Condensed matter systems out of equilibrium

Theory and numerical implementations

COMPUTE 2012

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The division of Mathematical Physics

- Solid State Theory:
  - Claudio Verdozzi (COMPUTE contact)
  - Carl-Olof Almbladh
  - Ulf von Barth
  - Ferdi Aryasetiawan
  - Phd students:
    - Alexey Kartsev
    - Daniel Karsson
    - Valeria Vettchinkina
    - Marc Puig von Friesen
    - 2 new PhD students coming soon
- Common research area:
  Condensed matter systems in and out of equilibrium

Other groups:

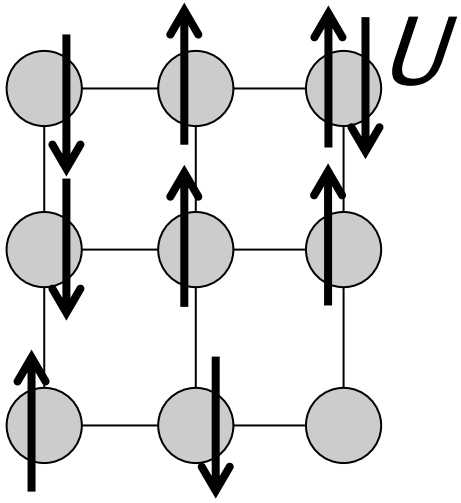
S. Reimann (Mesoscopic Physics)
A. Wacker (Quantum Transport)
P. Samuelsson (Quantum Information)
S. Åberg (Nuclear Structure)
I. Ragnarsson (Nuclear Structure)
T. Brage (Atomic physics)

Condensed matter systems out of equilibrium at the nanoscale

- Numerous applications:
  - Quantum transport
  - Cold atoms in optical lattices
  - Spin transport
  - Quantum information
  - Transient effects
  - …

- **Major challenge**:
  Strongly correlated systems out of equilibrium

The Hubbard model: Our favourite toy model



- Strongly correlated lattice model
- Fermions tunnel to different sites, experience contact interaction
- Can describe metals, spin physics, electron transport etc.
- Simple enough to solve exactly for small systems: Numerical experiments possible

