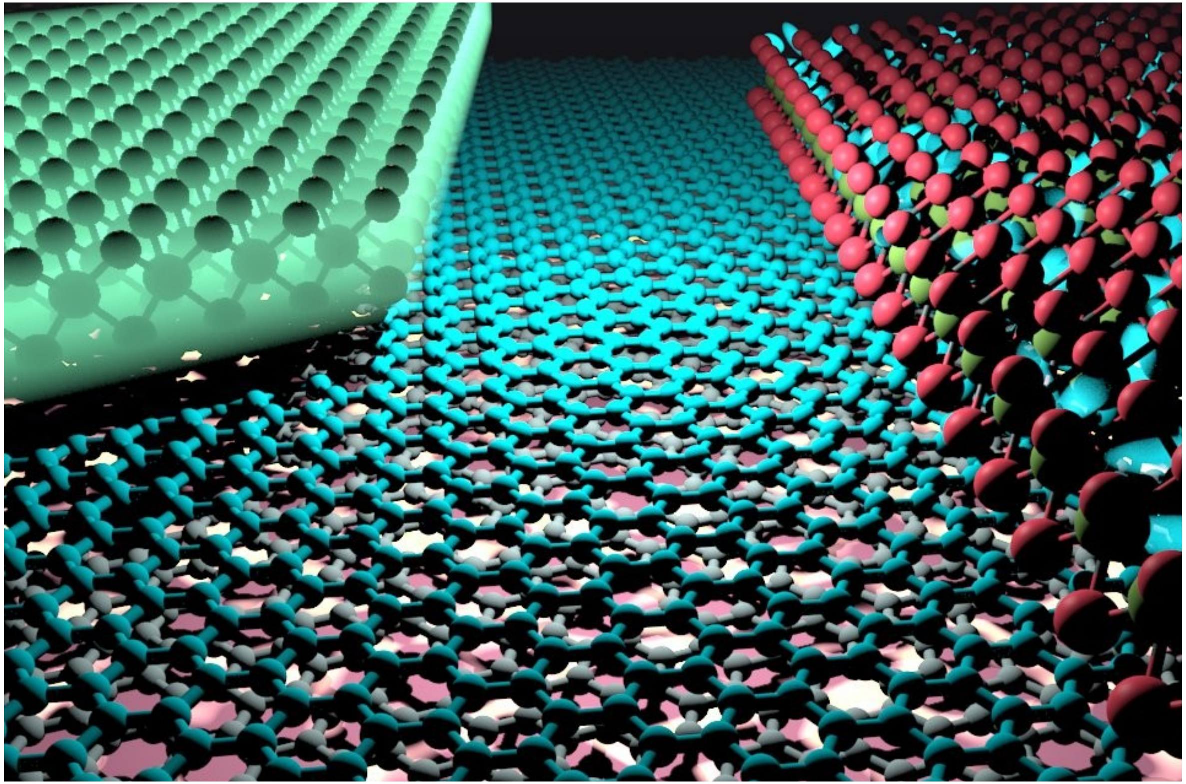
Session #1: Introduction, second quantization, mean-field and spontaneous symmetry breaking



March 1st 2021

Today’s learning outcomes

- What is a quantum material
- Why do we need quantum mechanics to understand quantum materials
- Basics of second quantization
- Mean-field and spontaneous symmetry breaking

Humankind and materials ages

Stone age

8700 BCE

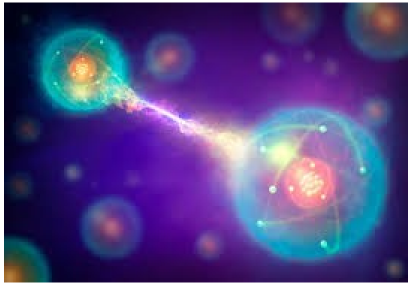
Copper age

3500 BCE

Silicon age

20th century

Quantum age



21th century

Some of the future materials will rely on controlling quantum properties of matter

