UNIVERSITY OF CAMBRIDGE

Many-body theory: Concepts

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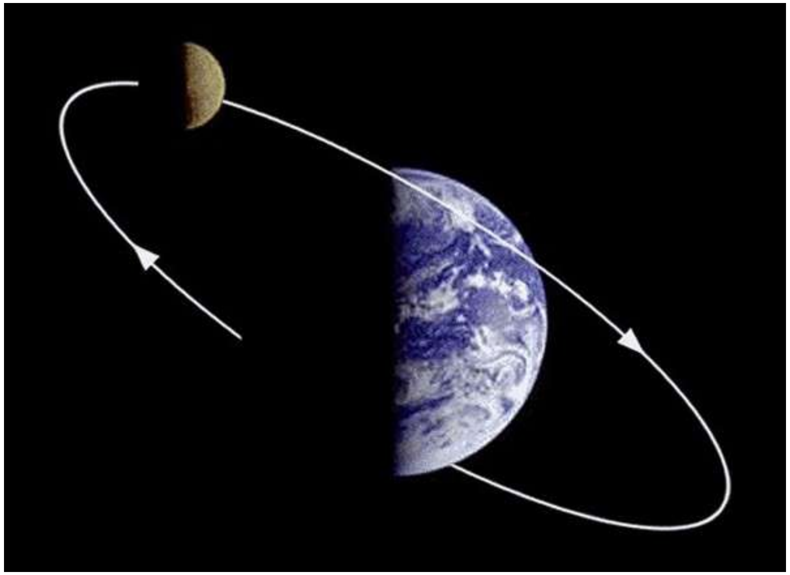
Characteristics of a many-body interacting system



