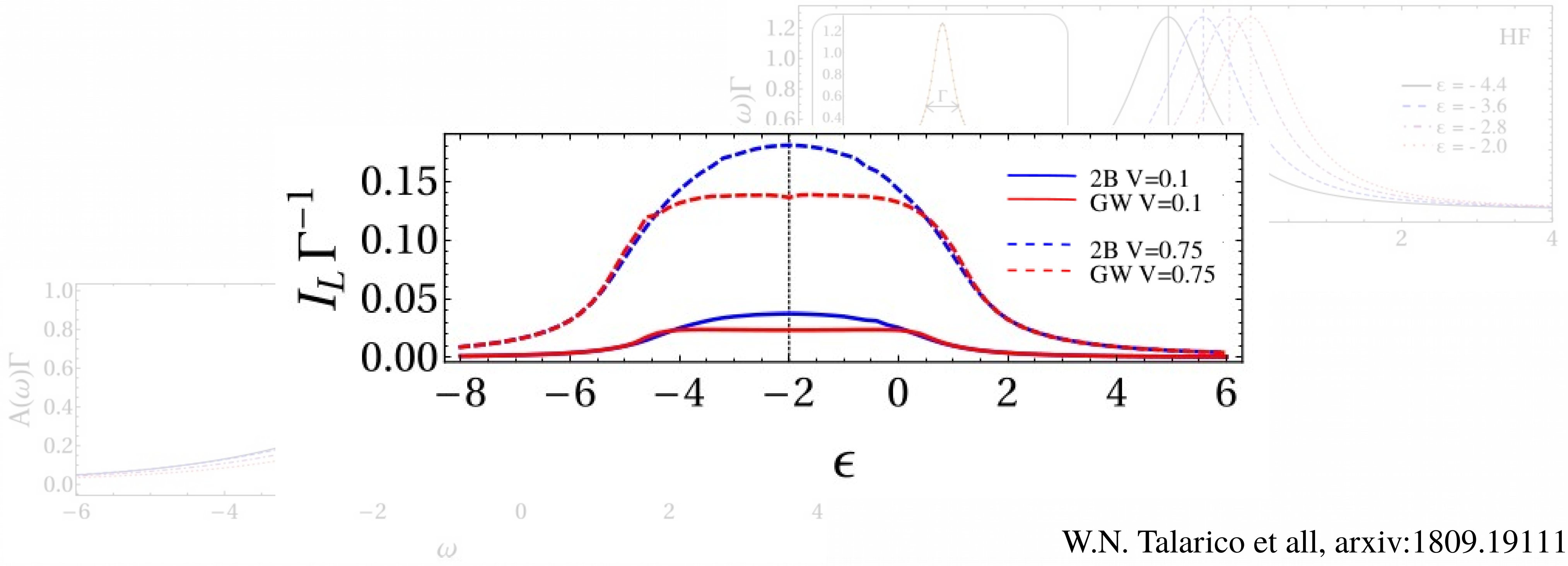


W.N. Talarico et all, arxiv:1809.19111

A signature of the Kondo regime



W.N. Talarico et all, arxiv:1809.19111

Open issues

The “inversion problem”

$$G^{R(l+1)}(t_n, t'_n) = [R^{R(l)} \circ G_0^R](t_n, t'_n)$$

$$R^{R(l)}(t_n, t'_n) = [(\mathrm{Id}_t - G_0^R \circ \Sigma^{R(l)})^{-1}](t_n, t'_n)$$

We need one inversion of a (ns × nt) × (ns × nt)

The "inversion problem" : eliminate the problem

$$G^{R(l+1)}(t_n, t'_n) = [R^{R(l)} \circ G_0^R](t_n, t'_n)$$

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We need one inversion of a (ns × nt) × (ns × nt)

Is it possible to avoid it? (In the KBE there is no inversion)

The "inversion problem" : eliminate the problem

$$G^{R(l+1)}(t_n, t'_n) = [R^{R(l)} \circ G_0^R](t_n, t'_n)$$

$$R^{R(l)}(t_n, t'_n) = [(\mathrm{Id}_t - G_0^R \circ \Sigma^{R(l)})^{-1}](t_n, t'_n)$$

We need one inversion of a (ns × nt) × (ns × nt)

Using, in the collisional integrals, the relation (?)

$$G^R(t;t') = \theta(t-t')\,(G^>(t;t') - G^<(t;t'))$$

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We need one inversion of a (ns × nt) × (ns × nt)

Using, in the collisional integrals, the relation (?)

$$G^R(t;t') = \theta(t-t')(G^>(t;t') - G^<(t;t'))$$

What about the singular parts? (Single-particle spectrum at HF level)