The impact of quantum materials

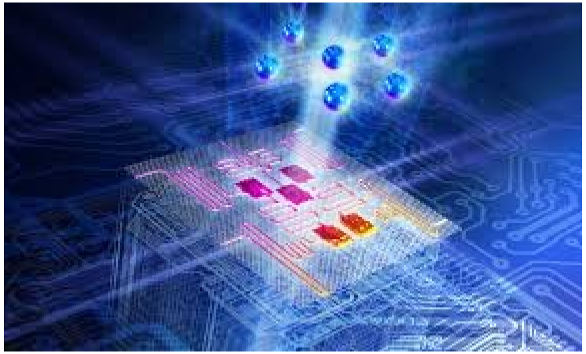
For medicine

Superconductors

For renewable energies

Semiconductors

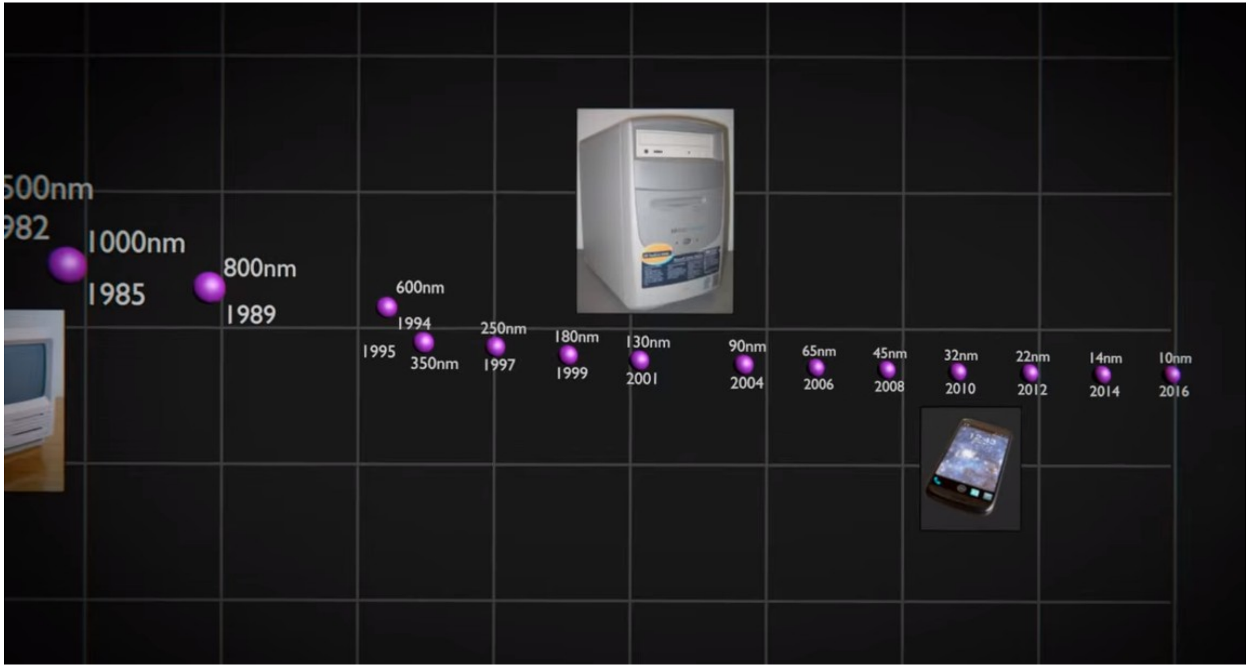
For quantum computing



Semiconductors & superconductors

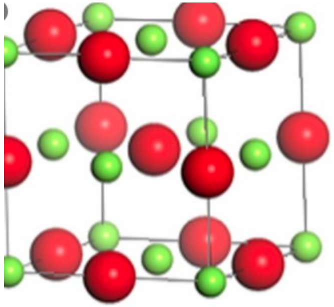
So close and such a stranger

https://www.youtube.com/watch?v=3De1rLxvzyU

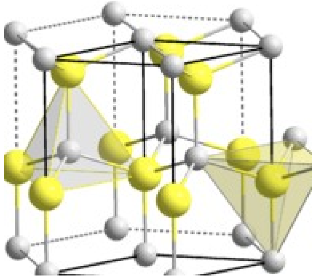


Which materials will we try to understand?