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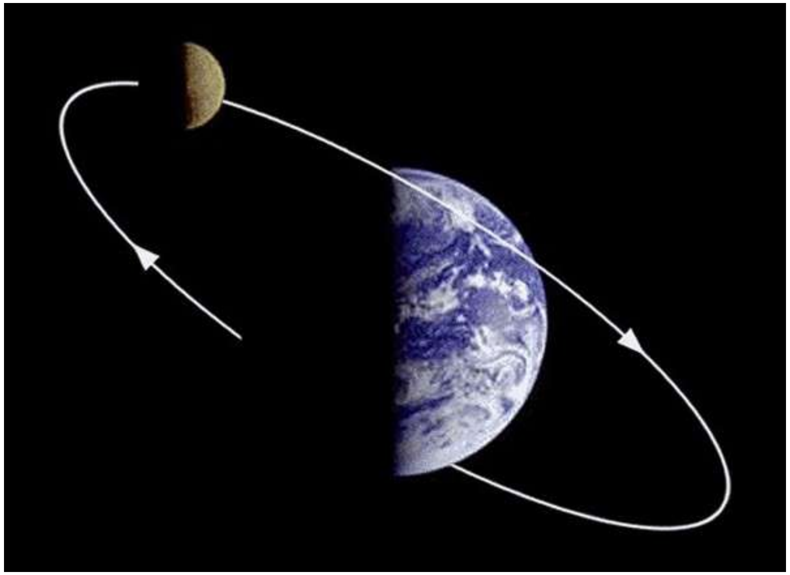
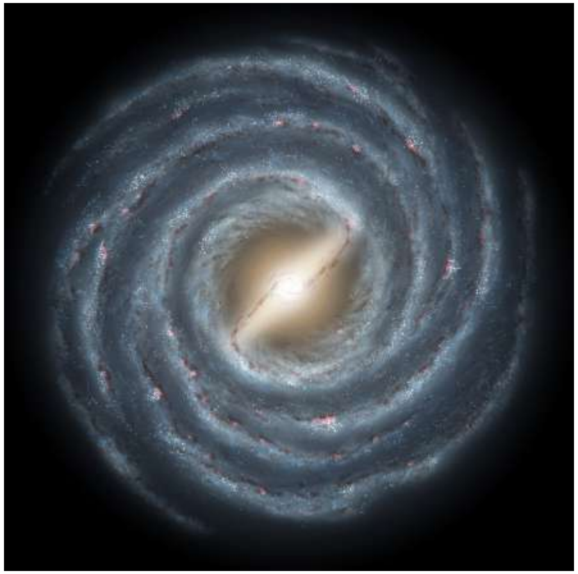
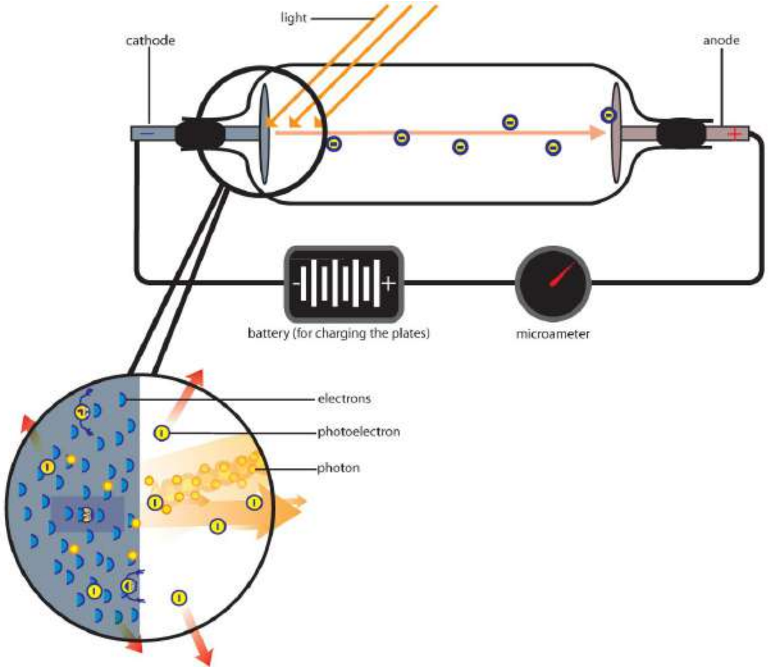
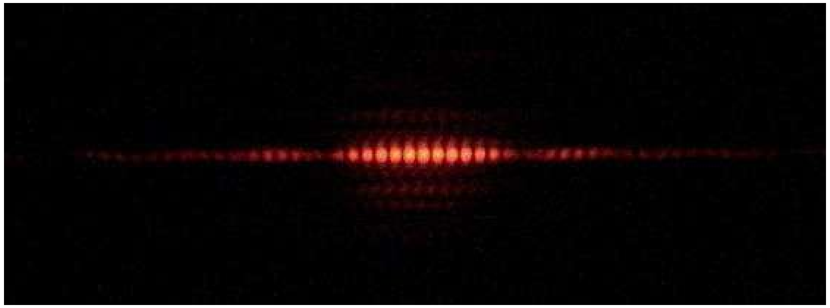




Characteristics of a quantum system



Photoelectric effect



Electron diffraction

Electrons: many-body interacting and quantum

10^{27} interacting electrons

Fermi temperature 30,000K

Electrons: Hamiltonian

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \sum_{i=1}^{M} \frac{\hat{P}_i^2}{2m}$$

$$+ \sum_{i=1}^{N} \sum_{j<i} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|}$$

$$+ \sum_{i=1}^{N} \sum_{j=1}^{M} \frac{Z_j e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{R}_j|}$$

$$+ \sum_{i=1}^{M} \sum_{j<i} \frac{Z_i Z_j e^2}{4\pi\epsilon_0 |\vec{R}_i - \vec{R}_j|}$$

$\hat{p}_i, \vec{r}_i$ Momentum and position of electron *i*

$\hat{P}_i, \vec{R}_i$ Momentum and position of ion *i*

N, M Number of electrons and ions

Ultracold atomic gas: many-body interacting and quantum

10^7 interacting atoms

0.1 T_F

Ultracold atomic gas: Hamiltonian

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \sum_{i=1}^{N} V(\vec{r}_i) + \sum_{i=1}^{N} \sum_{j<i} g\,\delta(|\vec{r}_i - \vec{r}_j|)$$

$\hat{p}_i, \vec{r}_i$	Momentum and position of atom *i*
V	External potential
g	Interaction strength

Energy stored in an elastic band

Potential energy in elastic band

$$E = \frac{1}{2} kx^2 = \frac{1}{2} Fx = \frac{1}{2} 10 \times 0.1 = 0.5\ \text{J}$$