The “inversion problem” : one out, one in

$$G^R(t;t') = \theta(t-t')\left(G^>(t;t') - G^<(t;t')\right)$$

Drive (but let us drop the HF part) $\hat{h} \rightarrow \hat{h}(t)$

The "inversion problem" : one out, one in

$$G^R(t;t') = \theta(t-t')\,(G^>(t;t') - G^<(t;t'))$$

Drive (but let us drop the HF part) $\hat{h} \to \hat{h}(t)$

$$g_0(1;1') \to G_0(1;1')$$

Only one inversion

$$G(1;1') = G_0(1;1') + G_0 \circ \Sigma \circ G(1;1')$$

$$A^R(t;t') = \theta(t-t')\,(A^>(t;t') - A^<(t;t'))$$

Turun yliopisto
University of Turku

The “inversion problem” : one out, one in

$$G^R(t;t') = \theta(t-t')\left(G^>(t;t') - G^<(t;t')\right)$$

What about the HF?

The “inversion problem” : one out, one in

$$G^R(t;t') = \theta(t-t')\,(G^>(t;t') - G^<(t;t'))$$

What about the HF?

$$g_0(1;1') \rightarrow G_0^{HF}(1;1')$$

$$G(1;1') = G_0^{HF}(1;1') + G_0^{HF} \circ \Sigma \circ G(1;1')$$

The “inversion problem” : one out, one in

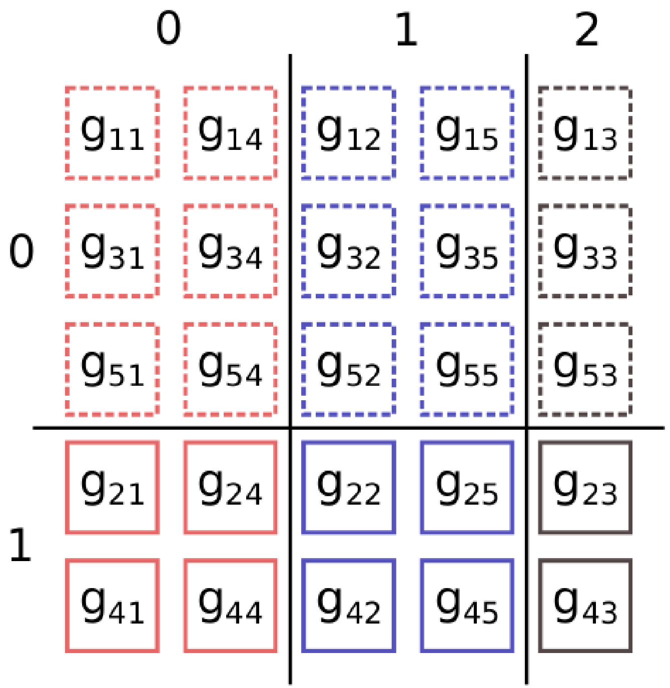
$$G^R(t;t') = \theta(t-t')\,(G^>(t;t') - G^<(t;t'))$$

What about the HF?

$$g_0(1;1') \rightarrow G_0^{HF}(1;1')$$

$$G(1;1') = G_0^{HF}(1;1') + G_0^{HF} \circ \Sigma \circ G(1;1')$$

Perhaps there is gain if done locally



The “inversion problem” : one out, one in

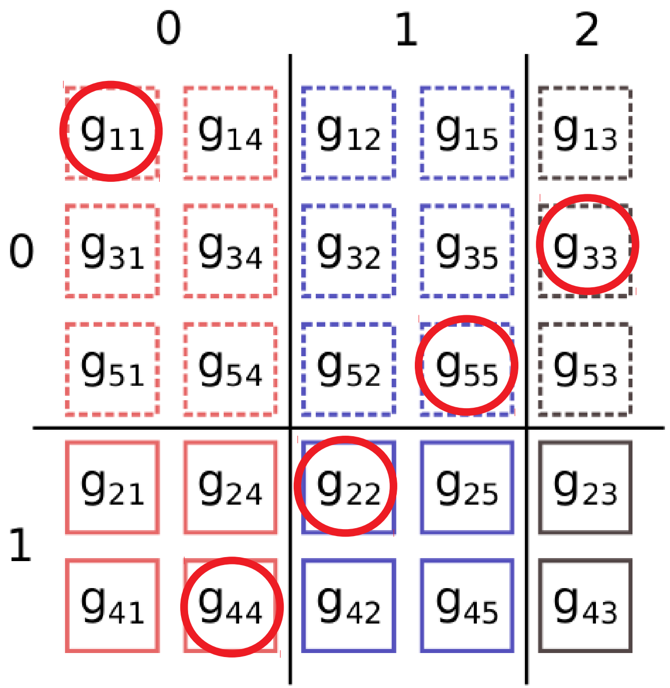
$$G^R(t;t') = \theta(t-t')\left(G^>(t;t') - G^<(t;t')\right)$$

