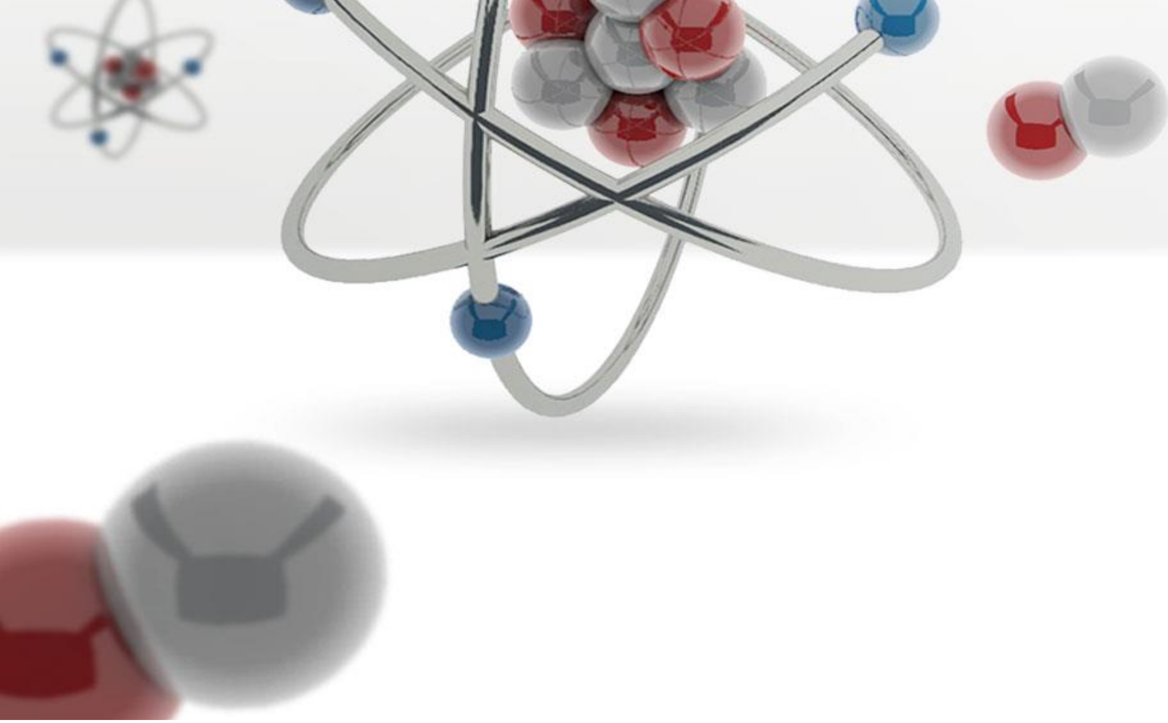


Computational Methods for Quantum Many-Body Systems (CMQMB) - from artificial atoms to high-temperature superconductors

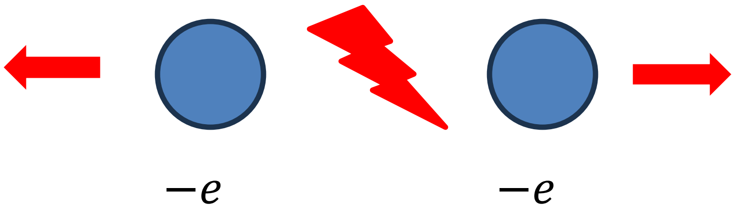
Lecture 1 – Introduction, Second Quantization

UNIVERSITÀ DEGLI STUDI DI TRIESTE

Prof. Dr. Thomas Schäfer
Università degli studi di Trieste (UNITS), Winter Semester 2025