Energy stored in an elastic band

Potential energy in elastic band $E = \frac{1}{2}kx^2 = \frac{1}{2}Fx = \frac{1}{2}10 \times 0.1 = 0.5\,\text{J}$

Kinetic energy in handgun bullet $E = \frac{1}{2}mv^2 = \frac{1}{2}0.005 \times 300^2 = 225\,\text{J}$

Energy stored in an elastic band

Potential energy in elastic band $E = \frac{1}{2}kx^2 = \frac{1}{2}Fx = \frac{1}{2}10 \times 0.1 = 0.5\,\mathrm{J}$

Kinetic energy in handgun bullet $E = \frac{1}{2}mv^2 = \frac{1}{2}0.005 \times 300^2 = 225\,\mathrm{J}$

Potential energy in enormous band $E = \frac{1}{2}kx^2 = \frac{1}{2}Fx = \frac{1}{2}100 \times 5 = 250\,\mathrm{J}$

Questions about solid state systems

Chemical and structural properties
Why does carbon form diamond, graphene, nanotube, or buckyballs?

Electrical properties
Why do some metals superconduct at low temperatures?

Optical properties
How does photosynthesis occur?

Magnetic properties
Why do high T_c superconductors display magnetic order?

Approaches to study the system

Analytical
Provides microscopic insights

Computational
More general
Complementary approximations

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \sum_{i=1}^{M} \frac{\hat{P}_i^2}{2m}$$
$$+ \sum_{i=1}^{N} \sum_{j<i} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|}$$
$$+ \sum_{i=1}^{N} \sum_{j=1}^{M} \frac{Z_j e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{R}_j|}$$
$$+ \sum_{i=1}^{M} \sum_{j<i} \frac{Z_i Z_j e^2}{4\pi\epsilon_0 |\vec{R}_i - \vec{R}_j|}$$

Experimental
Exact solution

Experiments: determining the ground state

Lattice of a solid	It is hard to predict from the many-electron Hamiltonian that copper crystallizes in a fcc crystal structure. Computational techniques can compare the energy of fcc Cu to bcc Cu, but cannot exclude other structures. X-ray diffraction experiments show that Cu crystallizes in a fcc structure, providing a platform for theoretical analysis.
Dominant terms in the Hamiltonian	There is currently no satisfactory theoretical understanding of the phenomenon of high-Tc superconductivity, but experimental techniques have delivered a lot of clues (and some red herrings) about how the physics of high-Tc materials differs from that of ordinary superconductors.
New strongly correlated effects	Within condensed matter physics, there is a very exciting interplay between experiment and theory: Sometimes theory is first to predict effects, often experiments discover interesting novel phenomena which then stimulate theoretical explanations, and may lead to general advances in understanding of many-body physical phenomena.

Experiments: probing the system response

Experimental stimulus promotes the system from its ground state into an excited state, and the response provides insights into the underlying microscopic properties

Response	Stimulus
Electrical	Applied electric field
Optical absorption	Electromagnetic wave
Temperature response	Heat flux
Magnetic moment	External magnetic field
Attenuation of sound waves	External source of sound

Computational approaches

Independent-electron approximation
Treats each electron as if it is moving in a periodic effective potential created by the ion cores
Neglect electron-electron correlations

Hartree-Fock theory
Includes “exchange” related correlations between electrons by forcing the wave function to be a single Slater determinant of optimal single-particle orbitals
Electrons of opposite spin remain uncorrelated

Computational approaches

Density functional theory

Includes both exchange and other correlations between valance electrons.

Correlations included by approximating the electron density as being locally uniform

Quantum Monte Carlo methods

Use the Monte Carlo method to handle the many-dimensional integrals that arise

Takes almost full account of electron-electron correlations

Exact diagonalization

Compute and diagonalize over all matrix elements

Captures all electron-electron correlations within limits of the basis set size

Analytical: emergent phenomena

Adopt a complementary approach to the reductionist approach of other areas of physics. Identify key organizing principles on the relevant macroscopic length scale inspired by experiment.