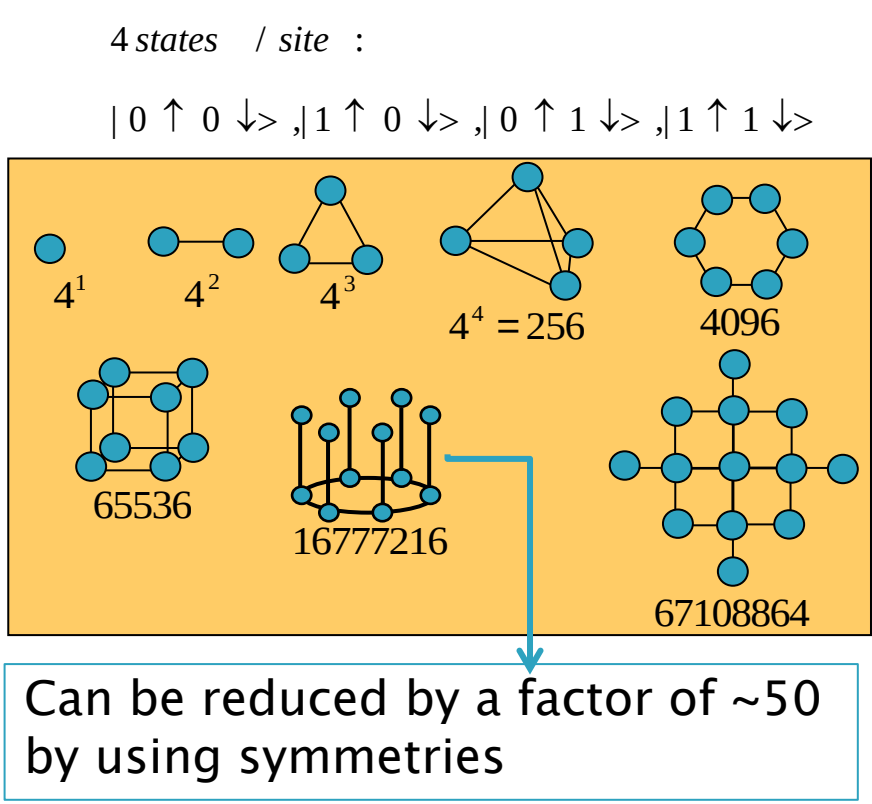
Solving the model

Time independent Schrödinger equation: $\mathbf{H}\,\psi = E\,\psi$
Energies / eigenstates: Diagonalizing Hamiltonian matrix **H**

Time dependent Schrödinger equation: $i\frac{d\psi}{dt} = \mathbf{H}(t)\psi$
Time propagate using various algorithms

Method 1: Exact Diagonalization

- **Basic variable**: Wave function
- **Method**: Solve by finding a basis and calculate ground state / time propagate with diagonalization.



Can be reduced by a factor of ~50 by using symmetries

- **Advantages**: Exact, Can benchmark other methods, get results of physical interest in few body problems
- **Limitations**: Only small systems manageable

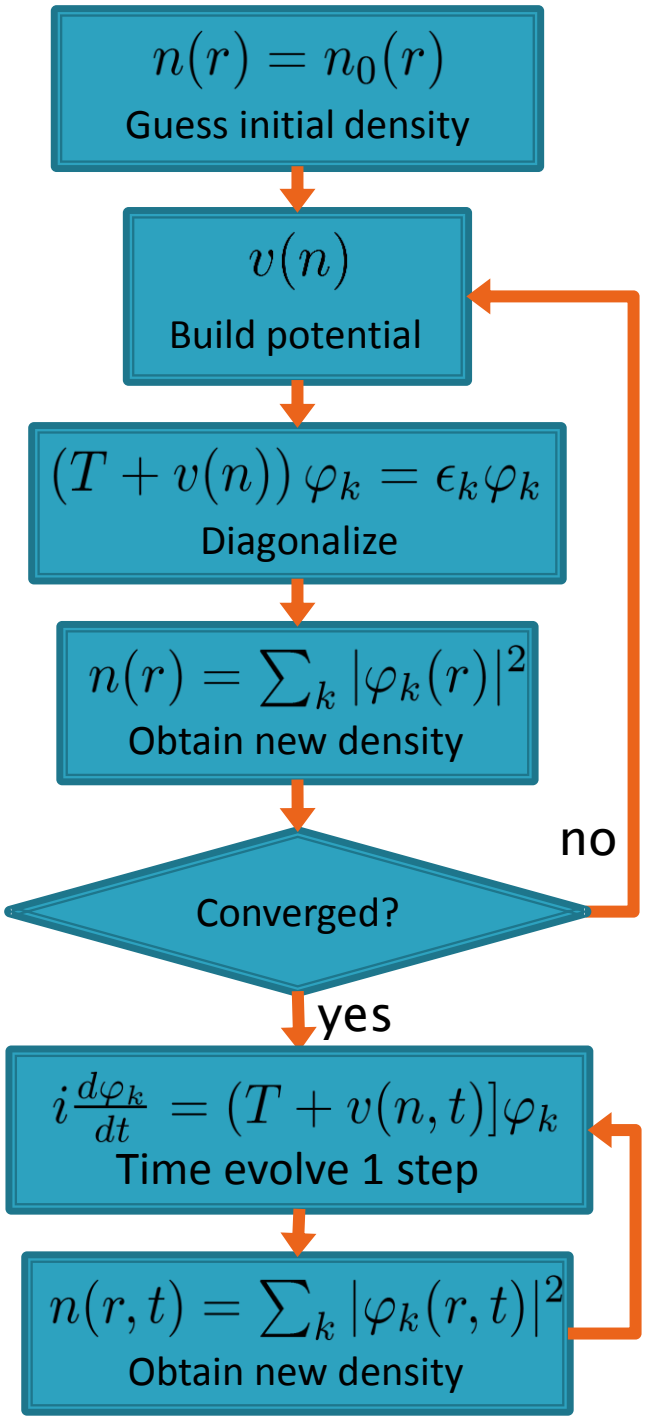
Lanczos algorithm avoids having to diagonalize the full matrix, useful for low lying states