Fascinating physics from electron-electron interactions

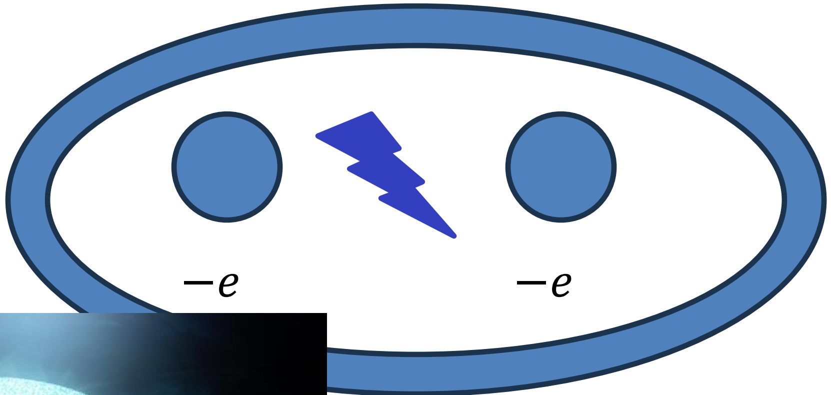
→ **repulsion**

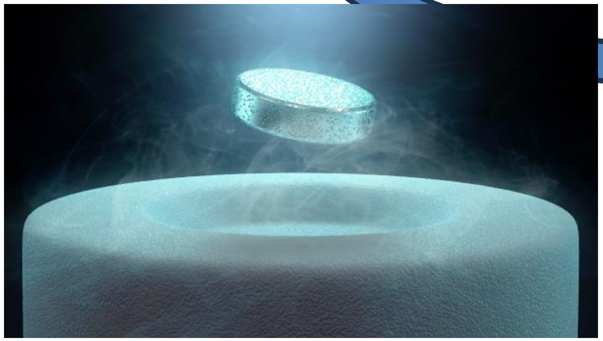


$$F = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r^2}$$

Classical electrostatics:
Coulomb force

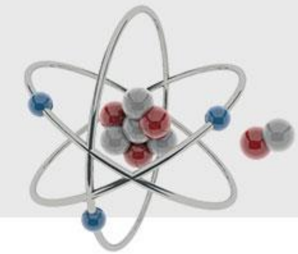
But Coulomb interaction can also lead to an (effective) **attraction!**





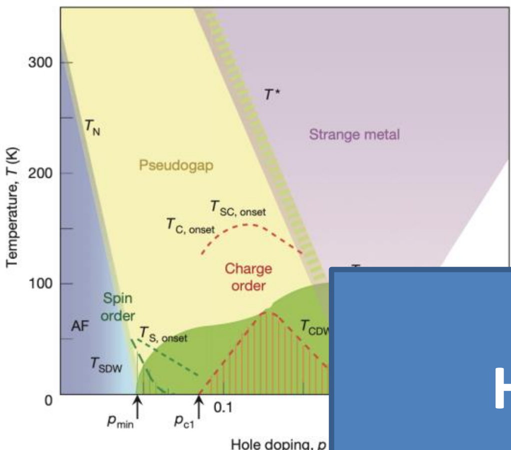
→ Cooper pairs and superconductors

Fascinating physics from electron-electron interactions



High-T_c superconductivity, pseudogap

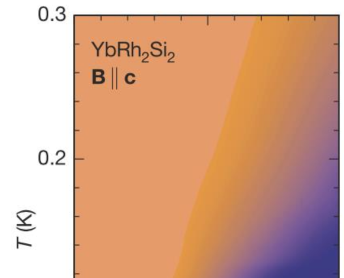
B. Keimer, et al., Nature (2015)



Tseng, …, TS, Hansmann, SciPost Ph. '25
Malcolms, …, TS, arXiv '24
Ortiz,…, TS, Hepting, PRR '22
Klett, …, TS, Front. Phys. '22
Kitatani, …, TS, Held, JPM '22
TS and Toschi, JPCM '21

Quantum criticality/Strange metals

J. Custers, et al., Nature (2003)

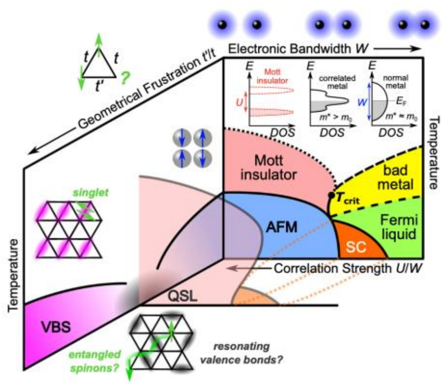


TS et al., PRL '17
TS et al., PRL '19
Adler, …, TS, …, arXiv '24
Kitatani, TS, …, arXiv '25

How can we treat such systems theoretically?