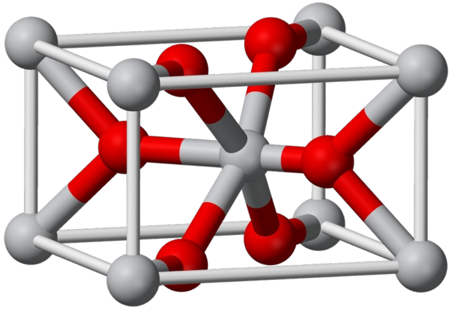
Insulators (MgO)



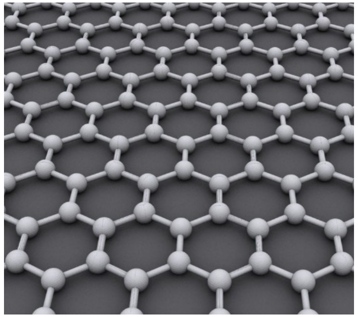
Semiconductors (GaN)



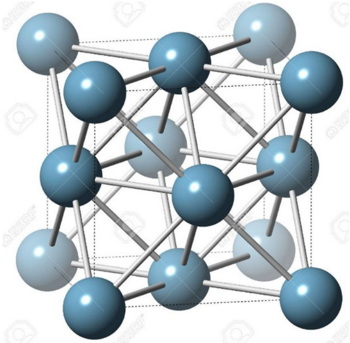
Ferromagnets (CrO_2)



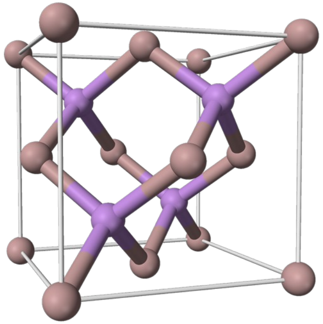
Dirac matter (graphene)



Superconductors (Al)



Fractional matter (GaAs)

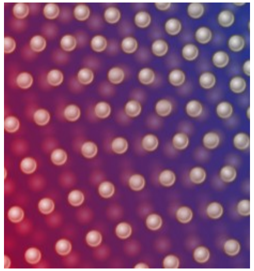


Quantum excitations in quantum materials

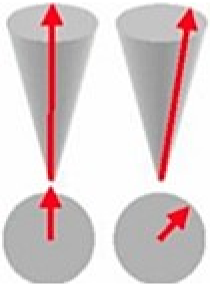
Solid state matter is made of electrons, protons, neutrons and photons

