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SPP Meetup Berlin, 14.10.2017

Quantum matter out of equilibrium - pathway to technological breakthrough?

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Achievements of quantum physics: highlights

- **Transistor**
  (1947, Bardeen, Brattain, and Shockley, 1956 Nobel Prize in Physics)
- **Superconductivity**
  (1911, Kammerlingh-Onnes, 1913 Nobel Prize in Physics;
  theory: 1957, Bardeen, Cooper, and Schrieffer, 1972 Nobel Prize in Physics)
- **High-temperature superconductivity**
  (1986, Bednorz and Müller, 1987 Nobel Prize in Physics)
- **Nuclear magnetic resonance**
  (molecules: 1938, Rabi, 1944 Nobel Prize in Physics;
  solids: 1946, Bloch and Purcell, 1952 Nobel Prize in Physics)
- **Magnetic resonance imaging (MRI)**
  (1973, Lauterbur and Mansfield,
  2003 Nobel Prize in Physiology or Medicine)

modern MRI scanner

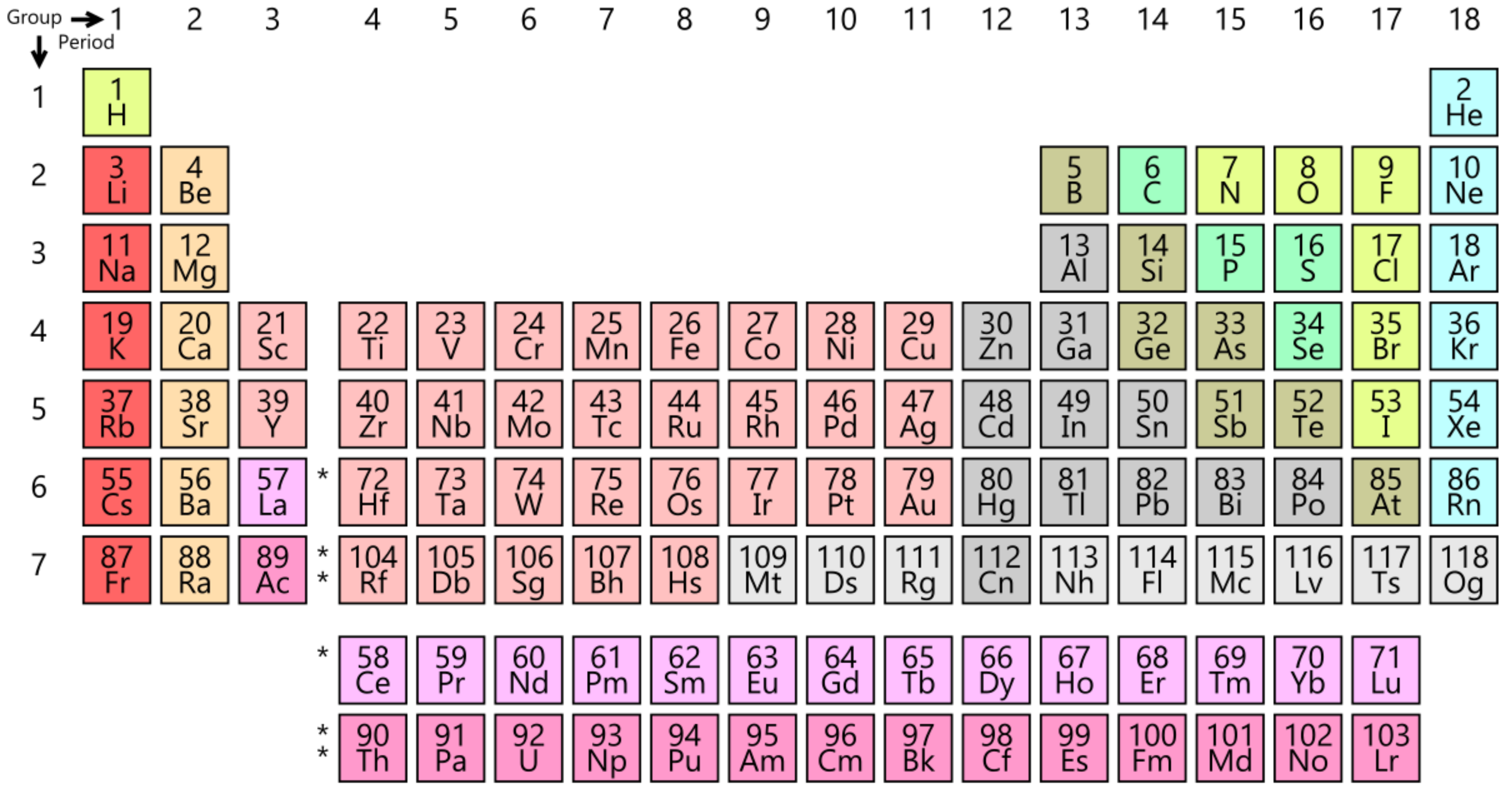
Challenges

- Next-generation electronics
  - ultrafast control