Mott metal-insu…

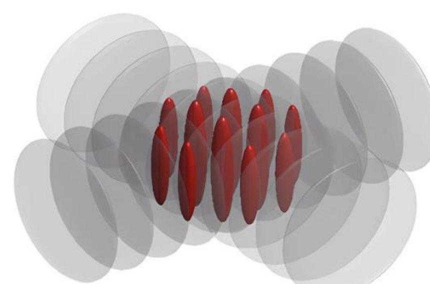
A. Pustogow, et al., Nat. Comm. (2023)



Menke, …, TS, PRL '24
Meixner, …, TS, arXiv '25
Kowalski, …, TS, PRL '24
Meixner, …, TS, SciPost Ph. '24
Wagner, …, TS, …, Sangiovanni Nat. Comm. '23
TS et al., PRX '21
Wietek, …, TS, Georges, PRX '21
Klett, …, TS, et al., PRR '20
TS et al., PRB '15
TS et al., JMMM '16

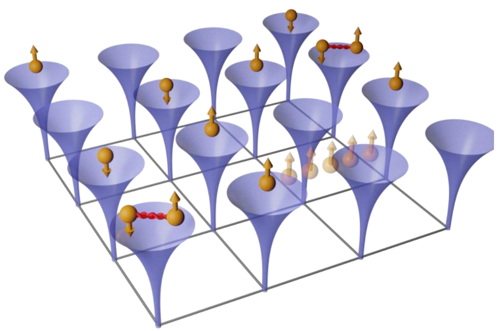
…ntum simulators (cold atoms, moiré, …)

Y. Huo, …, H.-C. Nägerl, Nat. Phys. (2024)



Tscheppe, …, TS, PNAS '24
D. Kiese, … TS, …, in preparation

The full many-body ('ab-initio', solid-state) Hamiltonian



$$\hat{H} = \sum_{\sigma} \int d^3r \; \hat{\Psi}^+(\mathbf{r},\sigma) \Big[-\frac{\hbar^2}{2m_e}\Delta + \underbrace{\sum_l \frac{-e^2}{4\pi\epsilon_0} \frac{Z_l}{|\mathbf{r}-\mathbf{R}_l|}}_{\equiv V_{\rm ion}(\mathbf{r})} \Big] \hat{\Psi}(\mathbf{r},\sigma)$$

$$+\frac{1}{2}\sum_{\sigma\sigma'} \int d^3r\, d^3r' \; \hat{\Psi}^+(\mathbf{r},\sigma)\hat{\Psi}^+(\mathbf{r}',\sigma') \underbrace{\frac{e^2}{4\pi\epsilon_0} \frac{1}{|\mathbf{r}-\mathbf{r}'|}}_{\equiv V_{\rm ee}(\mathbf{r}-\mathbf{r}')} \hat{\Psi}(\mathbf{r}',\sigma')\hat{\Psi}(\mathbf{r},\sigma)$$