But in solid state materials, we can have emergent collective new excitations

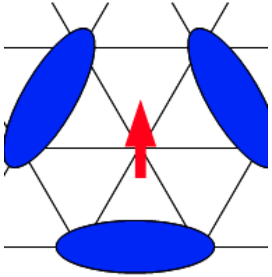
Phonons



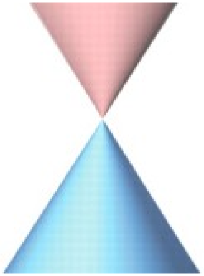
Magnons



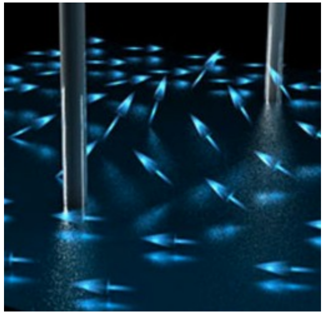
Spinons



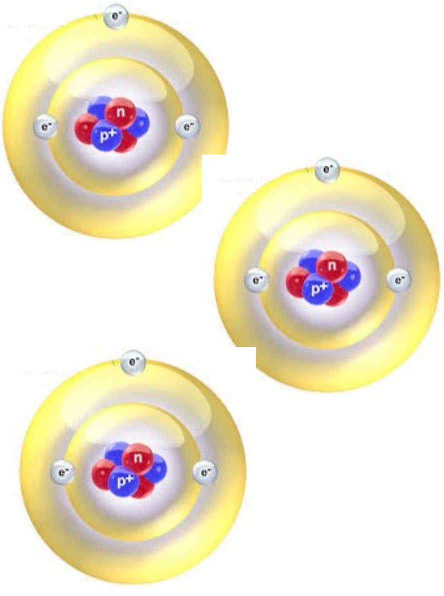
Dirac fermions

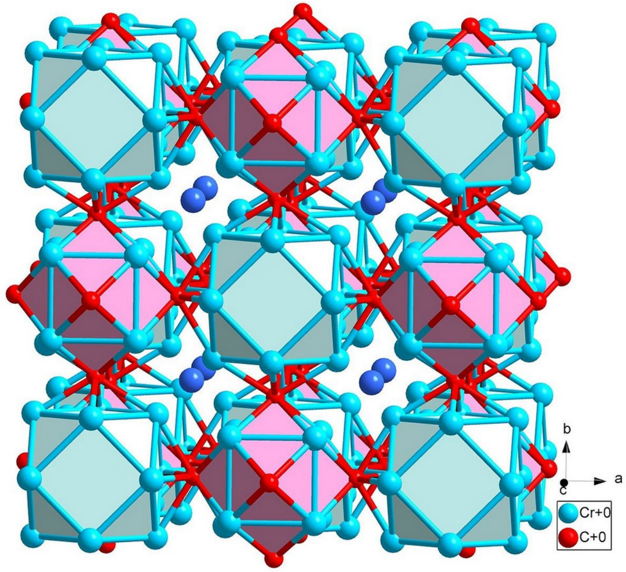


Vortexes



From atoms to quantum matter





How do we understand and predict properties as we put more and more atoms together?

How do we describe quantum matter?

We use quantum mechanics to understand electrons in materials

$$H|\Psi\rangle = -i\partial_t|\Psi\rangle$$

Hamiltonian

Wavefunction of the system

Two main kinds of phenomena can emerge

Single particle phenomena

Many-body phenomena

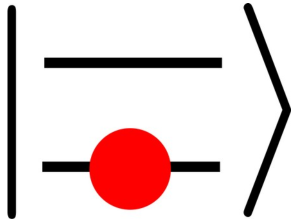
Two different kinds of quantum mechanical formalism

Systems where our number of particles is constant

First quantization, description based on a Hilbert space

Describes metals, semiconductors, insulators

<u>Highly successful and easy formalism</u>

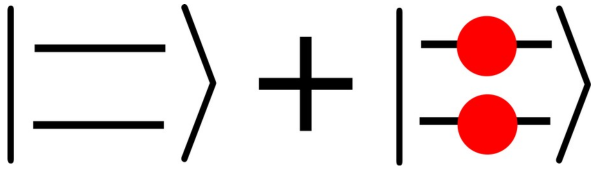


Systems where the number of particles fluctuates

Second quantization, description based on a Fock space

Describes superconductors, superfluids, correlated matter

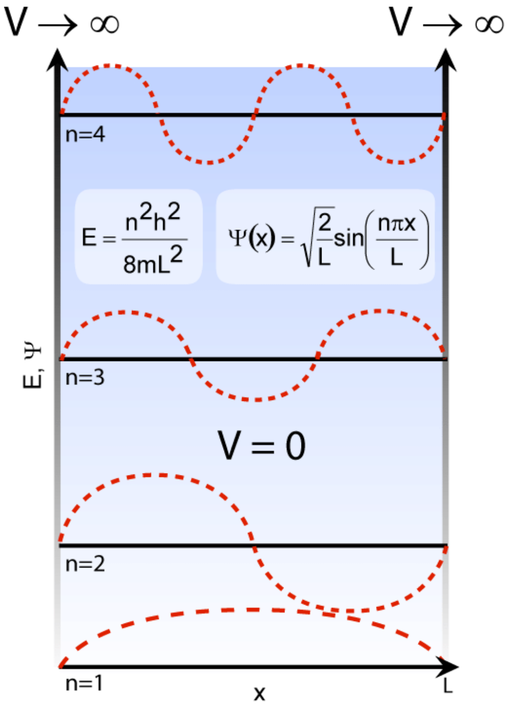
<u>Leads to much exotic phenomena, yet also more challenging</u>