$$H = \begin{pmatrix} \alpha_1 & \beta_2 & & & & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & & \beta_m & \alpha_m \end{pmatrix}$$

Method 2: Time Dependent Density Functional Theory

- **Basic variable**: Density
- **Method**: Solving non-interacting single-particle equations for ground state and dynamics
  Price: Density dependent effective potential => self-consistent procedure

- **Advantages**: Computationally inexpensive. Easy to implement.
- **Limitations**: Approximations hard to improve. No history dependence (Adiabatic approximation)



Method 3: Non-Equilibrium Green functions

- **Basic variable**: Single-particle Green function

$$G(12) = -i\langle T_C \left[\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\right]\rangle$$

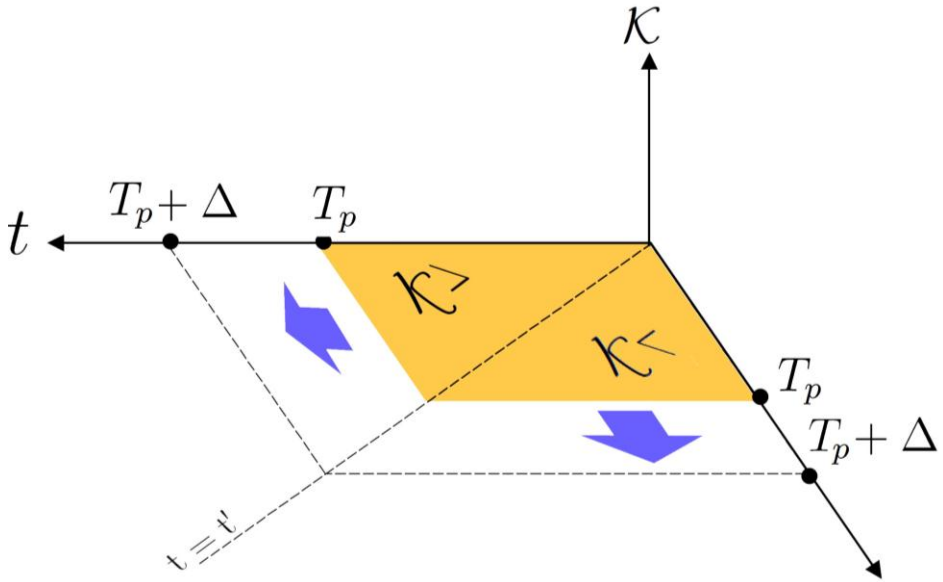
- **Method**: Solve self-consistent integral equations involving self-energy

$$(i\partial_{t_1} - h(t_1))\, G(t_1, t_2) = \delta(t_1, t_2) + \int_C \Sigma(t_1, t)\, G(t, t_2)\, dt$$