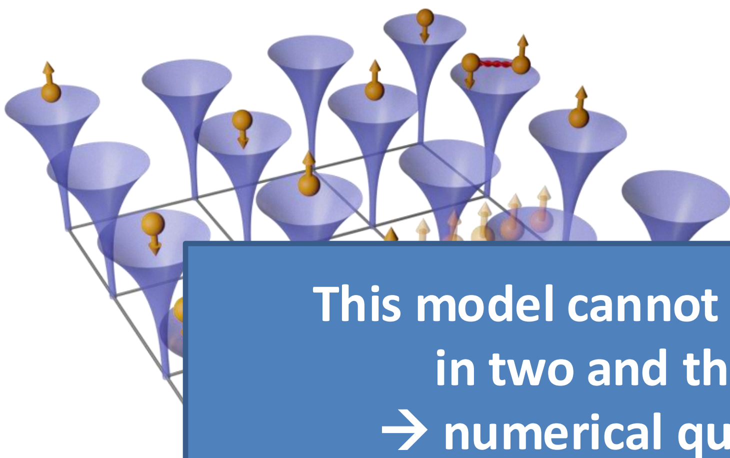
Problem: how can we treat a (quantum mechanical) system with 10^{23} constituents?

Approximate solutions to H:
density functional theory (DFT), perturbation theory, GW, etc.

Approximation to H:
capture essential physics

Interacting systems: fascinating physics - and a simple (?) modellization

Hubbard model




ANNUAL REVIEWS

Annual Review of Condensed Matter Physics

The Hubbard Model: A Computational Perspective

Thomas Schäfer,[2] Sabine Andergassen,[3] oz,[4] and Emanuel Gull[5]

https://doi.org/10.1146/annurev-conmatphys-090921-033948

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Abstract

The Hubbard model is the simplest model of interacting fermions on a lattice and is of similar importance to correlated electron physics as the Ising model is to statistical mechanics or the fruit fly to biomedical science. Despite its simplicity, the model exhibits an incredible wealth of phases, phase transitions, and exotic correlation phenomena. Although analytical methods have provided a qualitative description of the model in certain limits, numerical tools have shown impressive progress in achieving quantitative accurate results over the past several years. This article gives an introduction to the model, motivates common questions, and illustrates the progress that has been achieved over recent years in revealing various aspects of the correlation physics of the model.

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This model cannot be solved analytically in two and three dimensions!
→ numerical quantum many-body methods needed!

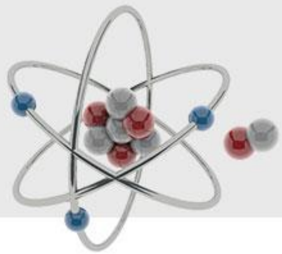
$$H = \boxed{-t} \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \boxed{U} \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

-t : hopping

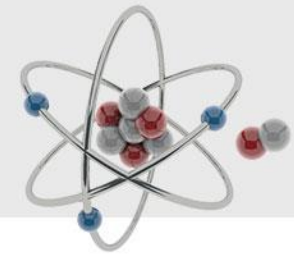
U: local Coulomb interaction

*J. Hubbard, Proc. Royal Soc. A, **276**, 238– 257 (1963)*
*M. Qin, TS, et al., „The Hubbard model – a computational perspective“, Annual Review of Condensed Matter Physics **13** (2022)*