Complex phenomena can emerge from very simple sets of rules, for example Conway’s life

Analytical: example of emergent phenomena

For a space that is populated

Cell with one or no neighbors dies

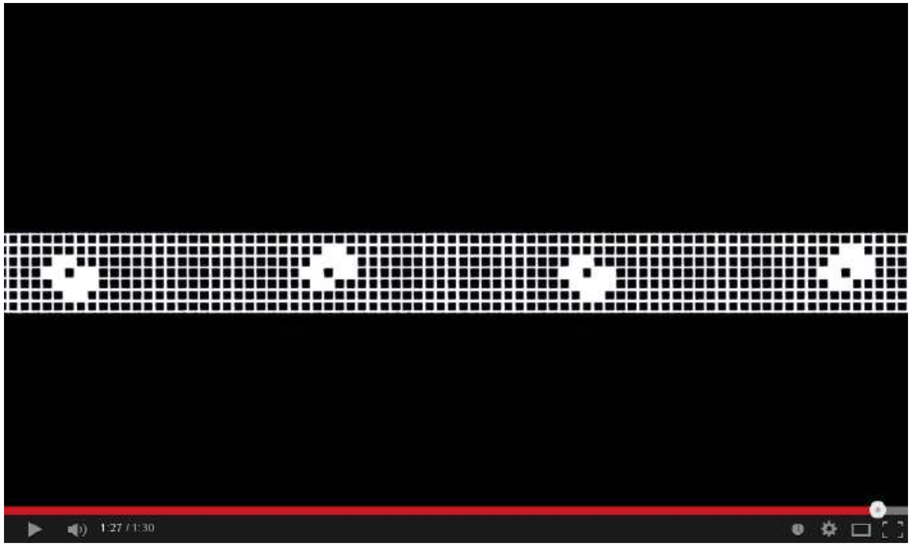
Cell with four or more neighbors dies

For a space that is unpopulated

Cell with three neighbors becomes populated

Analytical: critical phenomena

Critical phenomena: length scales diverge near to transitions insensitive to microscopic properties



Analytical: critical phenomena

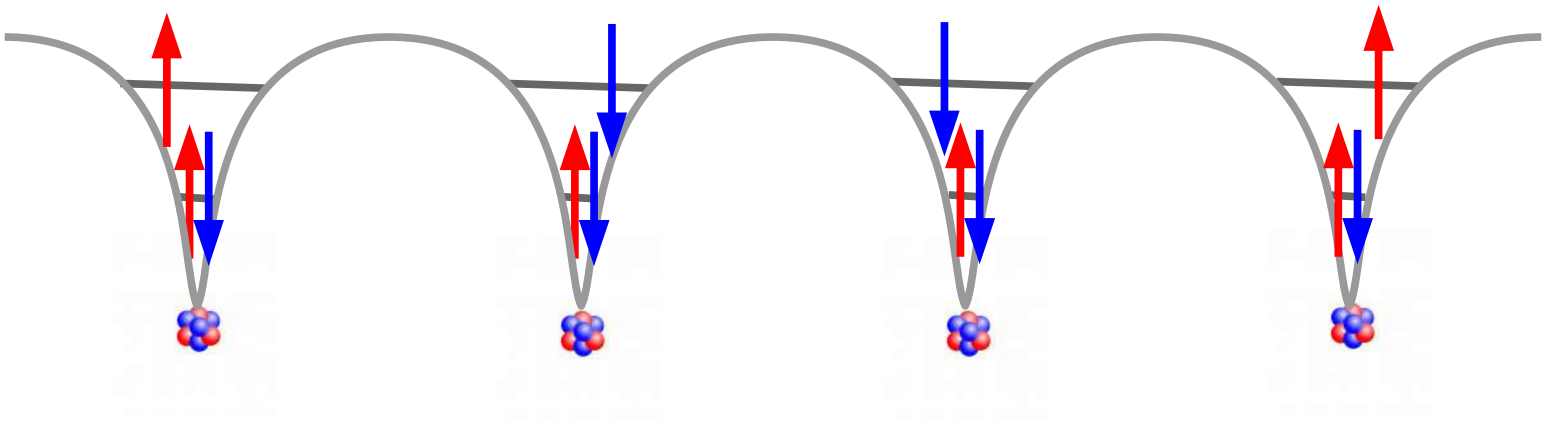
Analytical: construction of models

Solutions to the Schrödinger equation, whether numerical or exact, can be very hard to interpret or even connect with observed phenomena.

Phenomenological models that capture the essential physics of the system whilst blocking out non-relevant features often provide deeper, more applicable and predictive insight into a particular problem.

