

# Computational Methods for Quantum Many-Body Systems (CMQMB) - from **artificial atoms** to **high-temperature superconductors**

---

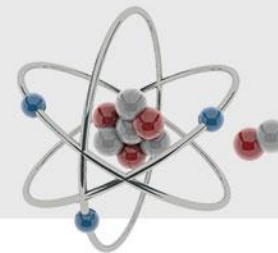
## Lecture 3 – Pictures of time evolution, linear response and Kubo formalism



**UNIVERSITÀ  
DEGLI STUDI  
DI TRIESTE**

Prof. Dr. Thomas Schäfer

Università degli studi di Trieste (UNITS), Winter Semester 2025



Please check, whether you can connect to:

sdsc-binder.flatironinstitute.org

Owner: ccq

Project: CMQMS



# TRIQS

## Toolbox for Research on Interacting Quantum Systems

01s-IPT\_and\_DMFT.ipynb Python 3 (ipykernel)

▼ A first DMFT calculation

The goal of this notebook is to make a first DMFT calculation using the iterated perturbation theory (IPT) to solve the impurity problem. You will proceed in two steps: first you will set up the IPT impurity solver and then you will set up the DMFT loop.


**The iterated perturbation theory**

The IPT is a cheap way to solve the impurity problem at half-filling, but fails away from half-filling ([further information](#)). It **approximates** the self-energy by second-order perturbation theory, just like in the last exercise of the notebook on Green's functions:

$$\Sigma(i\omega_n) = \frac{U}{2} + U^2 \int_0^\beta d\tau e^{i\omega_n \tau} \mathcal{G}_0(\tau)^3$$

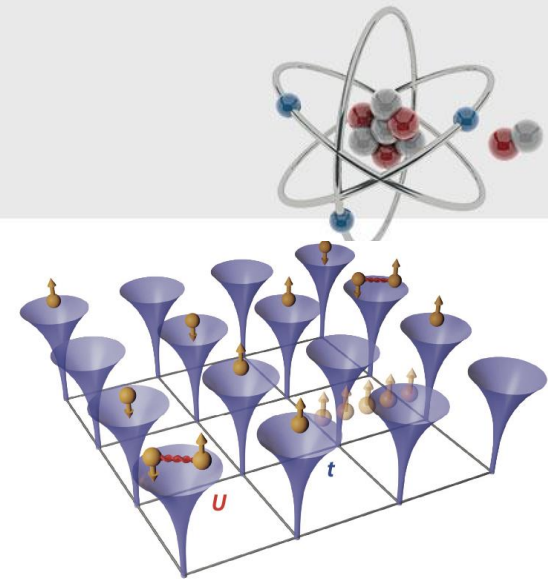
Note that the first term,  $\frac{U}{2}$ , is the chemical potential  $\mu$  for half-filling.

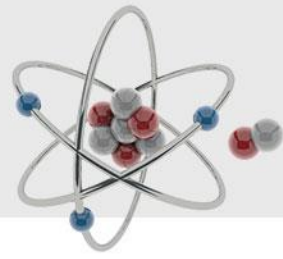
# The full solid-state Hamiltonian

$$H/E_0 = \boxed{-\frac{1}{2} \sum_i \frac{\partial^2}{\partial \tilde{\mathbf{r}}_i^2}} - \frac{1}{2} \sum_k \frac{m}{M_k} \frac{\partial^2}{\partial \tilde{\mathbf{R}}_k^2} \boxed{+ \sum_{i < j} \frac{1}{|\tilde{\mathbf{r}}_i - \tilde{\mathbf{r}}_j|}} \\ + \sum_{k < l} \frac{Z_k Z_l}{|\tilde{\mathbf{R}}_k - \tilde{\mathbf{R}}_l|} - \sum_{i,k} \frac{Z_k}{|\tilde{\mathbf{r}}_i - \tilde{\mathbf{R}}_k|}$$


Many fascinating phenomena like magnetism, superconductivity, quantum criticality, metal-insulator transitions, ...

However: advanced description necessary! One-particle picture does not hold!

