Quantum Theory of Magnetism

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Abstract

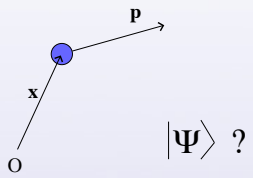
In this lecture I will give a brief introduction to the quantum theory of magnetism in real materials, especially, consisting of transition metal elements and their compounds. Starting from the Stoner theory of magnetism, we discuss several basic aspects of ferromagnetism and further expand the discussion into other models like Hubbard model, Anderson impurity model, and Kondo model as a way to understand the mechanisms behind such complex magnetic phenomena in real materials. We will also look into the theory of non-collinear magnetism, arising from spin-orbit coupling, which brings up multiferroic physics and topological properties of electronic states as well. If time permits, I will discuss a connection between magnetism and superconductivity in high T_c superconductors.

Outline

- What is all about condensed matter physics?
- Magnetic phenomena in real materials
- A quantum mechanical view of magnets:
  Pauli exclusion principle and Coulomb interactions
- Effective hamiltonians and phenomenological theory
  - Stoner theory
  - Hubbard model
  - Heisenberg model
  - Anderson impurity model
  - Kondo model
- Non-collinear magnetic ordering
- Berry phase and topological effects
- Magnetism and superconductivity

What is all about condensed matter physics?

... How do we understand the physical properties of single particle systems in a classical or quantum sense? In other words, what do we measure or observe?



... In classical dynamics, the state of a single particle is determined by the observables $\{\mathbf{x}(t), \mathbf{p}(t)\}$. It can be extended to the system with many particles where the state of the system is described by the set of observables $\{\mathbf{x}_i(t), \mathbf{p}_i(t) | i = 1, 2, ..., N\}$. However, when $N \sim 10^{25}$, it is practically impossible to trace the orbits of all, even the part of, the particles. Here it is the point where the statistical physics comes into playing a role. Instead of following each individual particles, we measure a quantity by an (ensemble or time) average of the given quantities adopted in classical dynamics. In addition, now we have to deal with new observables such as entropy, temperature, ...

The same thing applies for the case of quantum systems. The only difference is the dynamics state of the quantum system is determined by a state vector $|\psi(\mathbf{x}, t)\rangle$ for a single particle and $|\Psi(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N, t)\rangle$.

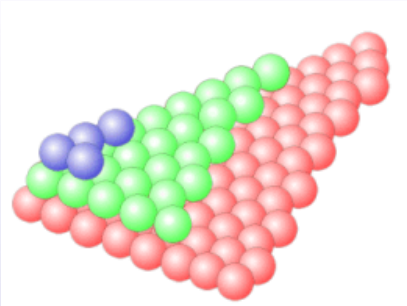
Macroscopic vs microscopic objects

- Observables for the macro object consisting of more than $\sim 10^{20}$ particles:
  - specific heat c_v $\longleftarrow$ entropy, temperature
  - bulk modulus or compressibility κ $\longleftarrow$ pressure P
  - polarization $\mathbf{P}$, magnetization $\mathbf{M}$ $\longleftarrow$ electro-magnetic field $\mathbf{E}$, $\mathbf{B}$
  - reflectivity, color, conductivity, ... etc.

For an example, what physical property of the cube (or disk) makes this happen, i.e., a cube float over a magnet against gravitation?

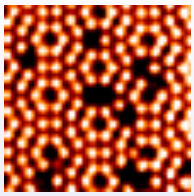
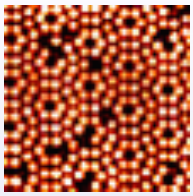
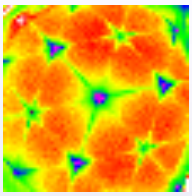



Observables for the micro or nano object of order $\sim 10^2$ particles:



- conductance G / electron tunneling current I
- force $\mathbf{F}$
- magnetic Flux Φ
- charge density distribution, electron cloud (bonding), ... etc.

an AFM image | an STM image | a LEED image

What do we really see in these images?
What physical quantities do they represent?

An example of the SEM System:



Most condensed matter systems are quantum mechanical by nature!

$$\lambda \sim \frac{\hbar}{p} \sim d$$

- Unfortunately, however, there is no quantum mechanical solution available except for free (i.e., non-interacting) particle systems.
- An example of exactly solvable models:

$$\mathcal{H} = \hbar\omega(a^+ a + \frac{1}{2})$$

$$a^+ a|n\rangle = n|n\rangle$$

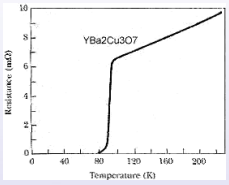
$$a|O\rangle = 0$$

How do we approach to the condensed matter system to understand the physics of a "black box"?