Models can be justified from first principles, and parameters determined by experiment.

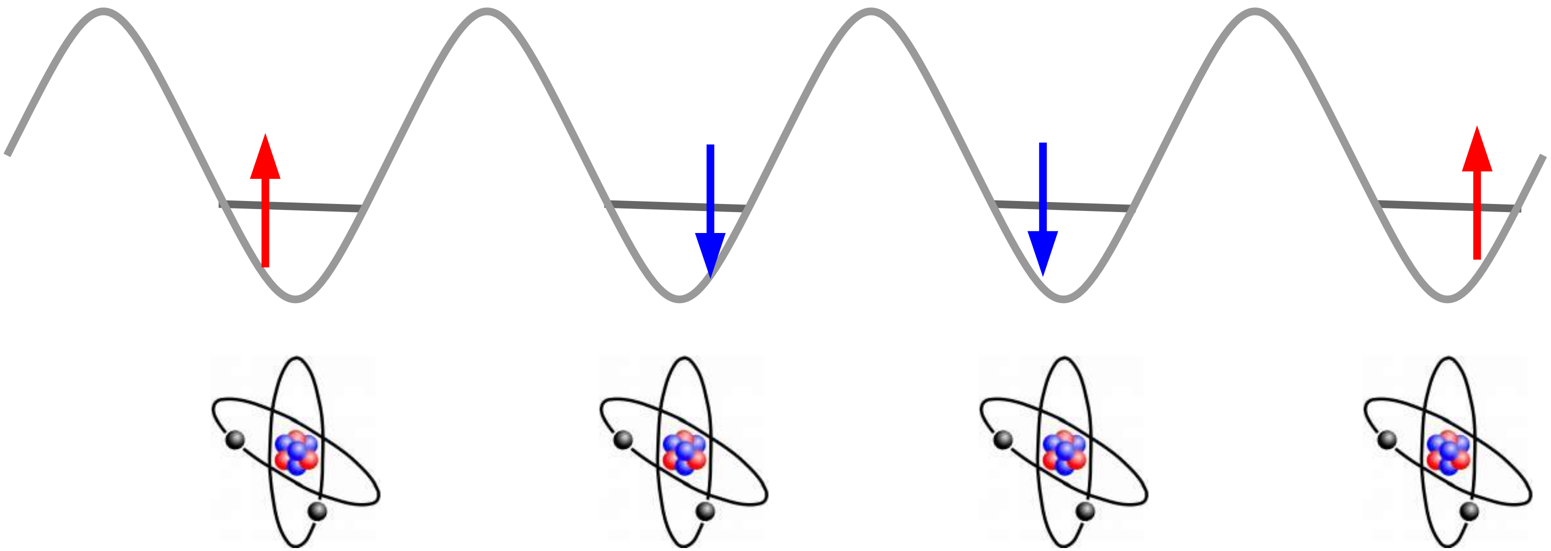
Analytical: constructing a model



$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \sum_{i=1}^{M} \frac{\hat{P}_i^2}{2m} + \sum_{i=1}^{N} \sum_{j<i} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|}$$

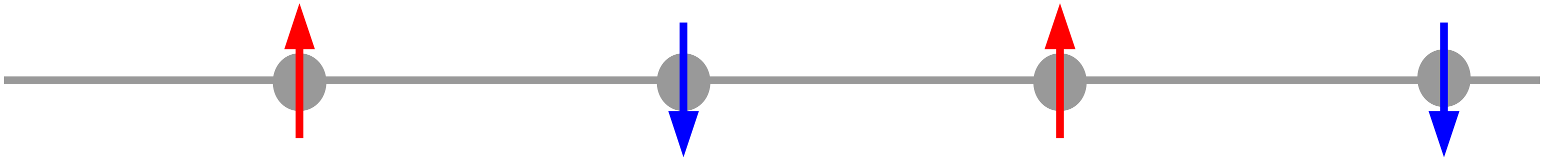
$$+ \sum_{i=1}^{N} \sum_{j=1}^{M} \frac{Z_j e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{R}_j|} + \sum_{i=1}^{M} \sum_{j<i} \frac{Z_i Z_j e^2}{4\pi\epsilon_0 |\vec{R}_i - \vec{R}_j|}$$