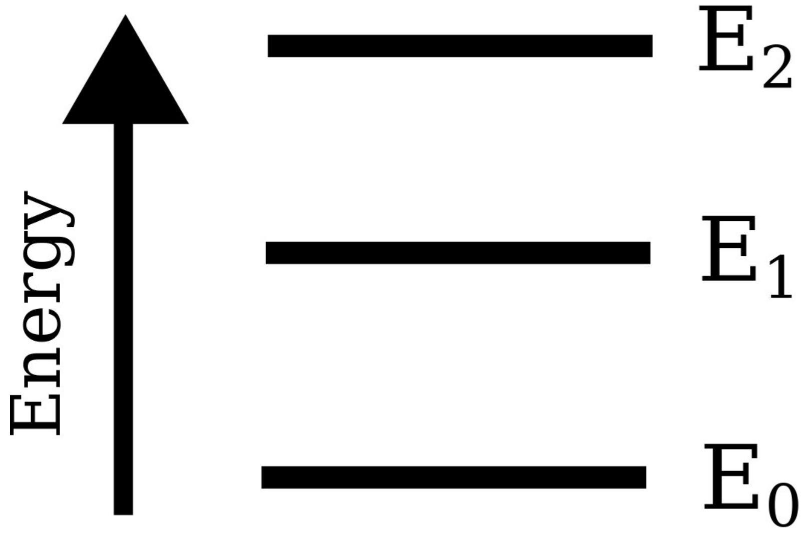


A reminder of a simple single particle state

Particle in a box

$$H|\Psi\rangle = E_n|\Psi\rangle$$





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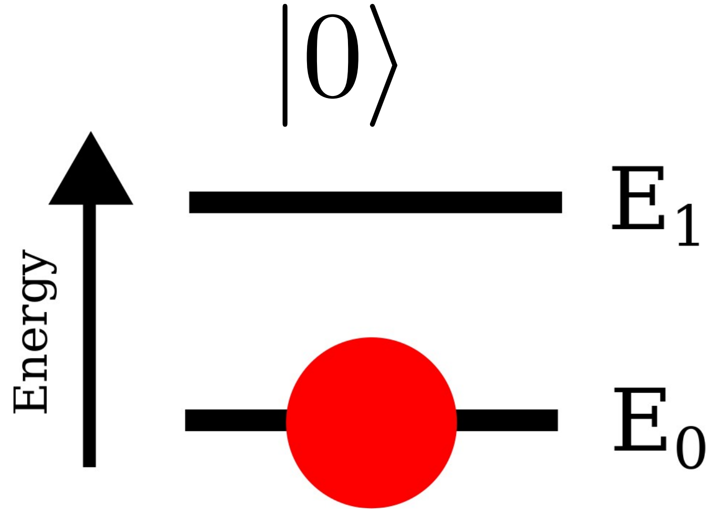
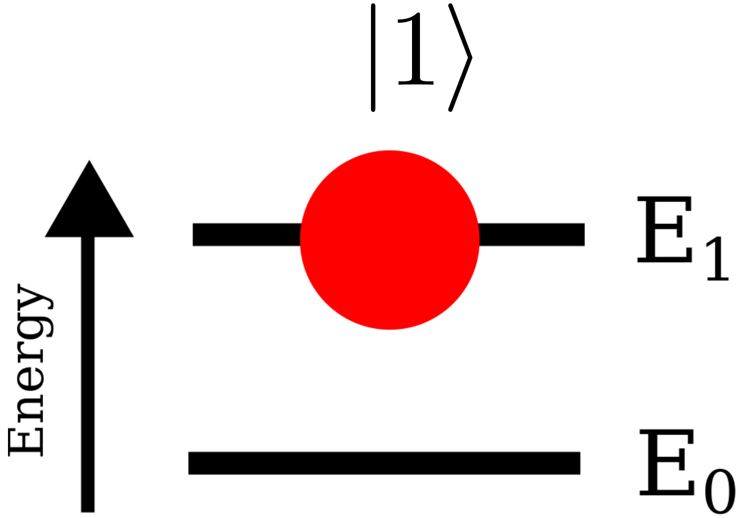