Non-interacting

Self-energy: Interactions

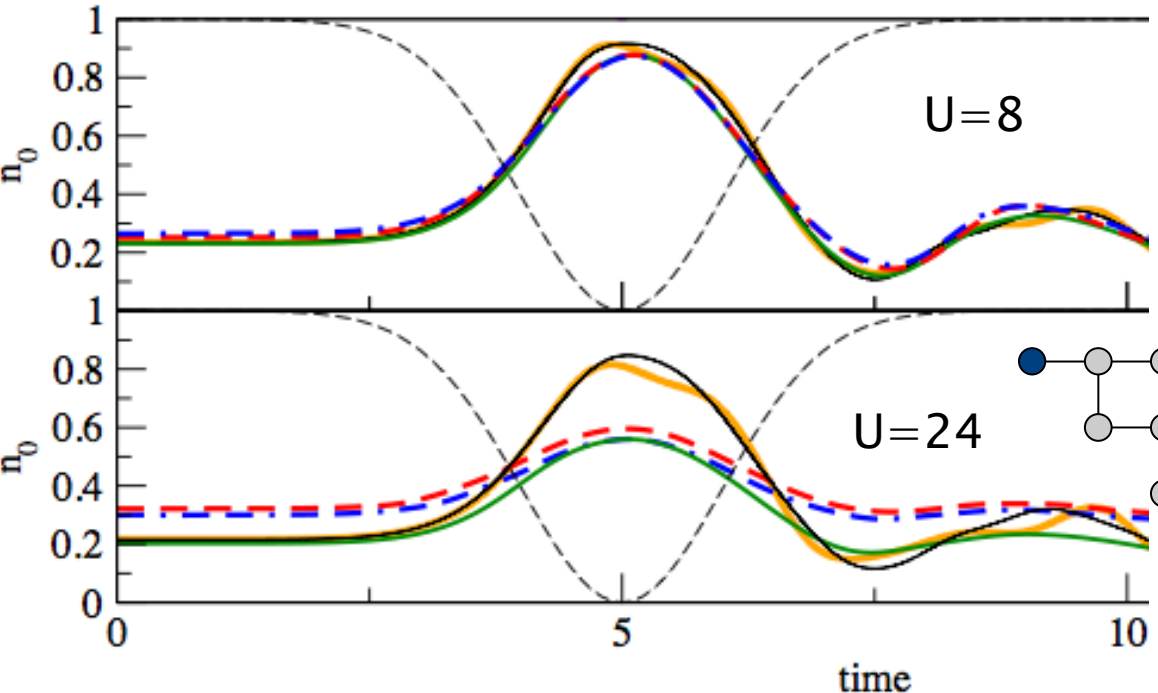
- **Advantages**: Can treat infinite systems, can be improved systematically
- **Limitations**: Computationally expensive. Two times: time propagation on square



Example of group work

- Benchmarking new effective potentials for use in 3 dimensions.
- Potential applications: Cold atoms
- Able to assess strengths and weaknesses of TDDFT and Green functions.

No approximation captures all the physics: Need to go beyond existing methods



Computational times:

Method 1: Exact diagonalization

~1 hour

Method 2: TDDFT

~1 minute

Method 3: Green function

~1 day

Summary of group work

- **In short, we do**
  - Development of new effective (exchange-correlation) potentials for use in TDDFT
  - Development of many-body methods to obtain new self-energies
  - Application to dynamics of ultracold atoms in optical lattices
- **Computational Outlook**
  - Treat larger matrices
  - Longer time propagations
  - Self-consistency calculations for larger systems
  - Solve non-linear equations more efficiently
  - ...
  - Parallelization feasible route?

For more information, see some of our articles
Verdozzi et al, Chem. Phys. **39**, 1 (2011)
Karlsson et al, Phys. Rev. Lett. **106**, 116401 (2011)

$$size = \binom{N_{\uparrow}}{L}\binom{N_{\downarrow}}{L}$$

Planned future research activity

Theoretical and computational research in non-equilibrium dynamics at the nanoscale.

Motivation

The variety of fascinating behaviors of matter in non-equilibrium

* Topology and low-dimensionality can enhance electronic correlations

novel physical behavior in a small systems coupled to a changing environment

* Inter-particle interactions tunable experimentally.

Promise of novel, groundbreaking technologies.

* Future nanodevices will operate under ever faster fields

Today's marginal transient effects: center stage features.

Major theoretical challenge:

Describing strong electronic correlations away from equilibrium

Essential feature: cannot be described effectively via non-interacting entities.

How ?