  - miniaturization

- Transformation of energy system
  - new sources of clean energy
  - efficient photovoltaic solar cells
  - improved energy storage and transmission
  - smart technologies for energy savings

silicon solar cell

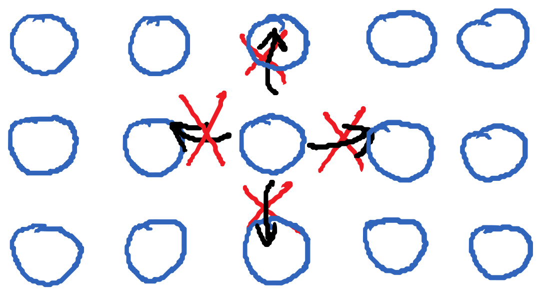
Strongly correlated electronic systems: *Quantum Matter*



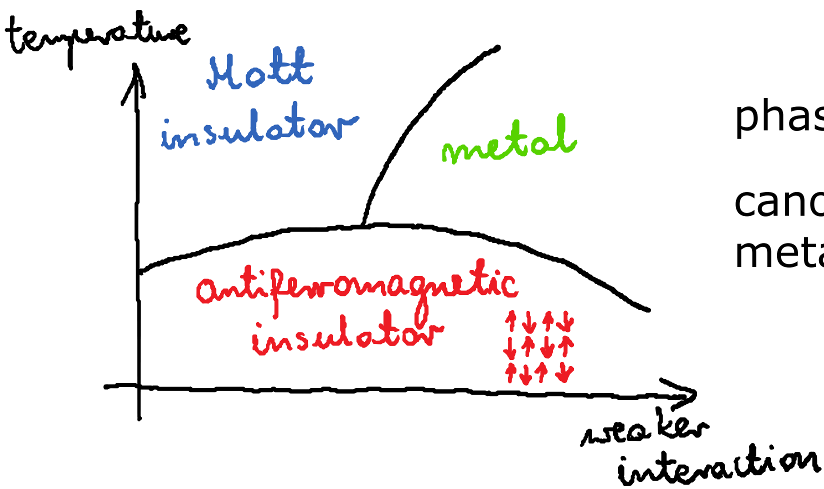
- Examples:
  - Mott insulators (transition metal oxides, V_2O_3)
  - high-temperature superconductors (cuprates, $YBa_2Cu_3O_{7-x}$)
  - heavy-fermion materials (rare-earth and actinide compounds, UGe_2)

Mott insulator

- Theoretical concept: 1937, Nevill F. Mott, 1977 Nobel Prize in Physics (1/3)
- Electrons frozen in their equilibrium positions due to Coulombic repulsion



- No transfer of charge possible
- Transition to metallic state when interaction strength decreased



phase diagram of V_2O_3

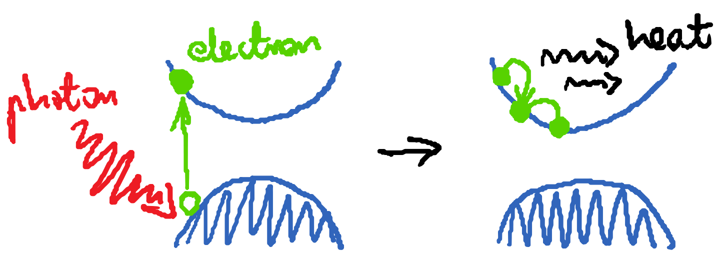
canonical example of Mott metal-insulator transition