What about the HF?

$$g_0(1;1') \rightarrow G_0^{HF}(1;1')$$

$$G(1;1') = G_0^{HF}(1;1') + G_0^{HF} \circ \Sigma \circ G(1;1')$$

Yes, but in a clever way



Improve integration scheme

$$[a \circ b](t_n, t'_m) = \sum_{p=0}^{n_t - 1} w_p \, a(t_n, t_p) b(t_p, t'_m)$$

Homogeneous grid $w_p = dt$

Improve integration scheme

$$[a \circ b](t_n, t'_m) = \sum_{p=0}^{n_t-1} w_p \, a(t_n, t_p) b(t_p, t'_m)$$

Choose different weights to improve the propagation scheme

Improve integration scheme

$$[a \circ b](t_n, t'_m) = \sum_{p=0}^{n_t-1} w_p \, a(t_n, t_p) b(t_p, t'_m)$$

Choose different weights to improve the propagation scheme

One has to be careful to certain issues

Improve integration scheme

$$[a \circ b](t_n, t'_m) = \sum_{p=0}^{n_t - 1} w_p \, a(t_n, t_p) b(t_p, t'_m)$$

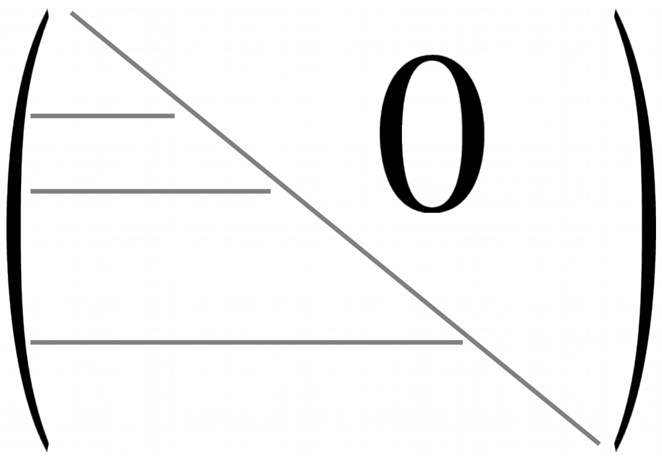
Choose different weights to improve the propagation scheme

One has to be careful to certain issues : identiy

$$\Delta(t_n, t_m) = \frac{\delta_{nm}}{w_n}$$

Improve integration scheme

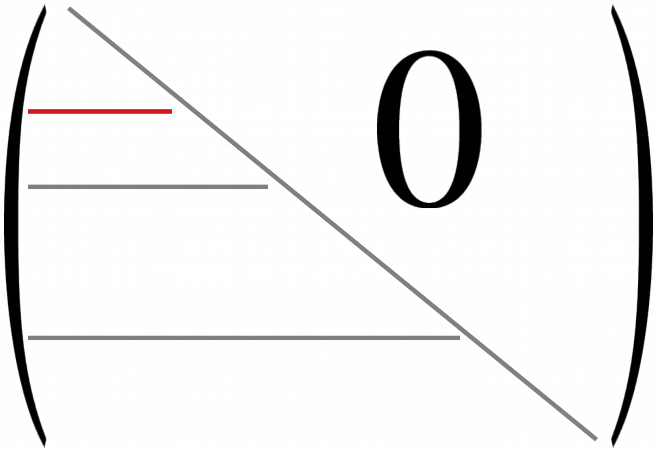
One has to be careful to certain issues : the integration interval



$$[a \circ b](t_n, t'_m) = \sum_{p=0}^{n_t - 1} w_p \; a(t_n, t_p) b(t_p, t'_m)$$

Improve integration scheme

One has to be careful to certain issues : the integration interval



$$[a \circ b](t_n, t'_m) = \sum_{p=0}^{n_t-1} w_p \; a(t_n, t_p) b(t_p, t'_m)$$

Improve integration scheme

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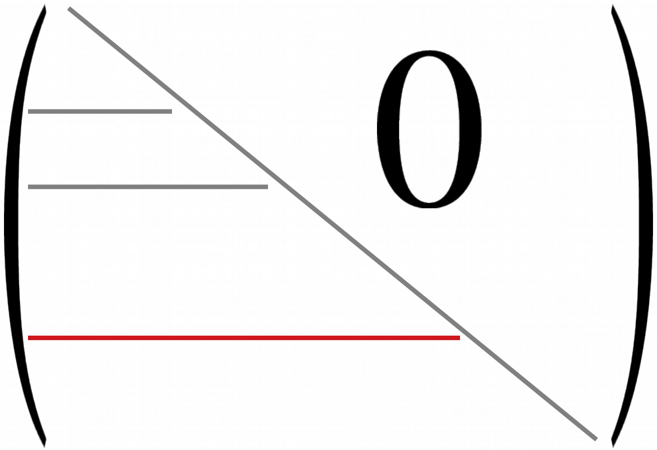

$$[a \circ b](t_n, t'_m) = \sum_{p=0}^{n_t - 1} w_p \; a(t_n, t_p) b(t_p, t'_m)$$

