Chair of Experimental Solid State Physics, LMU Munich

"Introduction to Graphene and 2D Materials"

SS24 Lecture 11, 01/07/2024

Outline - Lecture 11

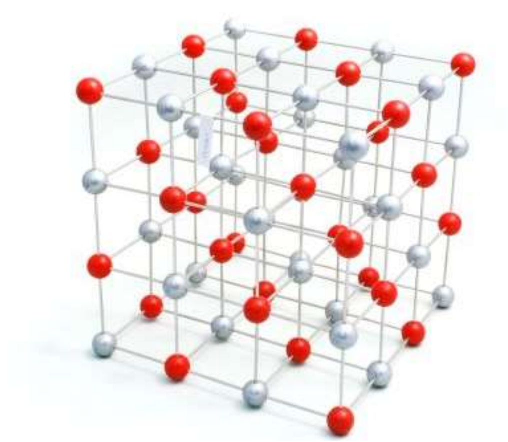
- Symmetry-breaking and phase transitions.
- Spin/valley symmetry breaking in graphene.
- Systems with strong electron-electron interactions.
- Fermi liquids.
- The Hubbard model.
- Flat-bands physics.
- Cascade of symmetry-broken phase transition in twisted bilayer graphene.

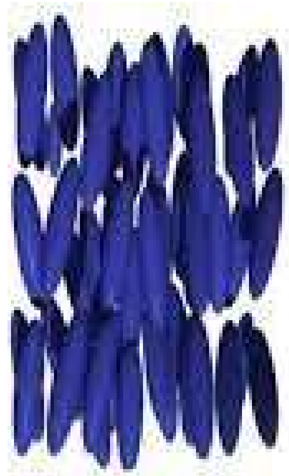
Types of order

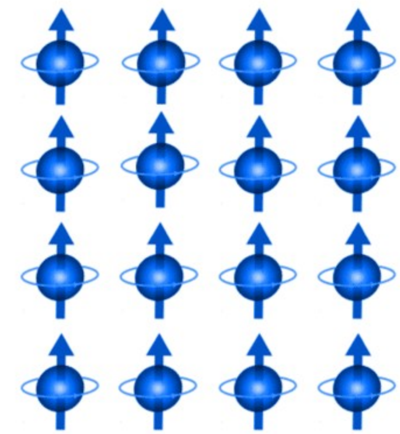
- Most of condensed matter physics is about how different kinds of **order** emerge from interaction between many simple constituents.

- Until 1980, all ordered phases could be understood being due to some sort of "symmetry breaking"

  → An ordered state appears at low temperatures when the system spontaneously loses one of symmetries present at high temperature and establishes a well-defined order parameter.







Examples:

- Crystals → break the **translation and rotation symmetries** of free space.

- Liquid crystals → break **rotational but not translational** symmetry.

- Magnets → break **time-reversal symmetry** and the **rotational symmetry of spin space**.

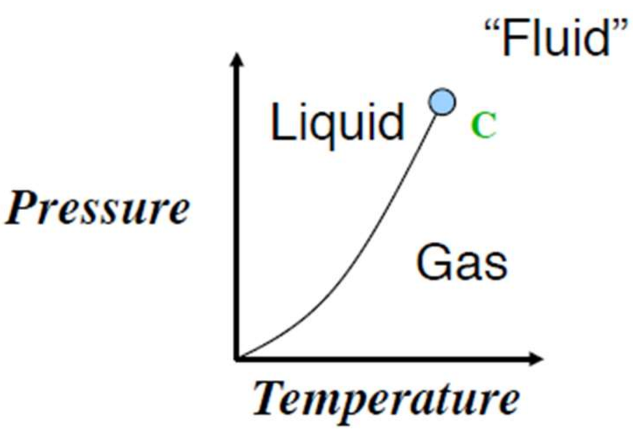
- Superfluids → break an **internal symmetry of quantum mechanics**.

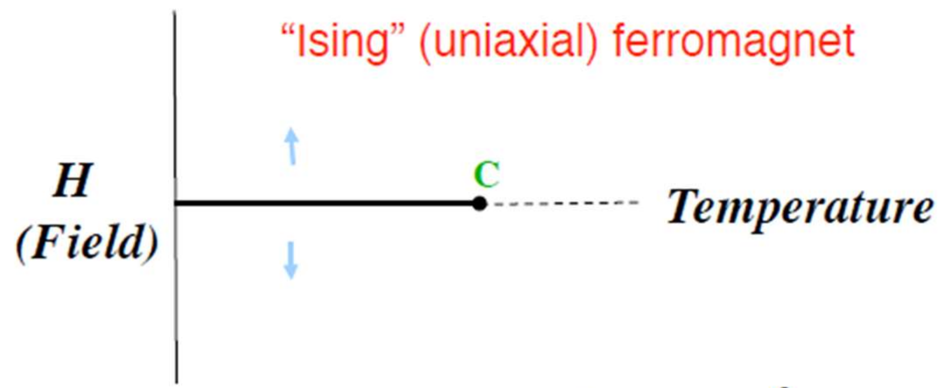
Types of order

- At high temperature, entropy dominates and leads to a disorder state.
- At low temperature, energy dominates and leads to an ordered state.

→ Landau theory of symmetry-breaking and phase transitions covers this physics in full. It states universality of phase-transitions, and defines an order parameter that spontaneously nucleates below a critical parameter (temperature, field etc.):

<u>Examples:</u>





$$\rho_L - \rho_G \sim \left(\frac{T_C - T}{T_C}\right)^{\beta}$$

$$M_{\uparrow} - M_{\downarrow} \sim \left(\frac{T_C - T}{T_C}\right)^{\beta}$$

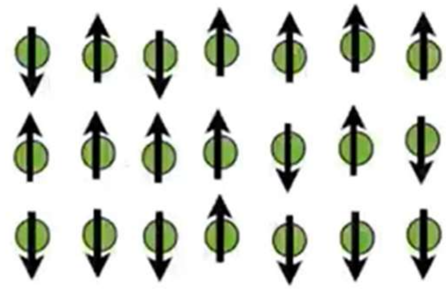
$$\text{Experiment}: \quad \beta = 0.322 \pm 0.005$$

$$\text{Theory}: \quad \beta = 0.325 \pm 0.002$$

The Ising model

- The Ising model captures qualitatively many of the key properties of ferromagnets and antiferromagnets.

$$H_{\text{Ising}} = g\mu_B B \sum_l \sigma_l - \frac{J}{2} \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$



- Let us first consider the absence of a magnetic field. Then, we set B=0, so that there are two possible energies depending on the value of σi, either:

$$E_{\sigma_i=+1/2} \quad = \quad -\frac{Jz}{2}\langle\sigma_i\rangle \qquad\qquad E_{\sigma_i=-1/2} \quad = \quad +\frac{Jz}{2}\langle\sigma_i\rangle$$

- The partition function for this spin can be written as:

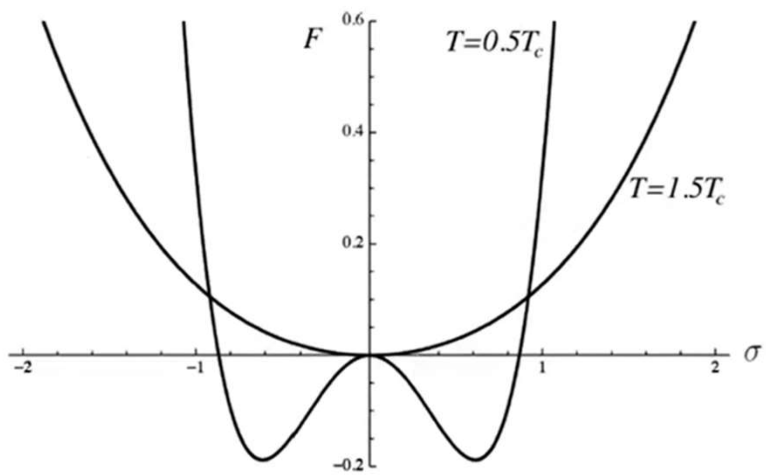
$$Z = e^{\beta Jz\langle\sigma_i\rangle/2} + e^{-\beta Jz\langle\sigma_i\rangle/2}$$