Mott insulator *out of equilibrium*

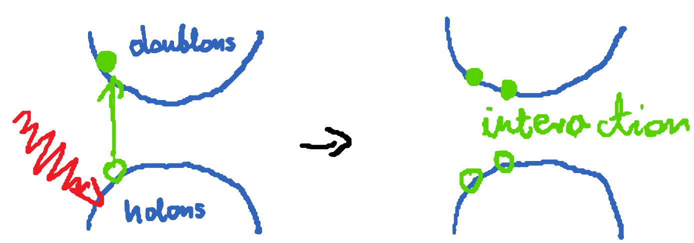
- Control of metal-insulator transitions by electric pulses: possibility to build resistive random-access memory (ReRAM)
  [L. Cario , C. Vaju , B. Corraze , V. Guiot , E. Janod , Adv. Mater., 225193 (2010)]

- Metastable hidden quantum states induced by laser pulses: another possibility for ReRAM
  [L. Stojchevska et al., *Science* 344, 177 (2014)]

- Solar-light driven Mott insulator: efficient photovoltaic device
  [E. Manousakis, Phys. Rev. B 82, 125109 (2010)]



silicon solar cell



Mott insulator solar cell

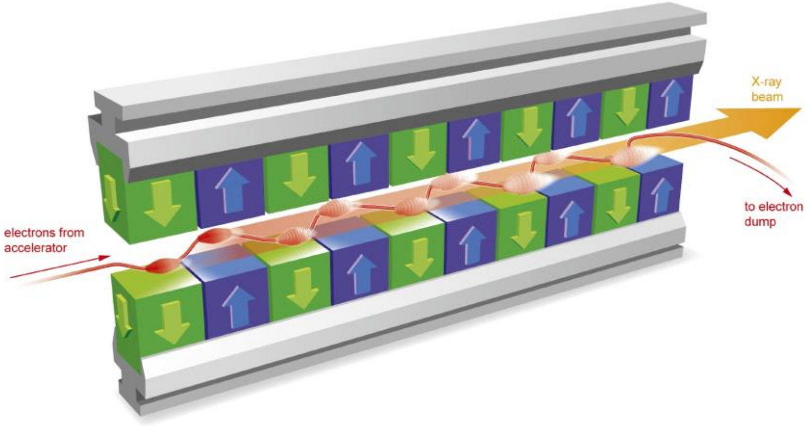
Europen X-Ray Free Electron Laser (XFEL)

- Source of ultrashort and ultra intense X-ray laser pulses
- Enables the study of real-time atomic-scale ultrafast dynamics of complex materials and biomolecules
- Official inauguration: 1 September 2017

total length = 3,4 km

electron accelerator: 2,1 km

undulators: 125 m, 212 m



Theoretical description: Solving many-body quantum problem

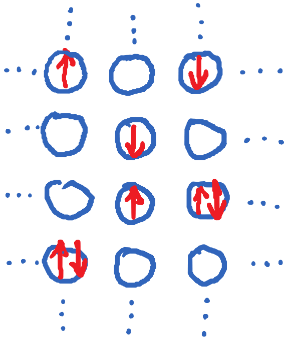
- Classical systems can be only in one state at a time
- Quantum systems can be in a superposition of many different states

$$\psi(t) = \sum_{i}^{M} c_i(t)\, \phi_i$$

- Goal: find probability amplitudes $c_i(t)$ by solving Schrödinger equation

$$i \frac{\partial}{\partial t} \psi(t) = H(t)\psi(t)$$

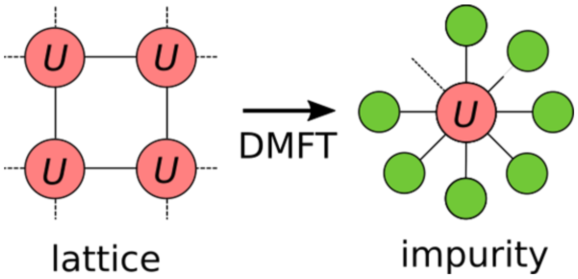
- In practice infeasible: example – Hubbard model
  - each site can be in one of 4 states:
    - empty 
    - occupied by spin-up electron 
    - occupied by spin-down electron 
    - doubly occupied 