Improve integration scheme

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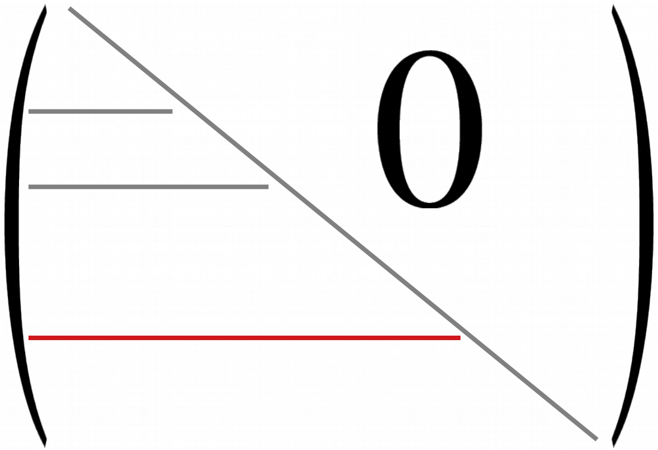
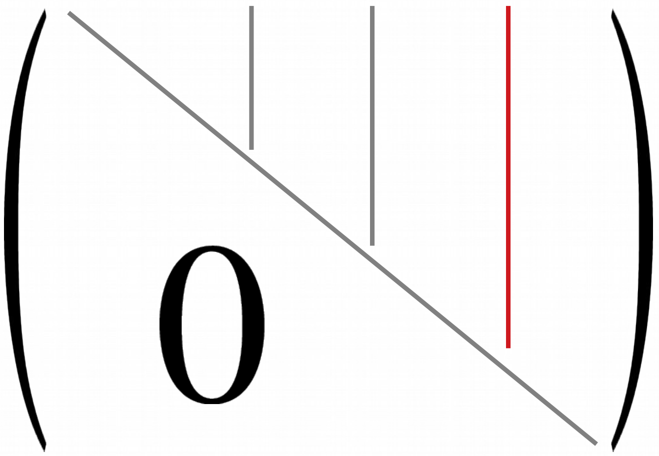


$$[a \circ b](t_n, t'_m) = \sum_{p=0}^{n_t - 1} w_p \, a(t_n, t_p) b(t_p, t'_m)$$

$$w_p \to w_p^{(n)}$$

Improve integration scheme

One has to be careful to certain issues : the integration interval



$$[a \circ b](t_n, t'_m) = \sum_{p=0}^{n_t - 1} w_p \, a(t_n, t_p) b(t_p, t'_m)$$

$$w_p \rightarrow w_p^{(m)}$$

Improve integration scheme

One has to be careful to certain issues : the inverse

$$\sum_p w_p^{(n)} K^R(t_n; t_p) G^R(t_p; t'_m) = g_0^R(t_n; t'_m)$$

Improve integration scheme

One has to be careful to certain issues : the inverse

$$\sum_p w_p^{(n)} K^R(t_n;t_p) G^R(t_p;t'_m) = g_0^R(t_n;t'_m)$$

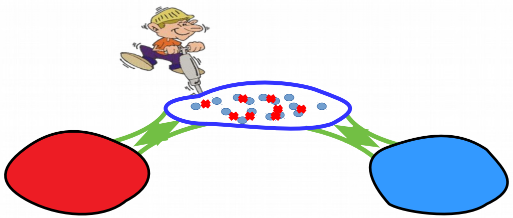
Improve integration scheme

One has to be careful to certain issues : the inverse

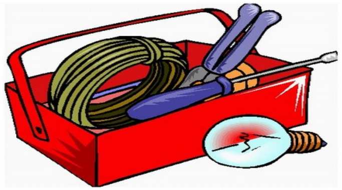
$$\sum_p w_p^{(n)} K^R(t_n;t_p) G^R(t_p;t'_m) = g_0^R(t_n;t'_m)$$

$$\sum_p w_p^{(n)} (K^R)^{-1}(t_n;t_p) K^R(t_p;t'_m) = \Delta(t_n;t'_m) = \frac{\delta_{nm}}{w_n^{(n)}}$$

Next



- Solve the "inverse problem"



- Distribute the library
- Extend it to other approximations and systems

Turku Collegium
for Science and Medicine

Turun yliopisto
University of Turku

Funding

ACADEMY OF FINLAND

HPC Europa3

Computational facilities

UNIVERSITÀ DELLA CALABRIA

MaTeRiA
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