Tentative outline of the course

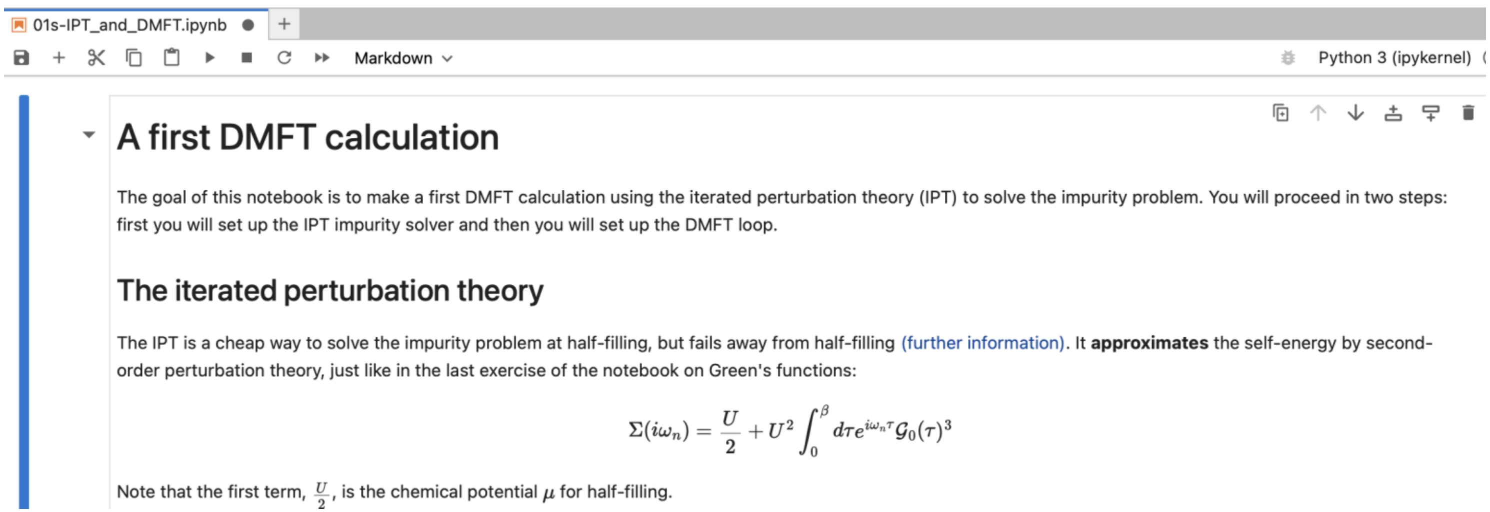


1. QFT and Green functions	Introduction, organization of the lecture, evaluation / Second quantization
	Second quantization (continued)
	Pictures of time evolution, Linear response theory and Kubo formalism
	From single-particle to many-particle Green functions
	Lehmann representation, spectral function, tunneling spectroscopy
	Finite temperatures and Matsubara formalism
	Perturbation theory, Feynman diagrams, self-energy and Dyson equation
	TRIQS I: Introduction to TRIQS, Python, Green functions
	TRIQS II: tight-binding, multivariable Green functions, dispersion relations, density of states
2. Quantum dots, Anderson impurity model	
3. Quantum magnetism, Hubbard model	
4. Mott transition, DMFT	



TRIQS

Toolbox for Research on Interacting Quantum Systems



01s-IPT_and_DMFT.ipynb

Markdown

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 μ for half-filling.

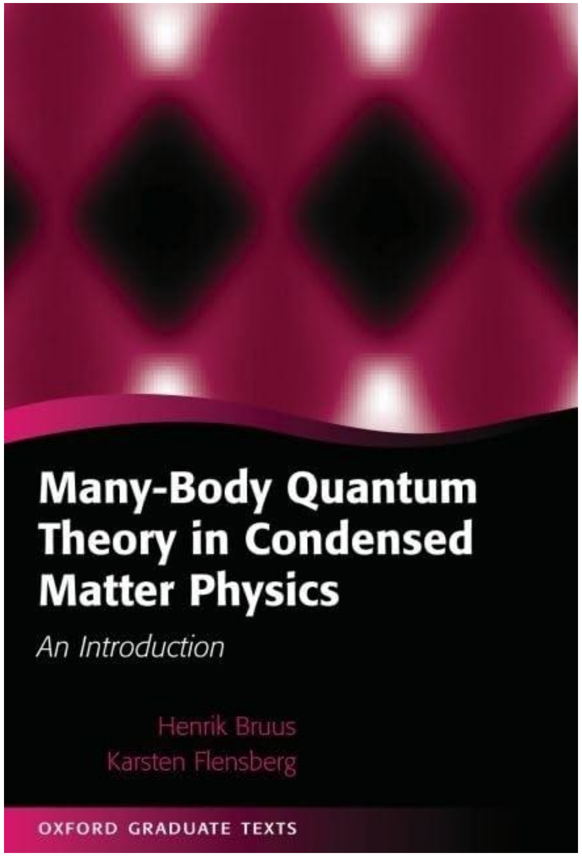
- Introduction to topic and presented example (30 minutes)
- Notebook to be worked on separately (40 minutes)
- Presentation of solution (20 minutes)