* Insight from models:

Even this field is at a very initial stage

* However for a quantitative study of the transient device response:

Ab-initio level required

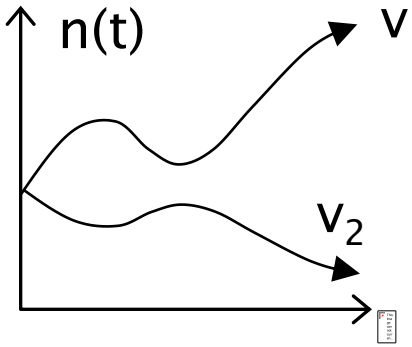
TDDFT schematics I : Runge-Gross Theorem (RGT)

$$\left[i\frac{\partial}{\partial t} - (\hat{T} + \hat{V}_1(t) + \hat{W})\right] \Psi_1(t) = 0$$

$$\left[i\frac{\partial}{\partial t} - (\hat{T} + \hat{V}_2(t) + \hat{W})\right] \Psi_2(t) = 0$$

$$\Psi_1(t_0) = \Psi_2(t_0) = \Psi_0$$

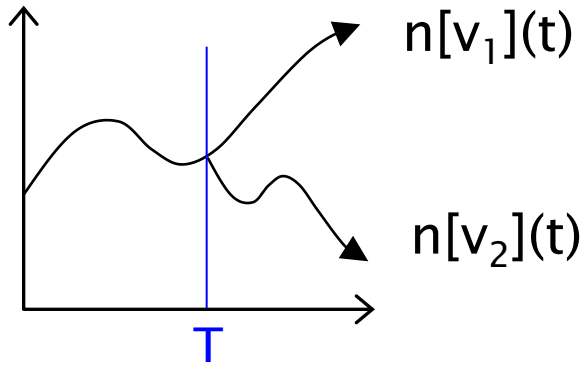
$$\hat{V}_1(t) \neq \hat{V}_2(t) + C(t) \Rightarrow n_1(t) \neq n_2(t)$$



Any observable is functio of density and initial sta

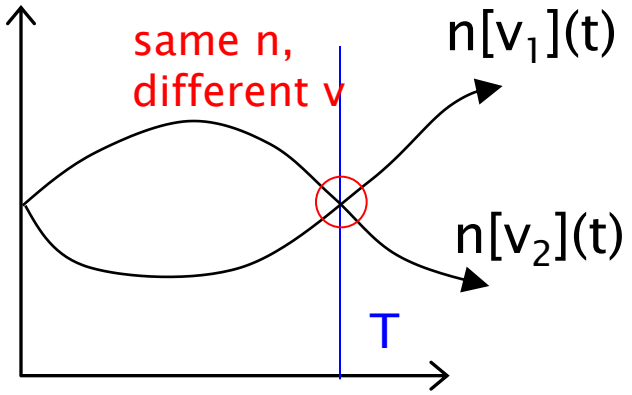
$$O[n, \Psi_0](t) = \langle \Psi[n](t) | \hat{O} | \Psi[n](t) \rangle$$

RGT and causality



If $v_1 = v_2$ for $t < T$ but different afterwards,
v[n] for t<T determined only by n(t<T)

RGT and memory



If v[n](T) not fixed by n(T) alone.
Must have **memory** of n at t<T

Kadanoff-Baym dynamics

- Basic quantity $G(12) = -i\langle T_C \left[\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\right]\rangle$

  Total energy, one-particle averages, Excitation energies with ± 1 particle

- Dyson Equation in time $(i\partial_{t_1} - h(t_1))\, G(t_1,t_2) = \delta(t_1,t_2) + \int_C \Sigma(t_1,t)\, G(t,t_2)\, dt$

- Conserving approximations: $\Sigma = \Sigma[G]$ functional derivative of generating functionals

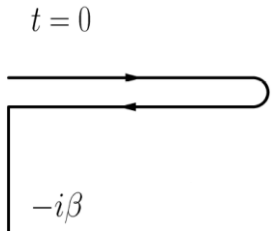
- Example of Many-Body approximations: TMA