- And the average value of σi can then be written as:

$$\langle\sigma_i\rangle = \frac{1}{2}\frac{e^{\beta Jz\langle\sigma_i\rangle/2} - e^{-\beta Jz\langle\sigma_i\rangle/2}}{e^{\beta Jz\langle\sigma_i\rangle/2} + e^{-\beta Jz\langle\sigma_i\rangle/2}} \equiv \frac{1}{2}\tanh\left(\frac{\beta Jz\langle\sigma_i\rangle}{2}\right)$$

Symmetry breaking

- It is instructive to see what happens to the free energy of the system as we pass through Tc. With the free energy, we can compute this is a function of $<\sigma i>$ from the partition function:
- We see clearly the different forms above and below Tc:
- For Tc>T, the free energy is perfectly symmetric with respect to $< \sigma_i >$, since there is no preferred direction for the spins in the absence of the external magnetic field.
- For T<Tc, the free energy curve remains symmetric in $< \sigma_i >$, but the system can move to lower energy by breaking this symmetry, picking an energy minimum with $< \sigma_i >$ unequal zero.
- For the solution $< \sigma_i >=0$ is a local maximum energy, so this state is unstable.
- We refer to the choice the system makes as spontaneous symmetry breaking, where the free energy is perfectly symmetric in $< \sigma_i >$, but the system will choose to make break it the other way.



$$F = -k_B T \log Z$$

Symmetry breaking

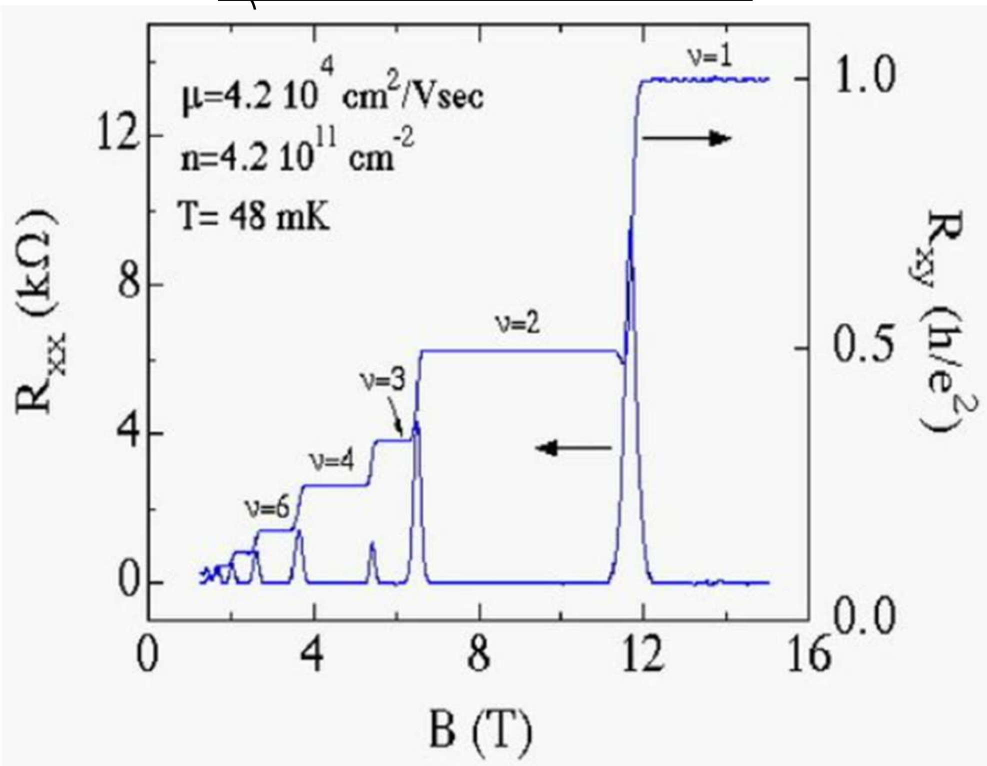
- We encounter this type of symmetry breaking regularly for phase transitions in condensed matter, and indeed also in high-energy physics and cosmology.

- In condensed matter physics, we can argue that there is always some stray magnetic field from outside the system (even if this is very small) which pushes the system in one direction or another. The system then amplifies this small asymmetry until it reaches a macroscopic average value of $< \sigma_i >$.

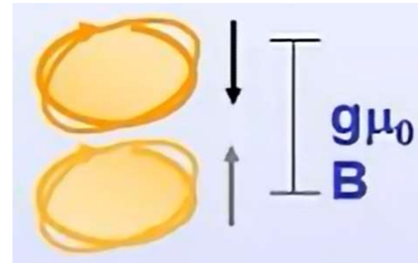
- If we apply an external field, we can explicitly break the symmetry and determine the directions in which the spins align. This is what is usually done when we are creating a permanent magnet from iron.

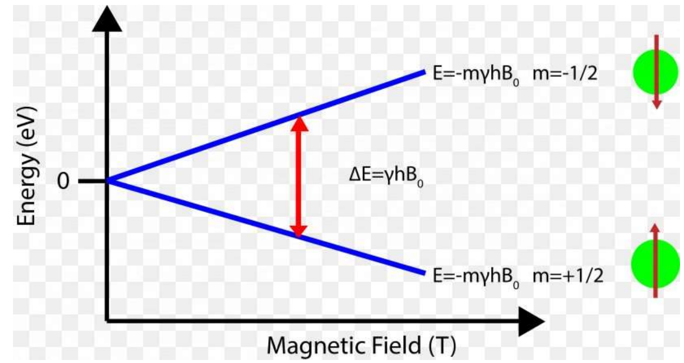
Analyzing the exact QHE – Zeeman splitting of LLs

QHE in a 2DEG device:



Zeemann splitting of the spins:



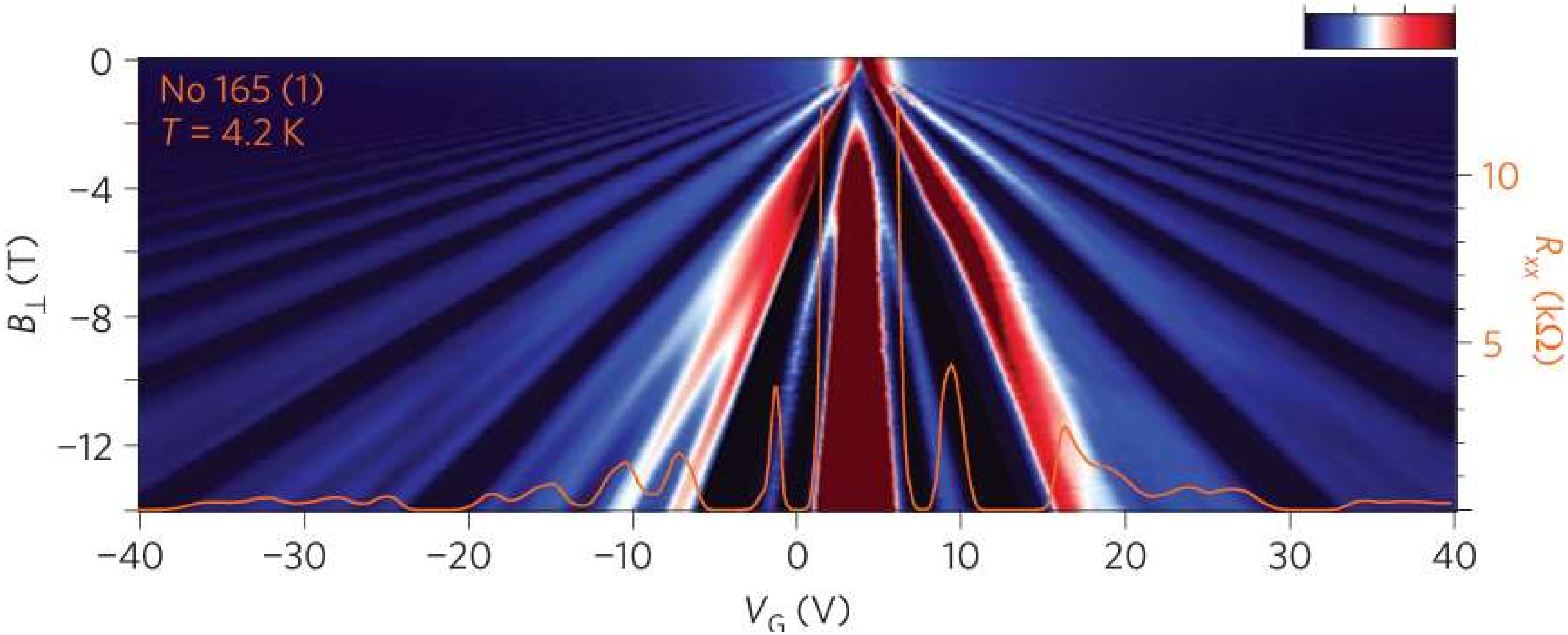


- Each Landau level holds the exactly same amount of states (electrons), where total number of states in each LL grows with B (gs = 2 accounts for spin):
  $N = g_s L_x L_y / 2\pi l_B^2 = g_s AB/\Phi_0 = g_s \Phi/\Phi_0$

- filling factor = number of occupied LLs (below Fermi energy) - total number of electrons ns devided by number of electrons in a LL (not accounting for degeneracy):
  $\nu = hn_s/eB$

→ At extremely high B-field we find QH states with odd filling factors and plateaus like ν=1 and ν=3. These states are states with broken spin symmetry due to the Zeeman energy – Quantum Hall ferromagnets.

Landau fan in the n vs. B phase space



- There is a linear dependence of the number of states in one of the LLs N vs. B: $N = g_s g_v L_x L_y / 2\pi l_B^2 = g_s g_v AB/\Phi_0 = g_s g_v \Phi/\Phi_0$

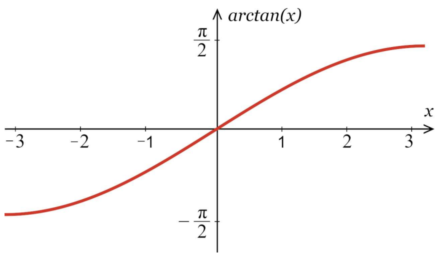
- For a fixed filling factor v there is a linear dependence of the carrier density in one of the LLs N vs. B:
$$n_s(\nu) = \frac{\nu e B}{h}$$

- Each Landau level has a 4-fold spin/valley degeneracy at low B-field.

Spin (SU(2)) X Pseudo-spin (SU(2)) = SU(4)

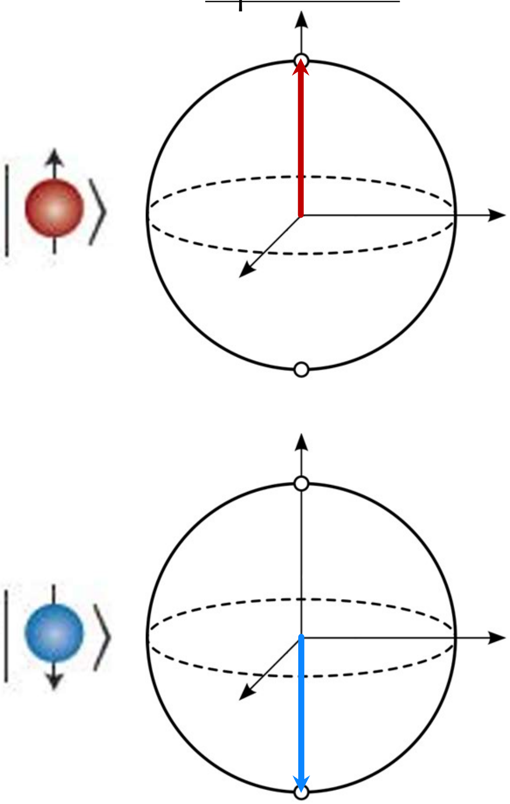
Wave-functions resemble spin:

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\vec{\kappa}\vec{r}} \\ e^{i(\vec{\kappa}\vec{r}+\theta_\kappa)} \end{pmatrix}$$

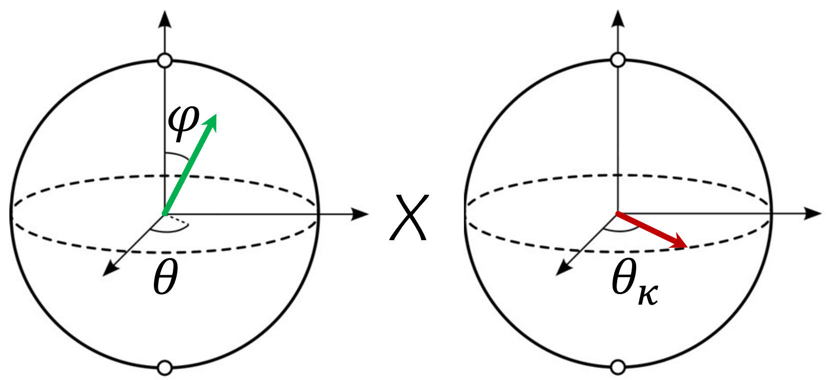


$$\theta_\kappa = arctan(\kappa_y/\kappa_x)$$

Spinors:



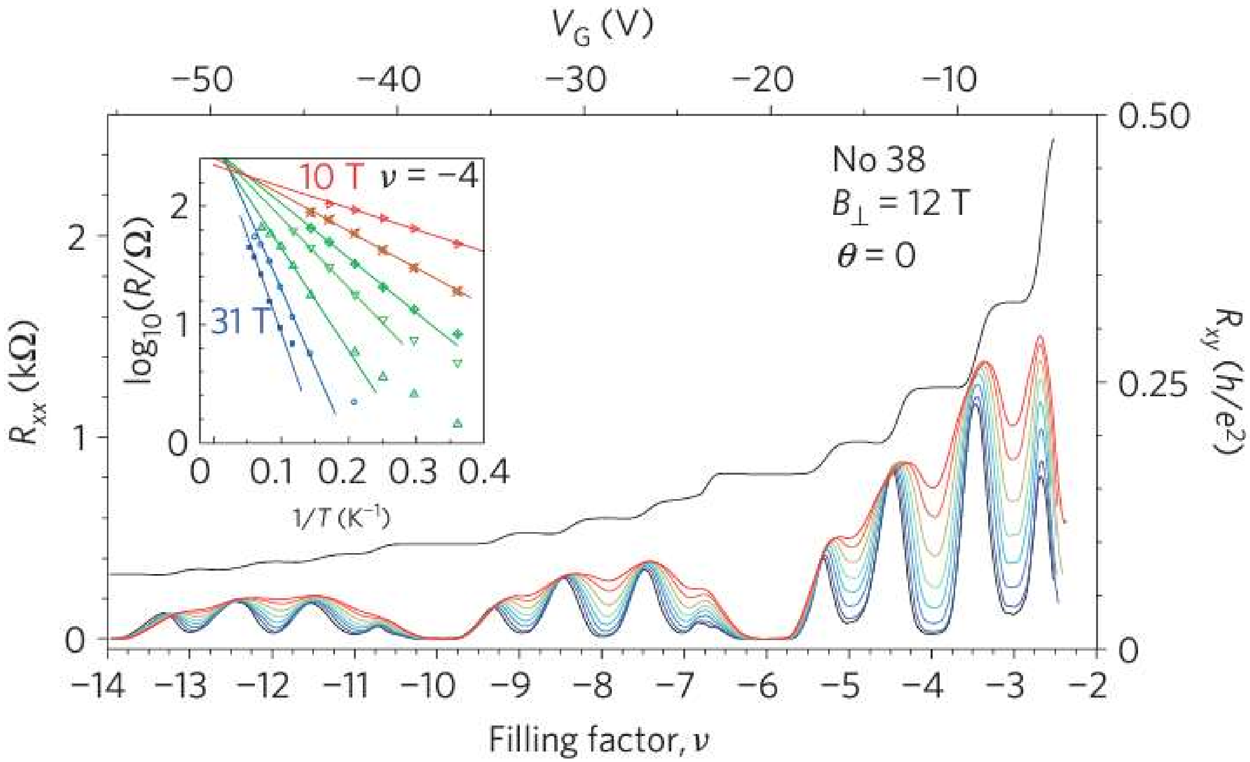
Two quantum numbers spin and pseudo-spin:

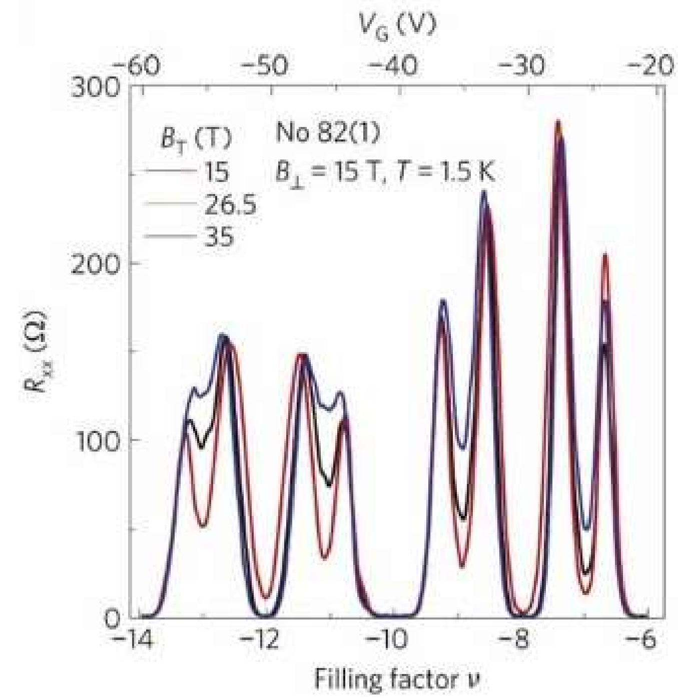


SU(2) x SU(2) = SU(4)

→ Also convenient to translate to SU(4) basis of spin x valley.

Spin and valley splitting at large B





- The 4-fold (spin/valley) degenerate LLs undergo symmetry-breaking, due to Zeeman splitting and electron-electron interactions, first to a 2-fold degeneracy, and then no degeneracy.
- The nature (spin vs. valley polarization) of the symmetry-broken LLs, can be tested by tilting the B field, while keeping the perpendicular B-field component fixed.
- The resulting states are no clearly spin or valley polarized, rather they form states within the allowed states in the SU(4) spin x valley phase space.

Strongly correlated electrons

- Electronic correlation is the interaction between electrons in the electronic structure of a quantum system. The correlation energy is a measure of how much the movement of one electron is influenced by the presence of all other electrons.

- Physical systems that we understand well correspond to ensembles of free particles. For example, semiconductors and most metals can be described as having non-interacting electrons. This simple approach is valid because the interaction (Coulomb) energy of electrons is much smaller than their kinetic energy.

- Another example is alkali atoms, that Bose condense at low temperatures. Alkali atoms can be treated as non-interacting bosons because their scattering length (i.e. the length at which they interact with each other) is much smaller than the average distance between the particles.

- However, there are important systems for which interactions between the particles are not weak, and these interactions play a major role in determining the properties of such systems.

Fermi liquids

1. Fermi liquid theory is a theoretical model of interacting fermions that describes describes the behavior of many-body systems of particles in which the interactions between particles may be strong. The theory explains why some of the properties of an interacting fermion system are very similar to those of the ideal Fermi gas.

2. The system's dynamics and thermodynamics at low excitation energies and temperatures may be described by substituting the non-interacting fermions with interacting quasiparticles, each of which carries the same spin, charge and momentum as the original particles. Physically these may be thought of as being particles whose motion is disturbed by the surrounding particles and which themselves perturb the particles in their vicinity.

3. Each many-particle excited state of the interacting system may be described by listing all occupied momentum states, just as in the non-interacting system. As a consequence, quantities such as the heat capacity of the Fermi liquid behave qualitatively in the same way as in the Fermi gas (e.g. the heat capacity rises linearly with temperature).

4. There are also clear differences to the Fermi gas, where f.e. the magnitude of the specific-heat, compressibility, spin-susceptibility can have strongly enhanced values. Also strong electron-electron scattering can highly limit the lifetime of the electrons.

Strongly correlated electrons

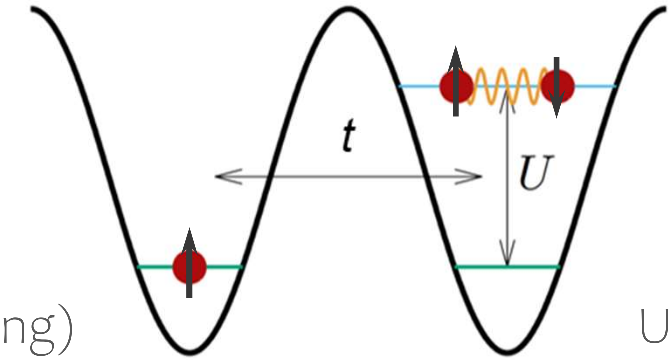
1. Conventional superconductors. Coulomb interaction between electrons and ions in these materials results in a new ground state that can support a dissipation less flow of electrical current.

2. High-temperature superconductors. The transition temperature for these materials is surprisingly high. The origin of superconductivity is still unclear, but it is commonly believed that it comes mostly from the Coulomb interaction between the electrons, rather than the electron-ion interactions that are important for the conventional superconductors. What is also intriguing about the high Tc cuprates is that superconductivity appears in materials that are not good metals to begin with. In fact their normal state properties are so unusual that they are often called "strange metals".

3. Magnetic systems. Coulomb and exchange interaction between electrons may lead to a variety of spin ordering patterns, including ferromagnetism (spins of all the particles are aligned), antiferromagnetism (spins of the neighboring particles are anti-aligned).

4. Fractional Quantum Hall systems. In the presence of a strong perpendicular magnetic field electrons confined in one or several two-dimensional layers form a new quantum liquid state, that may have such unusual properties as fractionally charged excitations or uncertain layer index.

Hubbard model



t – kinetic energy (hopping)

U – onsite energy (Coulomb)

$U = e^2\theta/(4\pi\varepsilon_0\kappa a)$

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

- If U and t are comparable in size → We have competition that arises between the interaction energy and the kinetic energy in the system (i.e. the energy of the electrons because of their position in the Bloch band):

- Each lattice site that hosts two electrons, pays an energy penalty that is defined by the Coulomb energy.