LAPTOPS NEEDED! GOOGLE ACCOUNT NEEDED!

https://triqs.github.io/triqs

Course material

- Lecture notes (blackboard and slides)
- Numerical parts: notebooks
- Book: H. Bruus and K. Flensberg
  “Many-body quantum theory in
  condensed matter physics”
  (Oxford Graduate Texts 2004)
- Research papers and reviews (given in lectures)



Interested in
Computational Methods for Quantum Many-Body Systems?

Thomas Schäfer

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thomas.schaefer@units.it

Mon 9:15 – 11:00
Aula B (Edificio F)
Tue 11:15 – 13:00
Aula A Idraulica (Edificio C2)
Via Valerio, 2 - 34127 Trieste

Possible exam modi of the course

Students can choose one of the following options (all orally):

- Examination with two questions on the course from two different topics (30 minutes).
- Presentation of a small numerical project worked out by the student (15 minutes) and one question on the course (15 minutes).
- Presentation of a current research publication by the student (20 minutes) and one question on the course (10 minutes).

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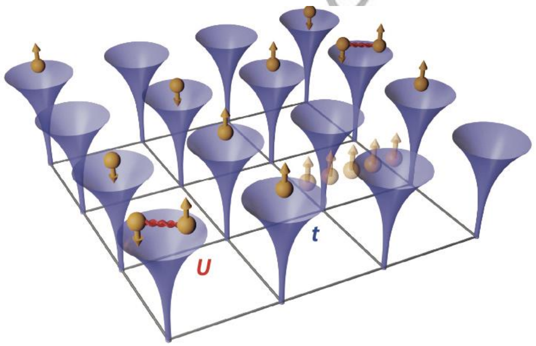
Lectures 1+2 – Second Quantization

The full solid-state Hamiltonian



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

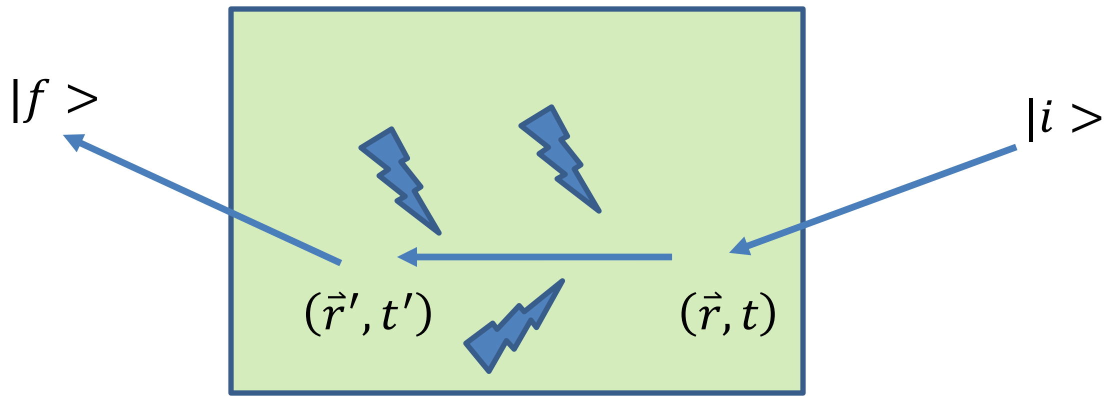
Many fascinating phenomena like magnetism, superconductivity, quantum criticality, metal-insulator transitions, …

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)



<u>Three ingredients necessary:</u>

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

Lectures 1 + 2

Content and goals

- Many-body wave functions in first quantization
- Operators in first quantization
- Occupation number representation
- Creation and annihilation operators for bosons and fermions
- Operators in second quantization
- Change of basis and quantum field operators
- Examples