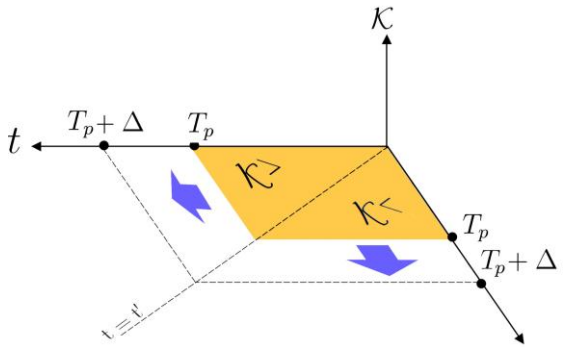
TMA) 

$$\Sigma_{TM}(12) = \Sigma_{HF} + iU^2 G(21)\, T(12).$$

$$T = \phi - \phi \mathcal{U} T, \;\; \phi(12) = -iG(12)\, G(12)$$

- Time propagation on the time square



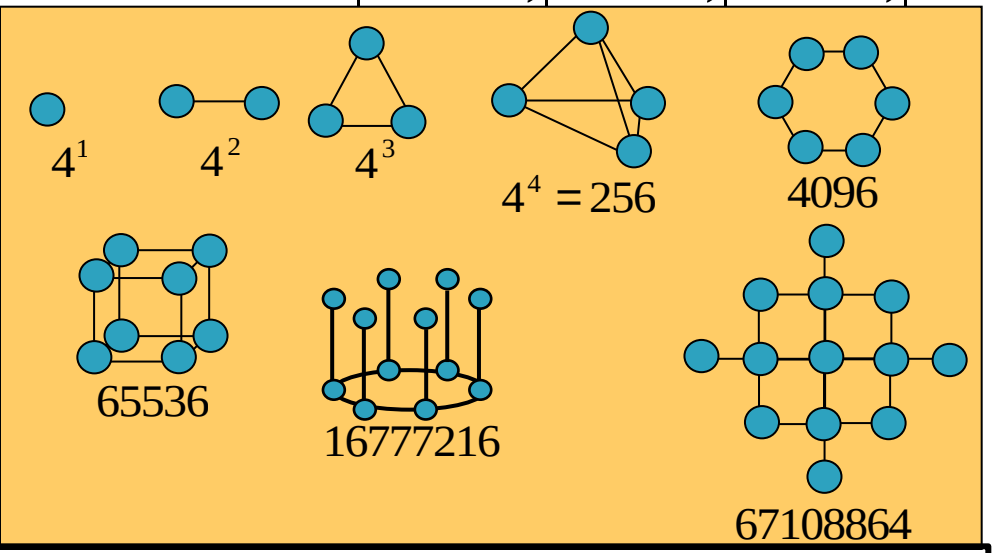


1) GWA and BA: negative double occupancy. TMA. Always positive (Theorem)
2) Finite systems & conserving MBA:s artificially damped dynamics (Puig, CV, Almbladh, 2009-11)

Scaling of Diagonalization

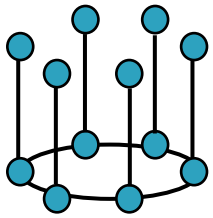
$$\text{basis state } |b\rangle = |n_{1\uparrow}\rangle \otimes |n_{N\uparrow}\rangle \otimes |n_{1\downarrow}\rangle \cdots \otimes |n_{N\downarrow}\rangle$$

4 states/site: $|0_\uparrow 0_\downarrow\rangle, |1_\uparrow 0_\downarrow\rangle, |0_\uparrow 1_\downarrow\rangle, |1_\uparrow 1_\downarrow\rangle,$