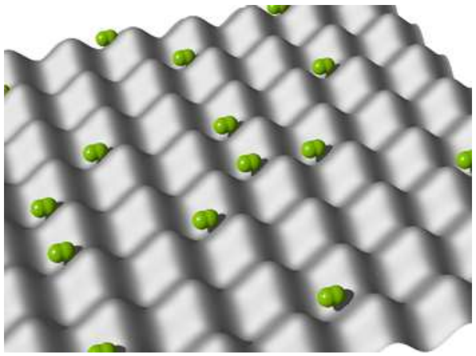
- If U >> t, the Coulomb energy cost is too high, so the electrons cannot tunnel and localize.

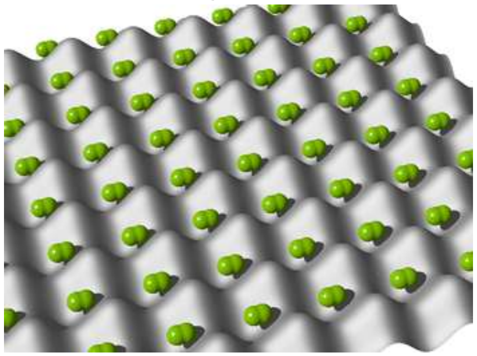
- Two electrons at each lattice site cannot have the same spin (Pauli principle), which further restricts possible hopping events.

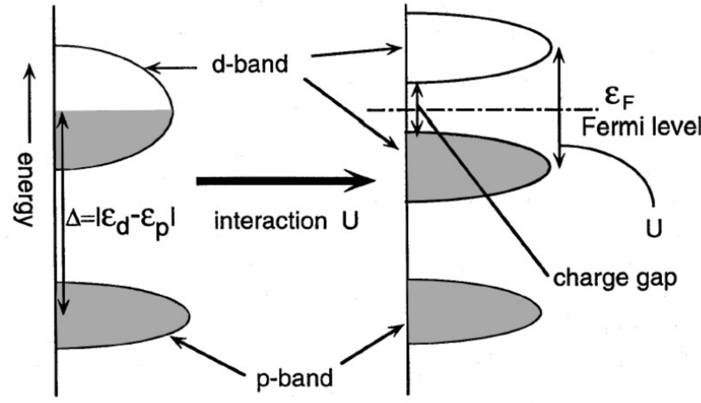
Mott insulator picture

At integer filling – gapped Mott insulator:

U/t >> 1





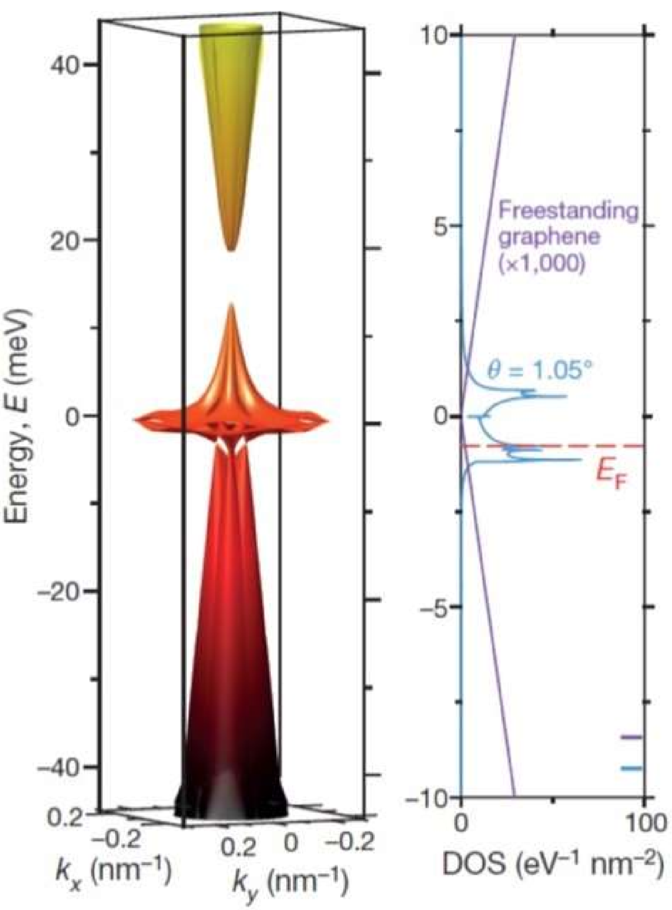


- For a partially filled band, there are always free lattice sites, so that electrons can freely tunnel between these and so propagate in the crystal.

- At integer filling (half-filling for a spin ½ system), all the lattice sites are occupied with one electron. Iif U >> t, the Coulomb energy cost is too high, so the electrons cannot tunnel and localize. An energy gap is formed in the spectrum and an insulating state is formed, called a correlated or Mott insulator.

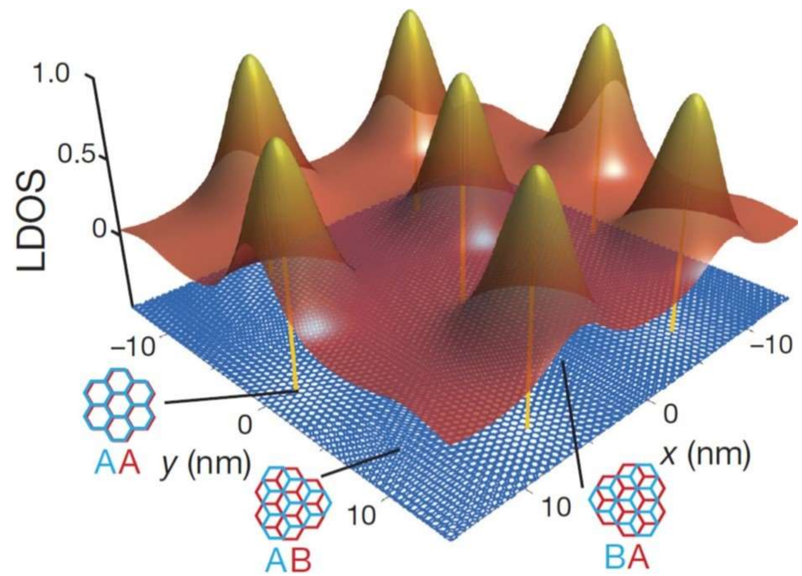
Flat bands and ultra-high DOS at the magic angle of 1.1°

Flat bands and ultra-high DOS:



R. Bistrizer, et. al. PNAS (2011);
2x - Y. Cao, et. al. Nature (2018);

Spatial distribution of DOS:



Strongly enhanced electronic interactions

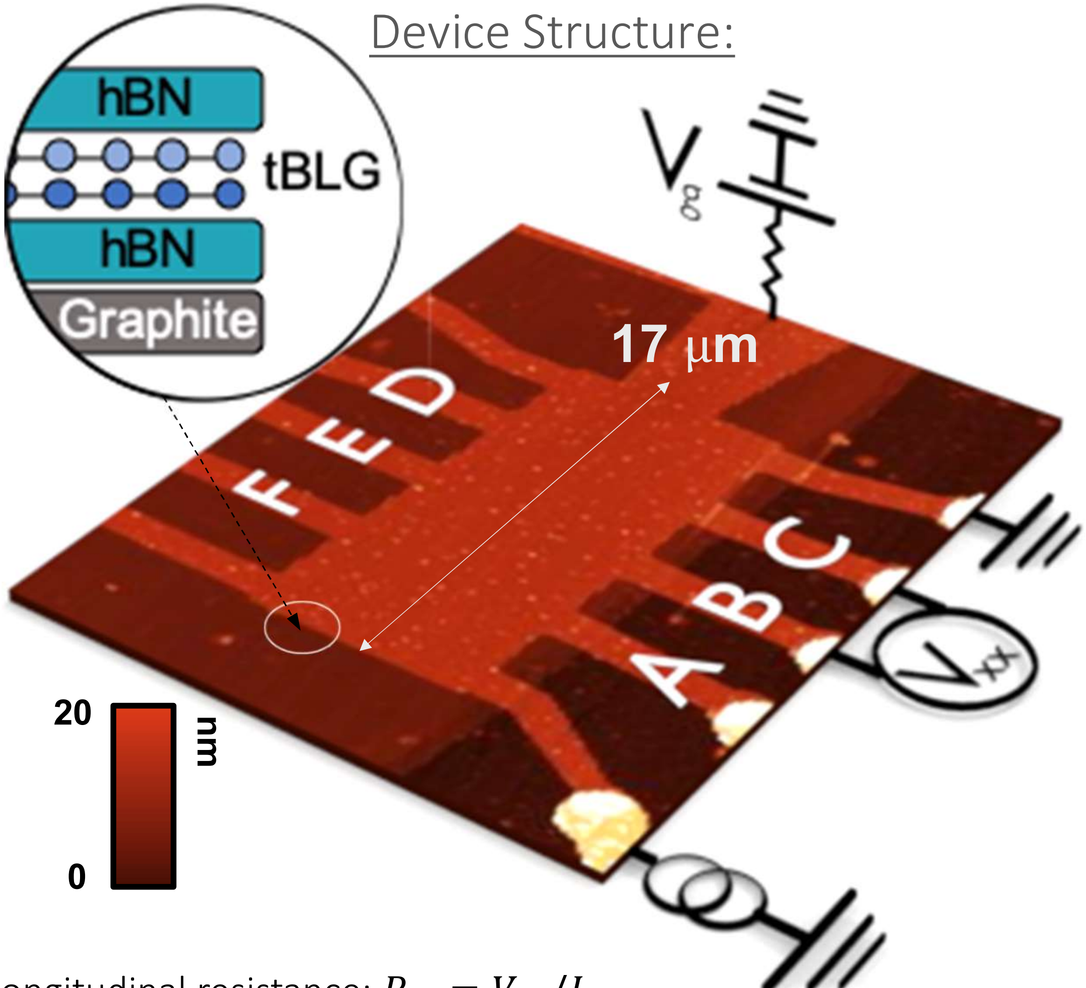
→ Correlated states
→ Superconductivity
→ Magnetism
→ Charge density wave
→ etc.

$$k_B T_c = 1.13\omega_D \exp\left(-\frac{1}{N(0)V}\right)$$

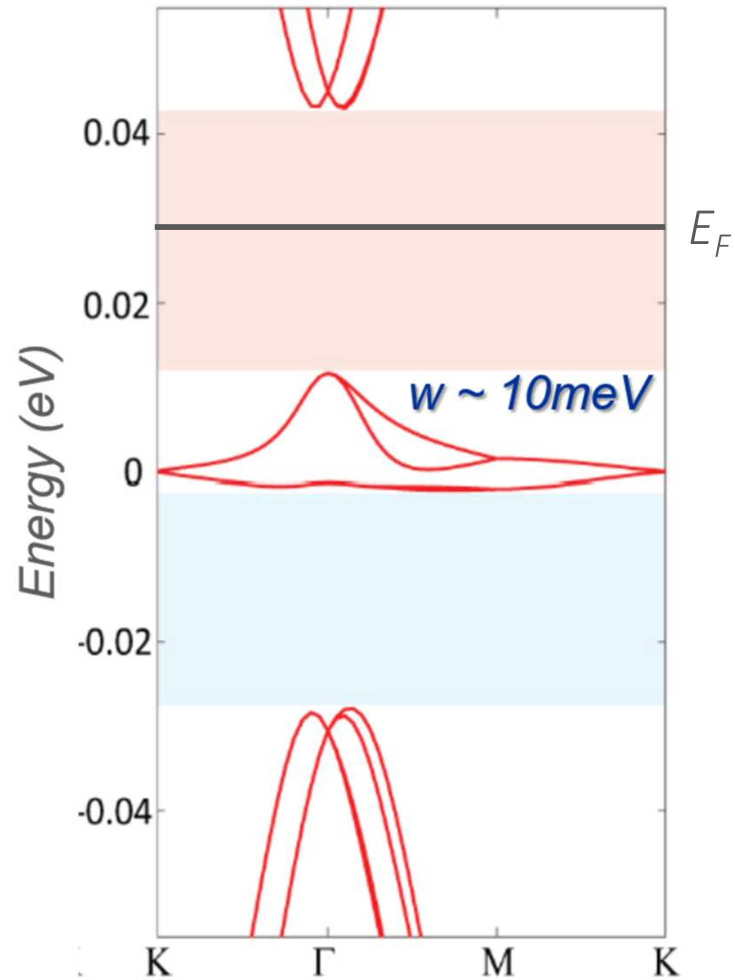
- quenched kinetic energy – t
- dominant interaction energy – U
- bands are topological

Transport Measurements

Device Structure:



Tuning Fermi Energy:



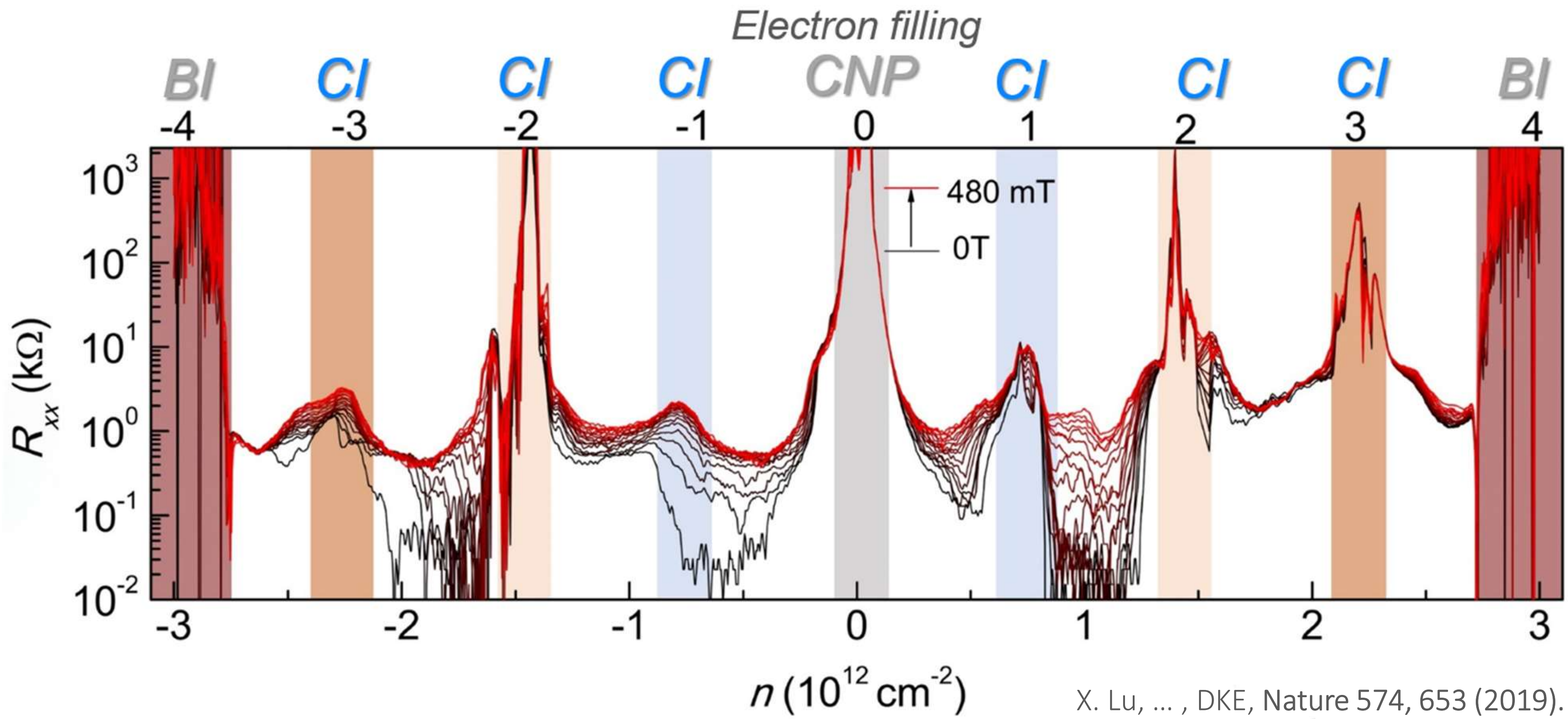
Longitudinal resistance: $R_{xx} = V_{xx}/I$