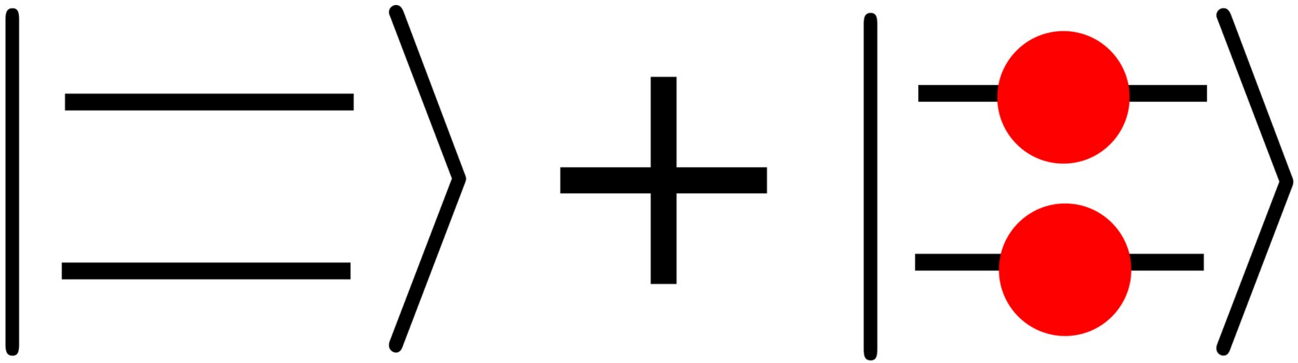


These two states describe having one particle, in one of the possible energy level

From single particle to many body

But what if our state is a combination of states with different numbers of particles?

A state having both 0 particles and 2 particles

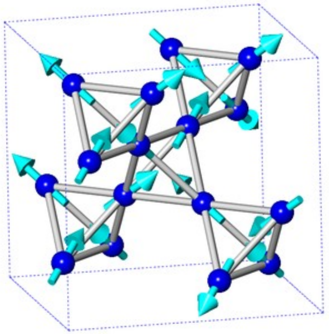


How do we describe states like these?

Non-constant number of particles

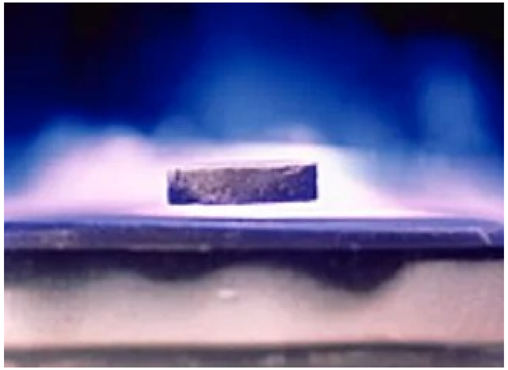
Why is this even relevant to understand materials?

Magnetic ordering of materials depends on processes in which the number of electrons fluctuates



Goodenough-Kanamori rules

The effective description of superconductors does not conserve electron number



Bogoliubov-de Gennes formalism

The idea of second quantization

Define operators that can create or destroy particles

c_i Annihilation operator, destroys a particle in site i

$c_i^\dagger$ Creation operator, creates a particle in site i

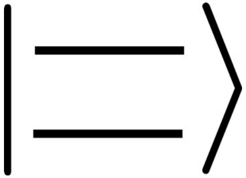
The empty vacuum state $|\Omega\rangle$ is defined as $c_i|\Omega\rangle = 0$

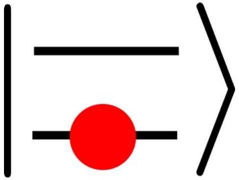
The Hamiltonian is written in terms of creation and annihilation operators