- Experimental Methods:
  By disturbing the black box by phtons, phonons, electrons, and/or neutrons, try to get a hint on elementary excitations in the system.
- Theoretical Methods:
  By guessing possible elementary excitations and working out the QM equation of motions, see if we can predict the physics of the system. If wrong, correct the model for the elementary excitations for the better description.
- How to disturb the "black box"?

Question: Measuring the dc resistance is a way of disturbing the system? What really happens inside the black box when we apply a bias voltage?

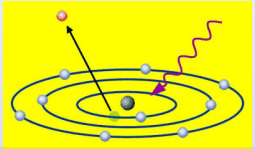
♠ Current-Voltage curve of a YBCO high T_c superconductor



Question: What happens when we shine a light on the matter?

Light scattering experiment: (Photoemission / IR spectroscopy)





"elementary excitations in solids"

- quasi-particles: electrons, holes, polarons, excitons, Cooper pairs, ...
- collective excitations: phonons, magnons, zero-sound, plasmons, ...

Energy scale

The condensed matter system is merely a collection of atoms, where each atom consists of electrons and a nucleus ($m_e \ll m_N$).

From the uncertainty principle $\Delta x \Delta p \sim \hbar$,

$$\Delta p = \sqrt{2m_e E} \approx \sqrt{3mk_B T}$$

Thus, practically, the size of atom $\approx$ the size of electrons.

- atomic unit: $\hbar = e^2 = m_e = 1$

$$\Delta x \approx a_B = \frac{\hbar^2}{me^2} = 0.529177\text{Å (Bohr radius)}$$

$$E_B = -\frac{1}{2}\frac{e^2}{a_B} = -\frac{me^4}{2\hbar^2} = -13.6058\text{eV} = -1\text{Ry}$$

In atomic unit, $a_B = 1$, $E_B = -1/2$, $c = 1/\alpha \approx 137$, $k_B \approx 3 \times 10^{-6}$, ...

($\alpha = e^2/\hbar c$: fine structure constant)

- energy of an electron in a box of size L:

$$\Delta x \sim L \quad \longrightarrow \quad \Delta p \approx \frac{\hbar}{L}$$

$$E_o = \frac{p^2}{2m} \approx \frac{1}{2L^2}$$

- speed of electrons in a box:

$$v_e \sim \frac{1}{L} \sim \frac{\alpha c}{L}$$

- electrons in solid
  - Fermions: Pauli exclusion principle
  - Degenerate Electrons: lowest possible excitations near the Fermi energy

Quiz

- Estimate the scale in atomic unit:

  (a) ground state energy of an electron in a cube of length 1 nm.

  (b) energy and momentum of a photon with $\lambda = 10^4$ Å.

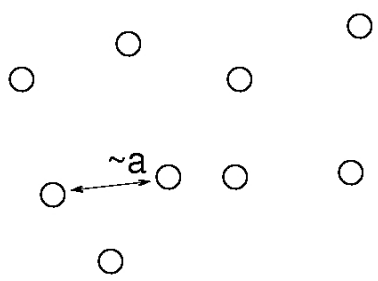
  (c) energy of an electron in a magnetic field of 1 T.

  (d) thermal wave length of an electron and a neutron in a thermal bath of 300 K.

  (e) Fermi energy of a degenerate electron (neutron) gas with its density 10^{22} cm^{-3} respectively.

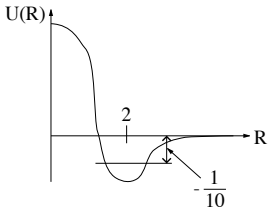
Hypothetical Hydrogen Solid

A solid, or, a condensed matter system in general, can be visualized as a mere collection of atoms. In this chapter, let us try to image what form of matter one can possibly get out of the collection of "hypothetical hydrogen" atoms as a function of temperature and density.



Basic assumptions

- The hypothetical hydrogen has a single electron-proton bound state with an energy of $-1/2$ a.u., which is equivalent to the $1s$ state of the hydrogen atom.
- Two hypothetical hydrogen atoms can also have a single bound state of an energy $-1/10$ a.u. and the mean separation between the atoms is about 3 a.u., leading to a H_2 hydrogen molecule.