  - whole system of N sites can be in $M = 4^N$ states
  - $N = 10^{23}$, then $M = 4^{10^{23}} \gg 10^{80}$ – number of atoms in the Universe

Theoretical description: approximations needed

- By neglecting interactions the electronic wavefunction factorizes: single-electron instead of many-electron problem (-> DFT)
- Not possible for strongly correlated systems: do some kind of mean field theory instead (-> DMFT)



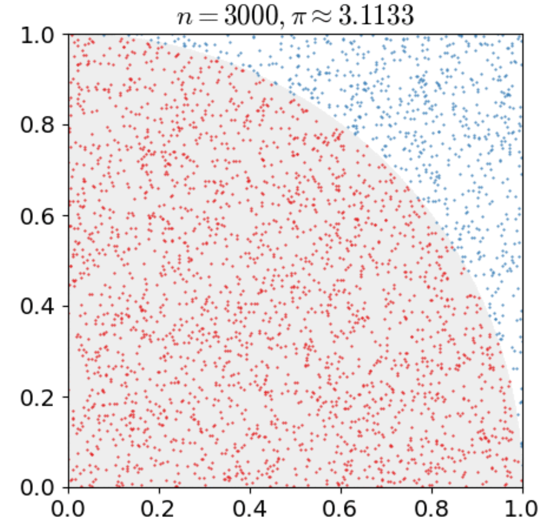
- Now solve the impurity problem: electrons interact only on the central site
- Idea:
  - solve the central site (M = 4) and bath (single-particle) separately
  - find the correction to the result for the full system by summing up all Feynman diagrams
  - there are too many Feynman diagrams to do this diagram-by-diagram
  - select diagrams randomly based on their importance: Monte Carlo

Quantum Monte Carlo

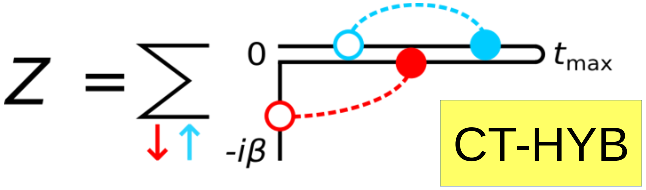
- Monte Carlo: stochastic way to evaluate integrals
- Example: area of a circle

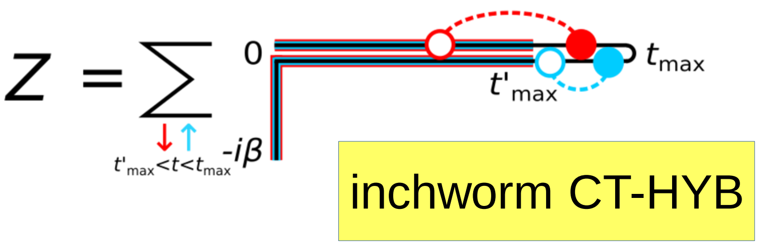
$$f(x,y) = \begin{cases} 1 \\ 0 \end{cases}$$

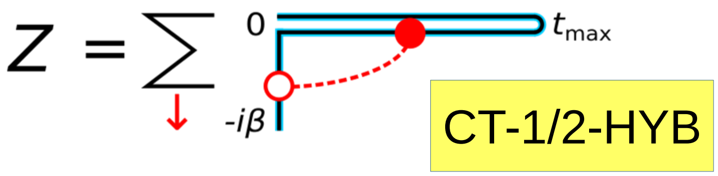
$$\int_0^1 dx \int_0^1 dy\, f(x,y) = \frac{\pi}{4}$$



- Quantum Monte Carlo: stochastic way to sum Feynman diagrams







Summary

- Quantum physics underlies many of the modern technologies
  - electronics
  - medical imaging (MRI)

- Strongly correlated electronic systems
  - fascinating macroscopic quantum phenomena (Mott insulators, high-temperaturę superconductors, …)
  - theoretical description challenging
  - possibilities for technological applications

- Nonequilibrium physics is an active field of research
  - European XFEL in Hamburg

Thank you for your attention!

References (for experts):

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Support from SFB925 gratefully acknowledged

SFB

SFB 925: Light induced dynamics and control of strongly correlated quantum systems