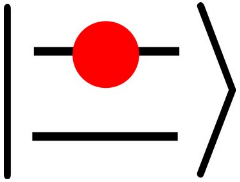
$$\mathrm{H} = \mathrm{c}_0^\dagger c_1 + h.c.$$

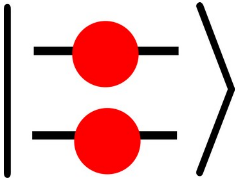
The idea of second quantization

Lets see some examples using the two-levels presented before

$$|\Omega\rangle =$$  The “vacuum” state

$$c_0^\dagger|\Omega\rangle =$$  One particle in level #0

$$c_1^\dagger|\Omega\rangle =$$  One particle in level #1

$$c_0^\dagger c_1^\dagger|\Omega\rangle =$$  Two particles in level #0 & #1

Fermionic quantum statistics in second quantization

Fermi-Dirac statistics for electrons
→ Wavefunctions are antisymmetric with respect to interchanging labels
→ There can only be 0 or 1 fermion per level

$$\{c_i^\dagger, c_j\} = c_i^\dagger c_j + c_j c_i^\dagger = \delta_{ij} \qquad \{c_i, c_j\} = 0$$

Anti-symmetric wavefunction $$c_0^\dagger c_1^\dagger |\Omega\rangle = -c_1^\dagger c_0^\dagger |\Omega\rangle$$

At most one fermion per site $$c_0^\dagger c_0^\dagger |\Omega\rangle = 0$$

Different kinds of Hamiltonians

Single particle Hamiltonians $$\mathrm{H} = \sum_{ij} t_{ij} c_i^\dagger c_j$$

Insulators, semiconductors, metals

Many-body Hamiltonian $$\mathrm{H} = \sum_{ij} V_{ijkl} c_i^\dagger c_j c_k^\dagger c_l$$

Fractional quantum Hall states, superconductors, quantum magnets

With second quantization, both cases can be treated on the same footing

What about interactions?

<u>But what happens when we put interactions?</u>

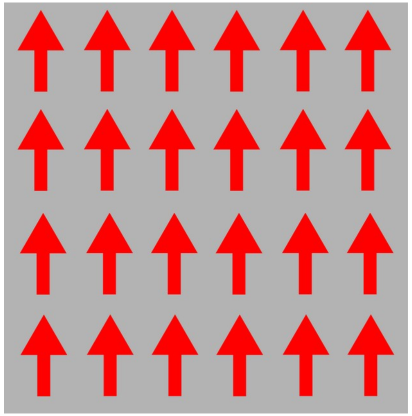
$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} V_{ijkl} c_i^\dagger c_j c_k^\dagger c_l$$