Hall resistance: $R_{xy} = V_{xy}/I$

Carrier density: $n = C_g * V_g$

Hall density: $n = n_H = -B/eR_{xy}$

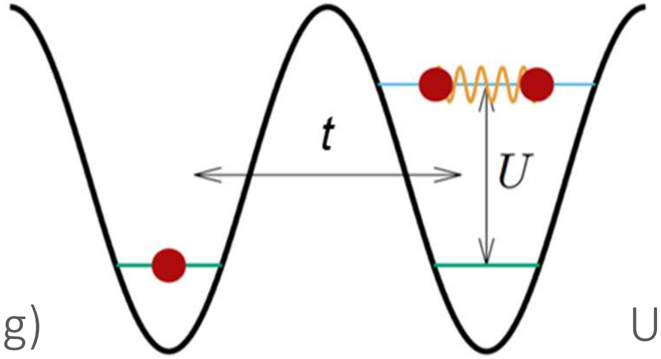
Transport measurements



X. Lu, ... , DKE, Nature 574, 653 (2019).

Symmetry broken correlated insulators at all integer fillings ν = 0,±1,±2,±3 e/uc

Mott insulator picture



t – kinetic energy (hopping)

U – onsite energy (Coulomb)

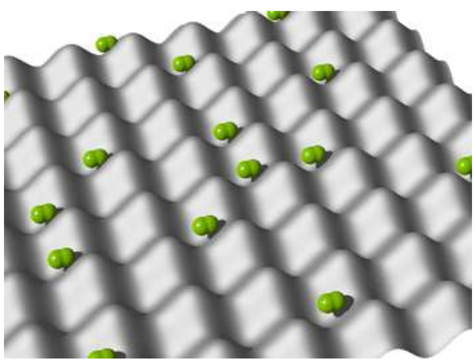
$U = e^2\theta/(4\pi\varepsilon_0\kappa a)$

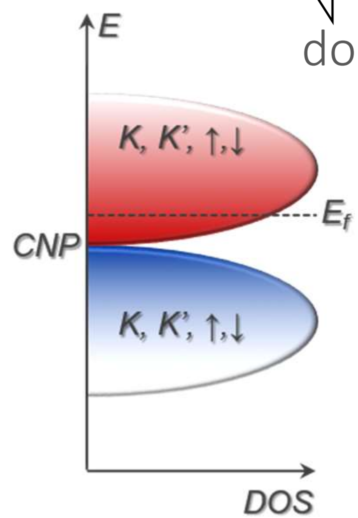
$$H = -t\sum_{i,j,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U\sum_i n_{i,\uparrow} n_{i,\downarrow}$$

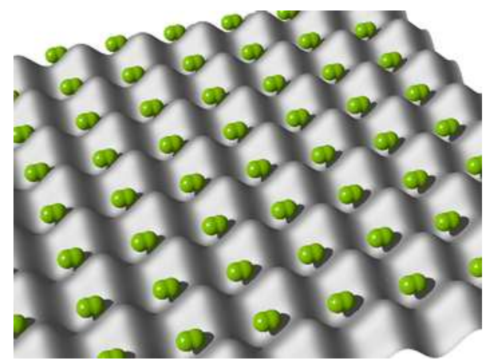
<u>partial filling - correlated metal:</u>

doping

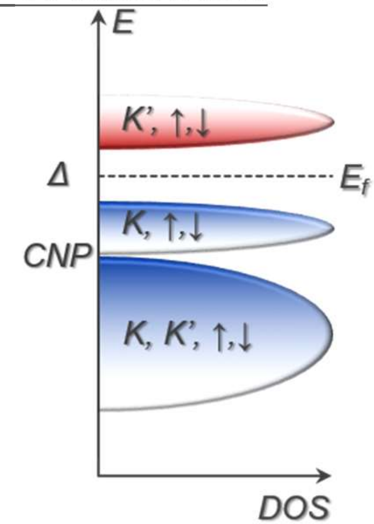
<u>integer filling – Mott insulator:</u>