Analytical: constructing a model



$$\hat{H}=\sum_{i=1}^{N}\frac{\hat{p}_i^2}{2m}+\sum_{i=1}^{N}\sum_{j<i}\frac{e^2}{4\pi\epsilon_0|\vec{r}_i-\vec{r}_j|}+\sum_{i=1}^{N}V(\vec{r}_i)$$

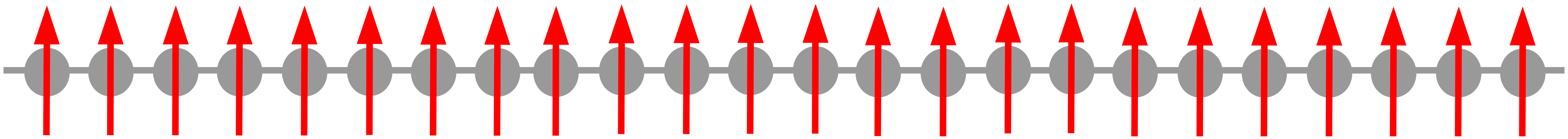
Analytical: constructing a model



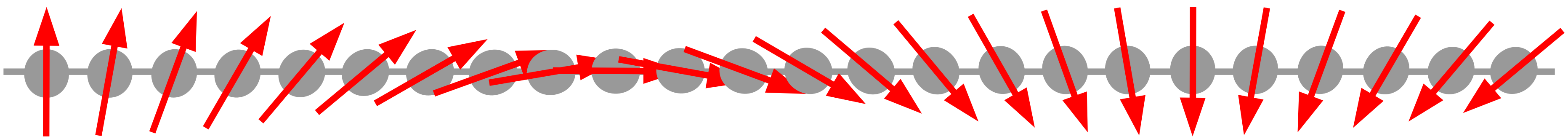
$$\hat{H} = -J \sum_{i=1}^{N} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_{i+1}$$

Collective excitations

Ground state



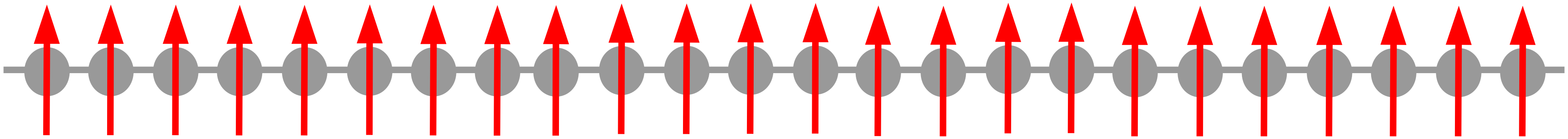
Spin wave



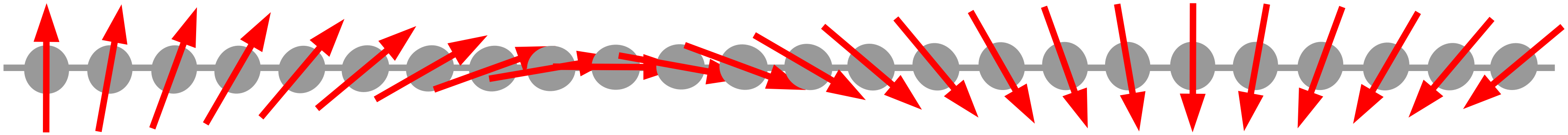
Magnon: wave-like deviations of spins

Collective excitations

Ground state

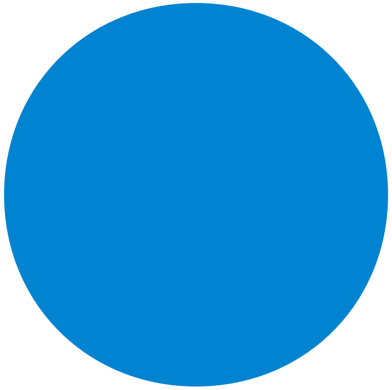


Spin wave



Magnon: wave-like deviations of spins
Plasmon: electron density displacements
Phonon: wave of atom displacements
Exciton: electron and hole bound
Polariton: electron and photon bound