The role of electronic interactions

Electronic interactions are responsible for symmetry breaking

Broken time-reversal symmetry

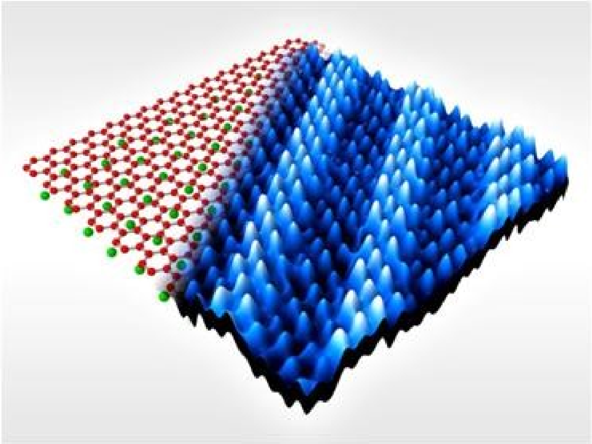
Classical magnets



$$\mathbf{M} \to -\mathbf{M}$$

Broken crystal symmetry

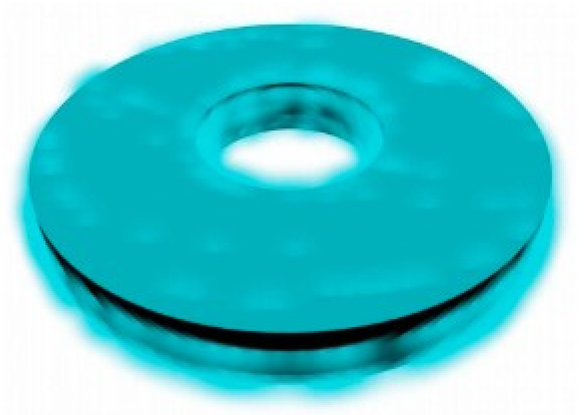
Charge density wave



$$\mathbf{r} \to \mathbf{r} + \mathbf{R}$$

Broken gauge symmetry

Superconductors



$$\langle c_\uparrow c_\downarrow \rangle \to e^{i\phi} \langle c_\uparrow c_\downarrow \rangle$$

A simple interacting Hamiltonian

Free Hamiltonian

Interactions (Hubbard term)

$$H = \sum_{ij} t_{ij} [c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}] + \sum_i U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

From now on lets consider we have a spin degree of freedom $\uparrow, \downarrow$

What is the ground state of this Hamiltonian?

$U < 0$ Superconductivity

$U > 0$ Magnetism

The mean-field approximation

Mean field: *Approximate four fermions by two fermions times expectation values*

Four fermions (not exactly solvable)	**Two fermions (exactly solvable)**

$$U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \approx U \langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \rangle c_{i\uparrow} c_{i\downarrow} + h.c.$$

$$U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \approx \Delta c_{i\uparrow} c_{i\downarrow} + h.c.$$

For $U < 0$

i.e. attractive interactions

$\Delta = \langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \rangle$ is the superfluid density

Gauge symmetry and superconductivity

What we know from quantum mechanics

"The phase of a wavefunction (field operator) does not have physical meaning"

This is what we know as gauge symmetry

$$c_n \to e^{i\phi} c_n$$

$$c_n^\dagger \to e^{-i\phi} c_n^\dagger$$

How does the superconducting pairing transform under a gauge transformation?

$$\Delta = \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle$$

Gauge symmetry and superconductivity

What we know from quantum mechanics

"The phase of a wavefunction (field operator) does not have physical meaning"

This is what we know as gauge symmetry

$$c_n \rightarrow e^{i\phi} c_n$$

$$c_n^\dagger \rightarrow e^{-i\phi} c_n^\dagger$$

How does the superconducting pairing transform under a gauge transformation?

$$\Delta \rightarrow e^{-2i\phi} \Delta$$

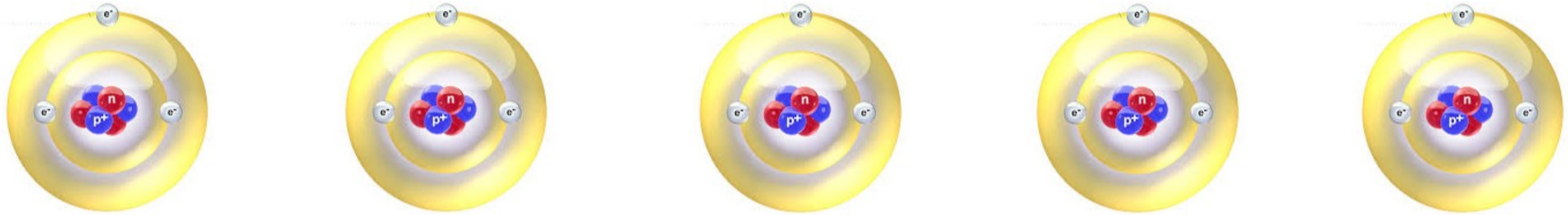
A superconductor breaks gauge symmetry

Take home

- Quantum materials realize a wide range of exotic phenomena
- Second quantization is a versatile language to understand quantum phenomena
- Symmetry breaking leads to new quantum states
- Read pages 9-24 from Solid State Lectures notes, by Titus Neupert

In the next session

Towards understanding crystals, when we have many, many atoms together arranged in a periodic manner



How to exploit symmetries to simplify quantum problems
How symmetries lead to conservation laws in quantum materials