H does not mix N subspaces:

$$N_0 \oplus N_1 \oplus N_2 \cdots N_{Max}$$



$$16777216 = \sum_{k=0}^{2N} \binom{N}{k} = \sum_{k=0}^{2N} N_k$$

Within N_{12}, fix how many spin-$\uparrow$ (i.e. S_z)

$$N_{12} = \sum_{q=0}^{12} \binom{12}{q}^2 = \sum_{q=0}^{12} n_q n_{12-q}$$

$$N_{12} = \binom{24}{12} = 2704156$$

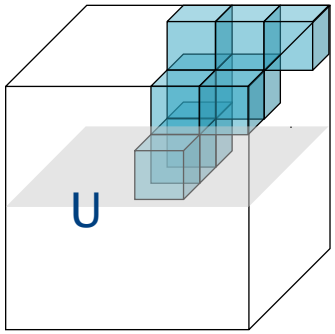
Finally, for $N_{6\uparrow,6\downarrow} = 853776$

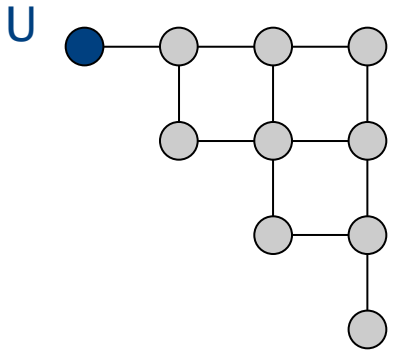
Total spin, pseudospin & space symmetry cuts further by ~

TDDFT-DMFT, exact and KBE dynamics in small 3D clusters

a 125-site cluster with one interacting impurity in the center

$5 \times 5 \times 5$





Interaction and perturbation only in the center *by symmetry, a 10-site ef*

TDDFT time propagation

- TDKS equations $\left(\hat{t} + \hat{v}_{KS}(\tau)\right) \varphi_\kappa(\tau) = i\partial_\tau \varphi_\kappa(\tau)\ ,$
- with $v_{KS}(i,\tau) = v_H(i,\tau) + v_{xc}(i,\tau) + v_{ext}(i,\tau)$
- In the ALDA $v_{xc}(i,\tau) \to v_{xc}^{DMFT}(n_i(\tau))$
- with $n_i(\tau) = \sum_\kappa^{occ} |\varphi_\kappa(i,\tau)|^2$

Open Problems

Time dependent Density Functional Theory

Advantage: Only one time variable

The hurdle: $v_{XC}(\mathbf{r},t)$

1) Complicated dependence on the density

$$v_{XC}(\mathbf{r},t) \equiv v_{XC}[n](\mathbf{r},t)$$

2) Local and memoryless approximations

$$v_{XC}[n](\mathbf{r},t) \approx v_{XC}(n(\mathbf{r},t))$$

may be not enough.

3) For strongly correlated systems, even local approximations not easy

Non equilibrium Green's Functions

The hurdle : two time variables

$$G(t_1,t_2) \not\equiv G(t_1-t_2)$$

Advantage: $\Sigma = \Sigma[G]$

Systematic many-body expansion for Σ

BUT

Simple (i.e. workable) many body schemes

may not be enough
for strongly correlated systems.

Still, these methods are at present regarded as the premier choice to deal with system out of equilibrium

Which systems and which physics -II

-Topic 3: European Spallation Source (ESS)

- New ESS: probing non equilibrium processes (structural + magnetic)
- Calculations can be important complementary tool to such experiments

Topic 4: Non-equilibrium behavior of Cold atoms trapped in optical lattices-

- Ideal benchmarking ground for methodological developments
- Dynamics of the coexisting phases & quantum entanglement
- Time-dependent collapse/segregation of fermionic and bosonic mixtures

The PhD Students:

M. Puig von Friesen: Green's function methods (methodology development)
D. Karlsson: TDDFT (methodology development)
A. Kartsev : Ab-initio implementation of TDDFT and lattice TDDFT
V. Vettchinkina : Applications of lattice TDDFT

Also, collaborations within and outside ETSF