Quasiparticles



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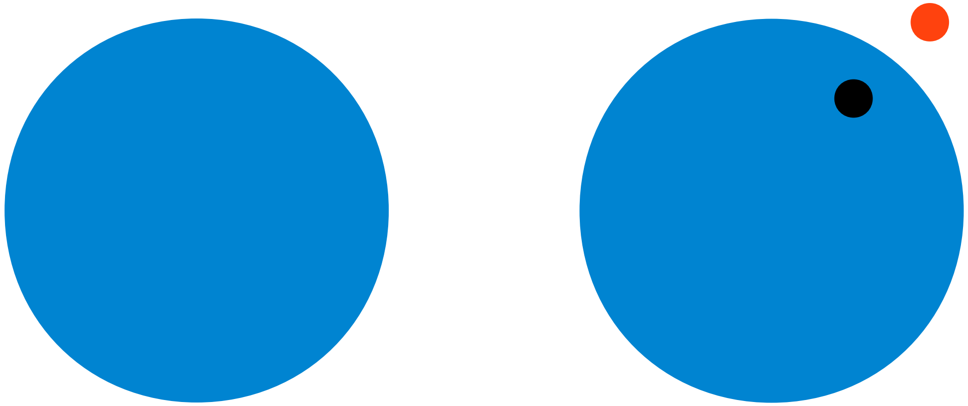

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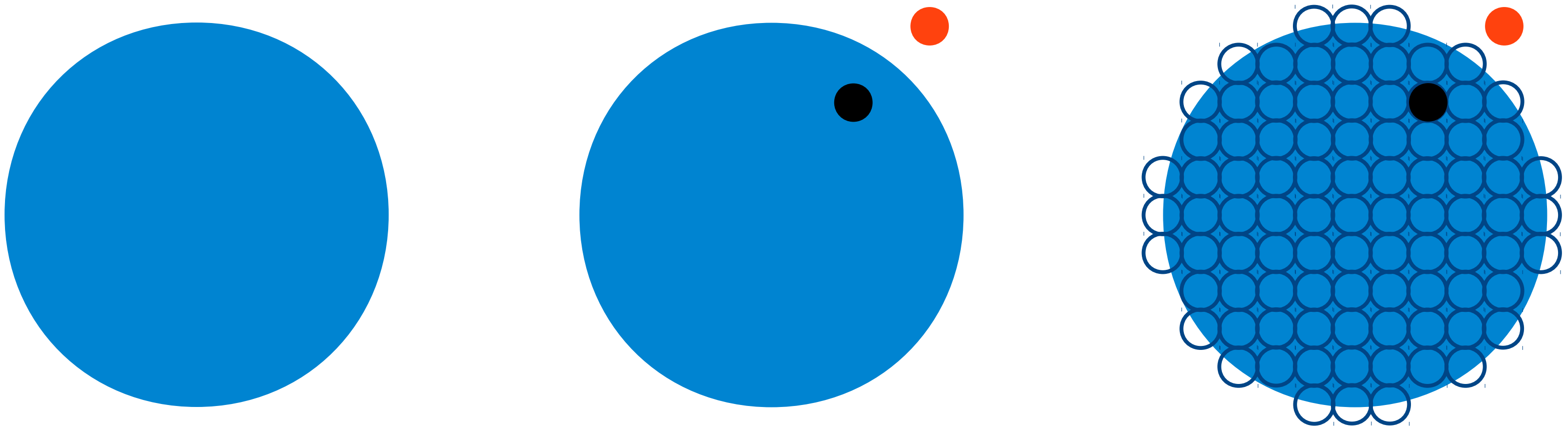