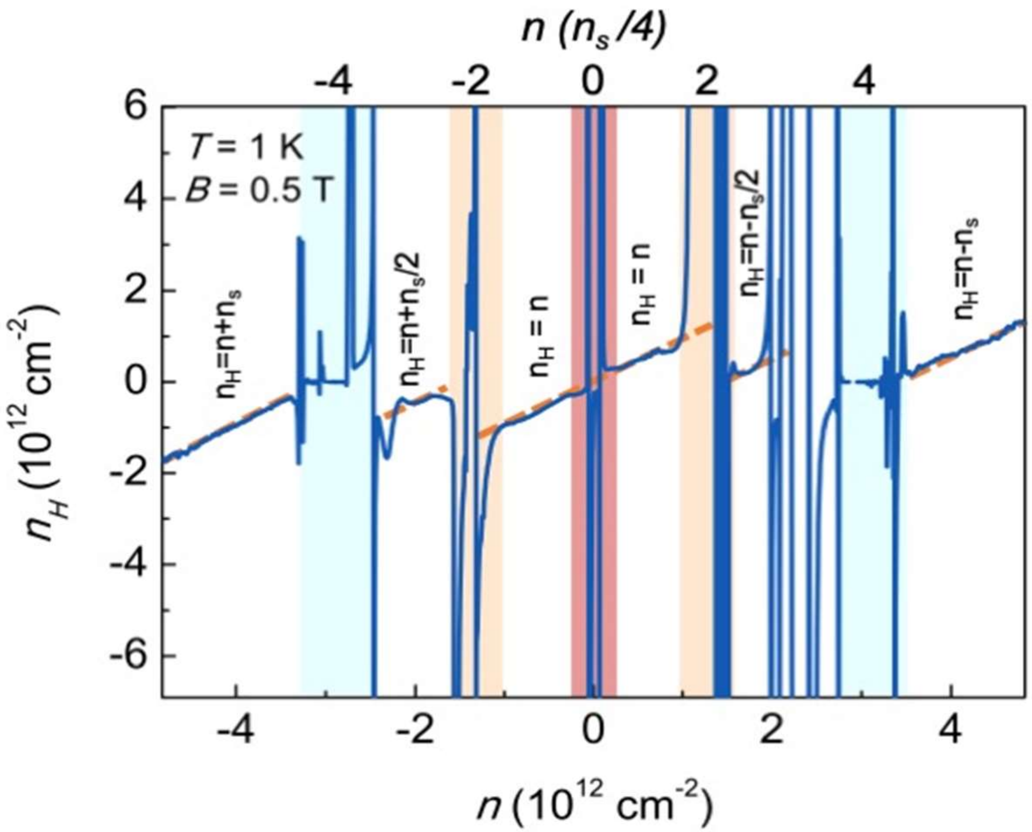
<u>*U/t >> 1*</u>



SU(4) spin/valley symmetry breaking

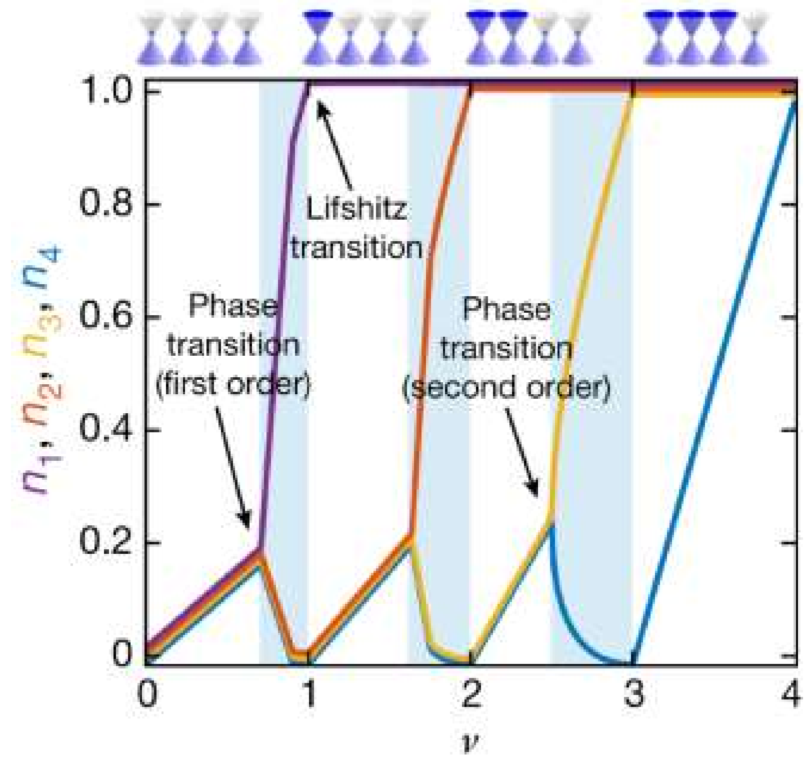
Interaction driven restructuring of Fermi surfaces

Hall density resets:



X. Lu, ... , DKE, Nature 574, 653 (2019).

Dirac revivals:



S. Ilani, Nature (2020).

Carrier density (Fermi level) resets at all integer fillings $\nu = \pm1, \pm2, \pm3$ e/uc

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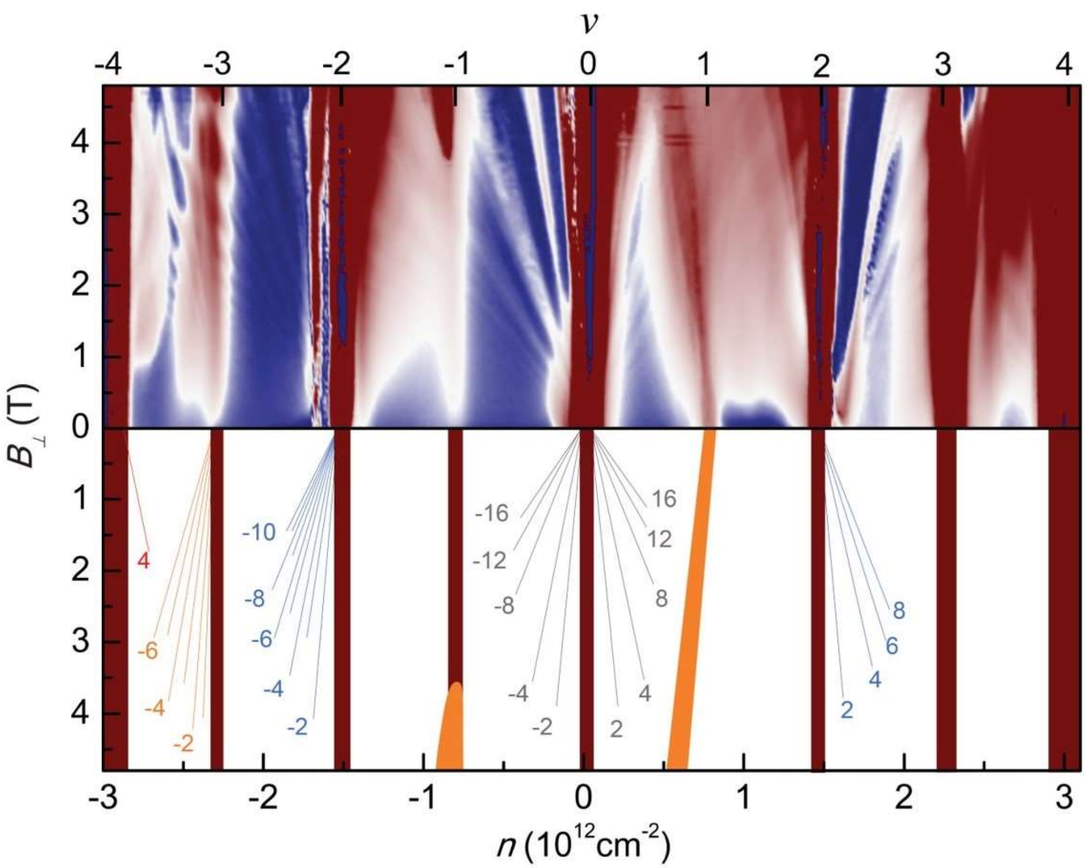
Chair of Experimental Solid State Physics

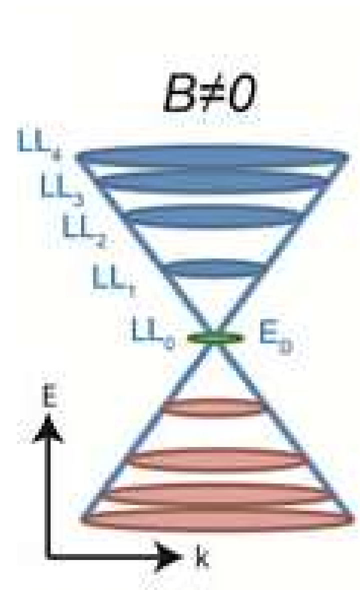
Quantum oscillations - Landau Fan diagram

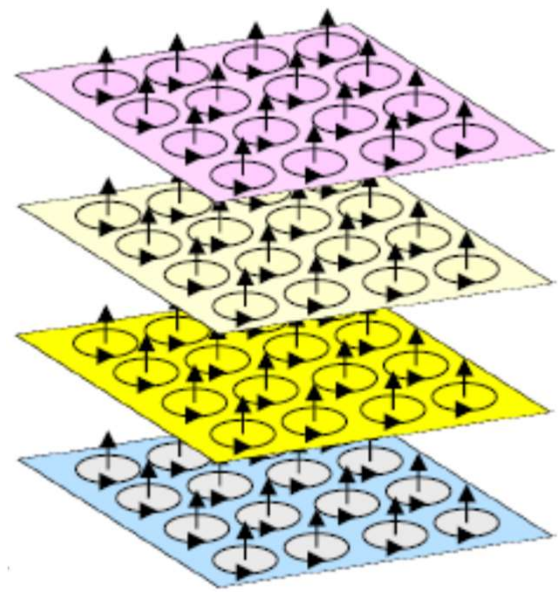
LL fan diagram:



X. Lu, … , DKE, Nature 574, 653 (2019).

Linear LL trajectories in *n*-*B* space:





$$\nu = 2\pi \ell_B^2 n \quad \Rightarrow \quad B = \frac{\phi_0}{\nu} n$$

Breaking of SU(4) spin/valley symmetry

→ different degeneracy of LL fans for different ν

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