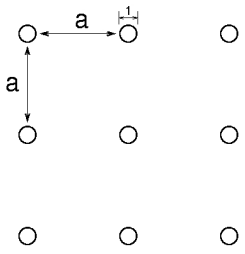
- The hypothetical H_2 molecules, interacting with each other through the van der Waals interaction, are assumed to have a single bound state of energy $-1/10^2$ a.u. and the mean distance between the atoms is about ~ 10.

In the limit of low density and low temperature

First, consider a regular array of the hypothetical atoms, for an example, in a cubic lattice. Suppose that the system is at $T = 0$ and the mean spacing between the atoms is relatively large, i.e., $a \gg 1$.

$$T = 0$$

$$a \gg 1 \quad \longrightarrow \quad n = \frac{1}{a^3} \ll 1$$



Question: Is this cubic lattice stable or not?

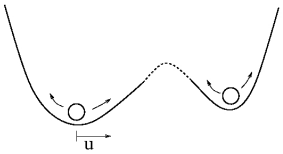
- What is a general criterion for the stability of a system?
  In classical mechanics, a particle in its equilibrium with restoring forces is called "stable". In other words, any displacement u from the equilibrium position has to be described by the equation of motion:

$$\frac{d^2u}{dt^2} = -\omega_o^2 u$$

  where ω_o^2 needs to be positive, i.e, $\omega_o^2 > 0$. If $\omega_o^2 < 0$, then it becomes unstable. In general, we can consider the energetics in its configuration space in order to identify the stability condition.

  - Energy curve:

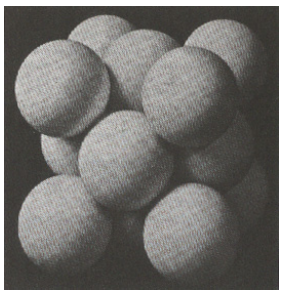
$$E = E(\{x_i^o\}) + (x_i - x_i^o) \cdot \nabla_x E|_{x_i^o} + \frac{1}{2}(x_i - x_i^o)(x_i - x_i^o) \cdot \nabla_x^2 E|_{x_i^o}$$



- If this system is not stable, what can cause such instability?

  For examples, one can consider external perturbations, quantum fluctuations, etc.

Question: Can you guess what the final form of the matter will be in its ground state? What kind of lattice structure will it have? Just try to make a wild, but reasonable, guess.



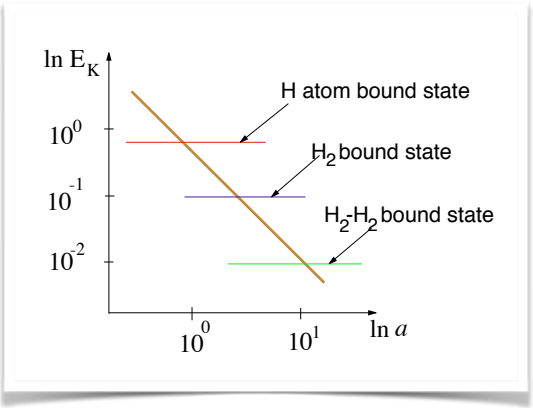
For an example, the inert gases form a close-packed lattice such as fcc or hcp structures. How does it apply for the case of hypothetical H_2 molecules? Could you also guess the density of such matter?

In the limit of high density and low temperature

Now, starting from the solid form of hypothetical hydrogen atoms, e.g., H_2 molecular solids, where the mean spacing between the atoms is about $a \sim 10$, let us apply an external pressure on the solid so that the mean spacing a becomes shorter and shorter as the pressure arises. Here we assume that the system is at $T = 0$.

As the mean separation decreases and becomes less than the size of molecules, we can imagine that each electron attached to the *hydrogen atom* or *molecule* will be squeezed into a box of size a^3. As a result, the electrons will gain a kinetic energy