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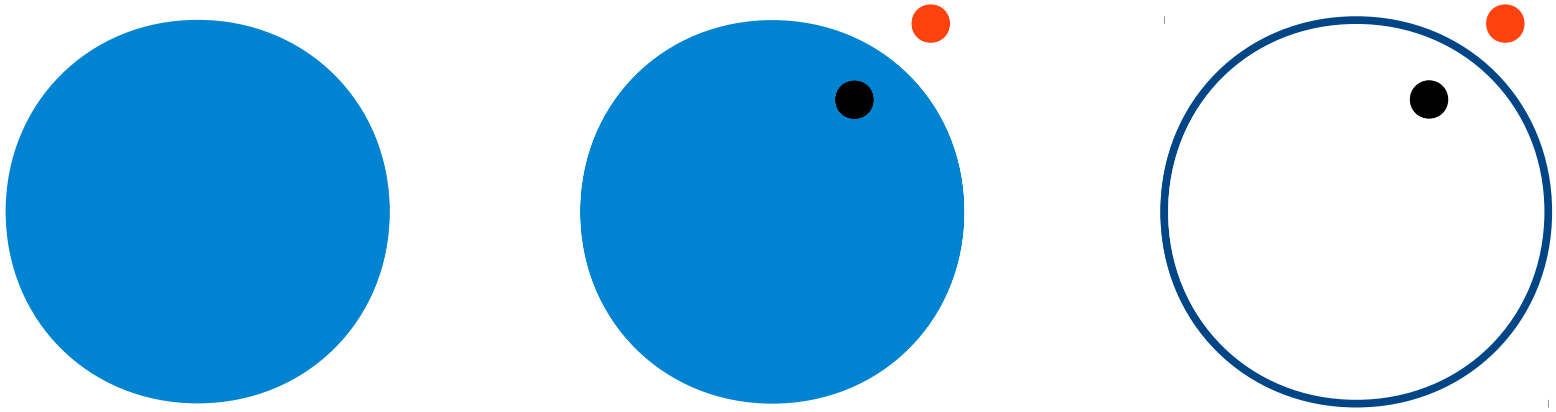

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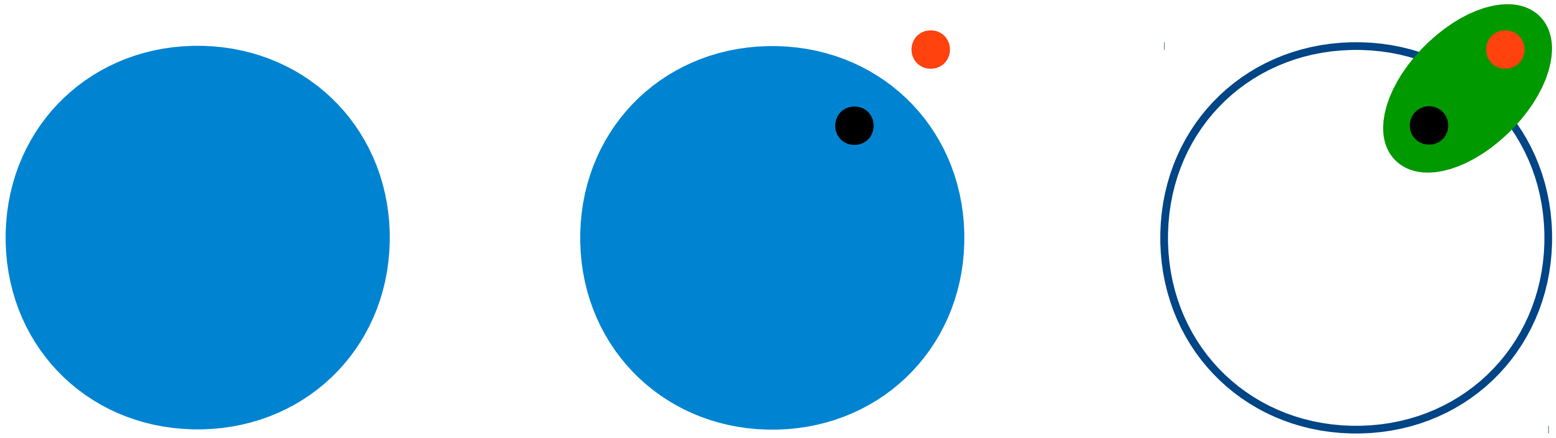

Outline of lectures

1) Concepts in many-body physics

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1) Concepts in many-body physics

2) Second quantization

3) Interactions

4) Correlation functions

5) Feynman diagrams

Books

Basic general

Principles of the Theory of Solids, Ziman (1979)
Solid State Physics, Ashcroft & Mermin (1976)
Introduction to Solid State Physics, Kittel (1996)

Advanced many-body theory

Quantum Theory of Solids, Kittel (1987)
Quantum Field Theory in Condensed Matter Physics, Nagaosa (1999)
Condensed Matter Field Theory, Altland & Simons (2010)