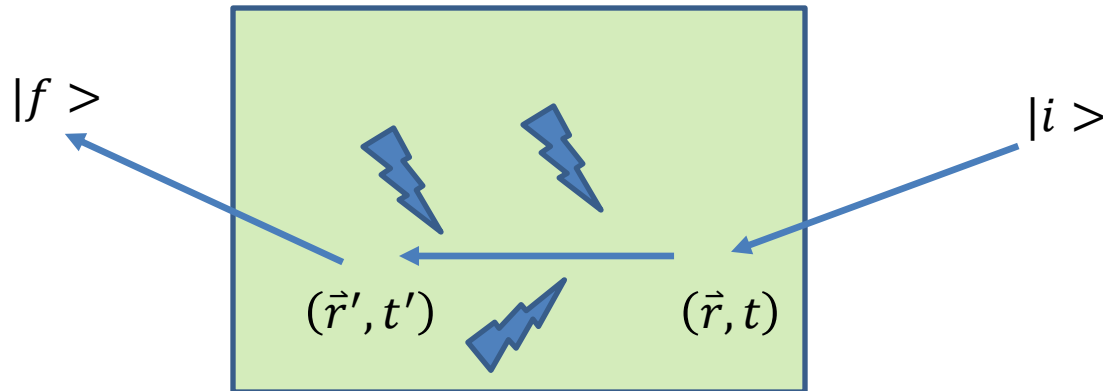




# Towards interacting systems...

How can we obtain information from an interacting system?

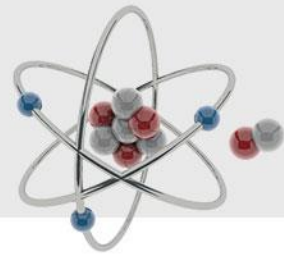
→ Scattering experiments (theory)



Three ingredients necessary:

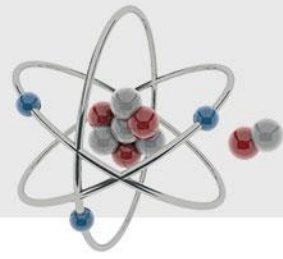
- 1) Many-body treatment → Second quantization ✓
- 2) Time evolution → Pictures of time evolution
- 3) How does the system respond? → Linear response theory

# Lecture 3



## Content and goals

- Pictures of time evolution in quantum mechanics
  - Schrödinger picture
  - Heisenberg picture
  - Dirac picture
- Linear Response Theory
  - Kubo-Nakano formula
  - Examples



# Lecture 3: Examples for correlation functions I

Density operator and variation of chemical potential

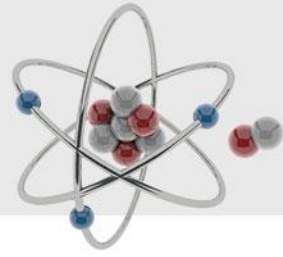
$$B(t) = - \int d^d r \, n(\vec{r}) \delta\mu(\vec{r}, t)$$

We also measure density: A=B

$$\delta\langle n(\vec{r}) \rangle = \int_{-\infty}^{\infty} dt' \int d^d r' \, \chi_{nn}(\vec{r} - \vec{r}', t - t') \delta\mu(\vec{r}', t')$$

Density-density (or charge) response function  
“Polarizability”

$$\chi_{nn}(\vec{r} - \vec{r}', t - t') = -i\theta(t - t') \langle [n(\vec{r}, t), n(\vec{r}', t')] \rangle$$



## Lecture 3: Examples for correlation functions II

Magnetic moment and external magnetic field in direction  $\alpha$

$$B(t) = - \int d^d r \mu_B g S_\alpha \cdot h_\alpha(\vec{r}', t')$$

We also measure spin:  $A=B$

Spin-spin (or magnetic) response function  
“spin susceptibility”

$$\chi_{S_\alpha S_\beta}(\vec{r} - \vec{r}', t - t') = -i\theta(t - t') \langle [S_\alpha(\vec{r}, t), S_\beta(\vec{r}', t')] \rangle$$