$$E_K \sim \alpha \frac{\hbar}{2ma^2} \sim \frac{\alpha}{2a^2}$$

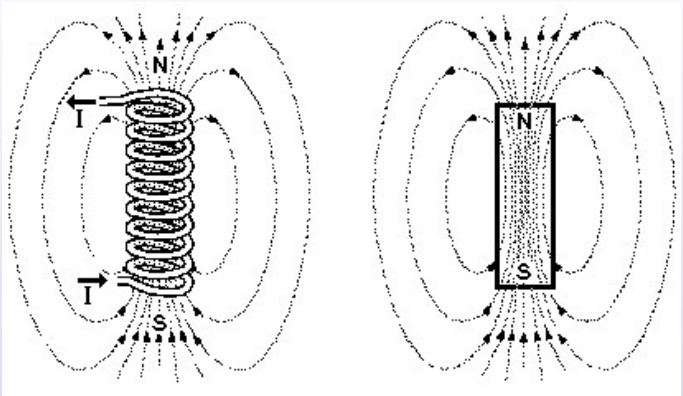


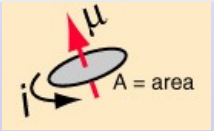
Magnetic phenomena in real materials

Magnets



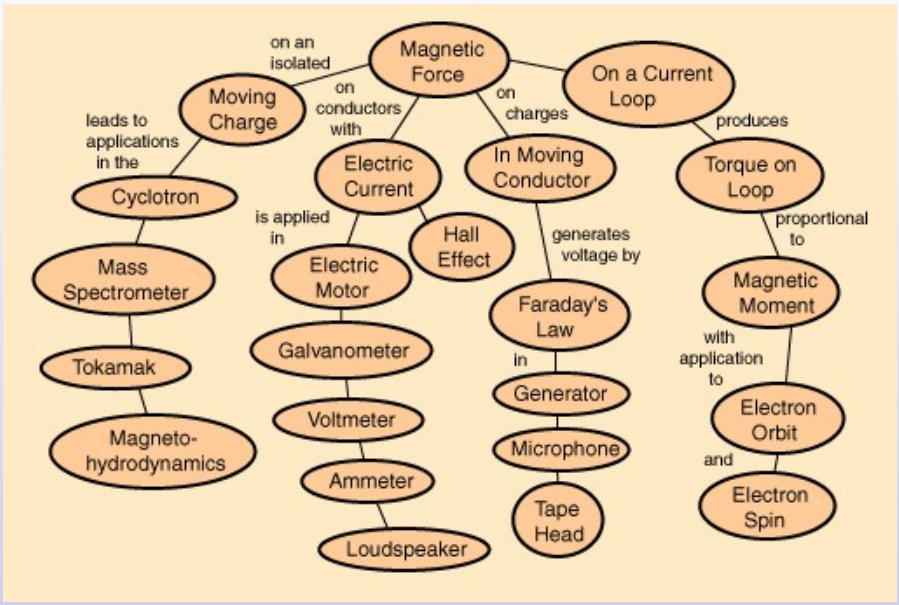
Solenoid vs. Bar Magnet

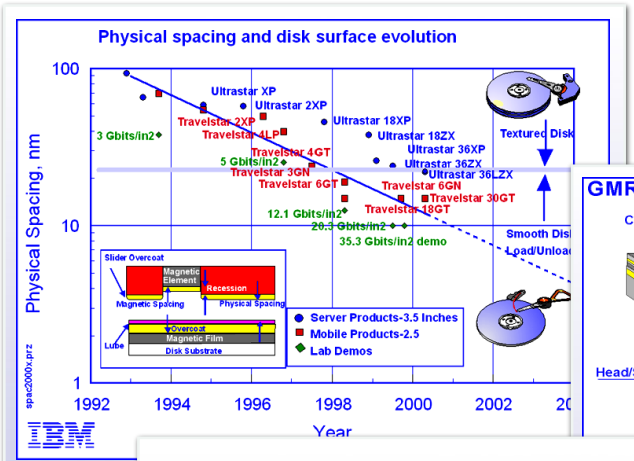


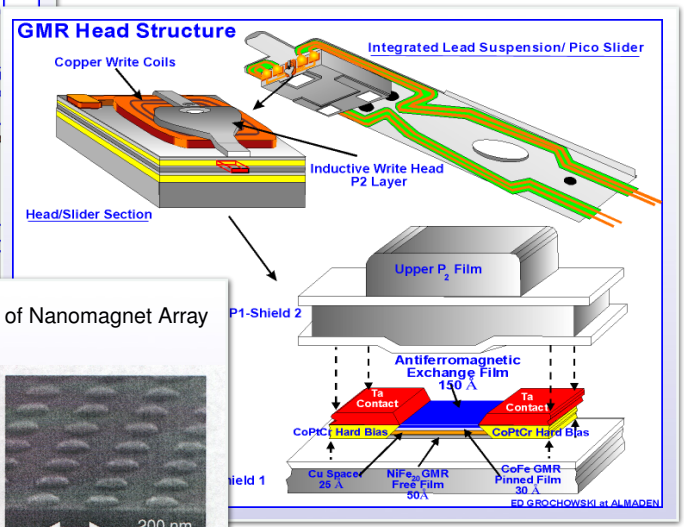


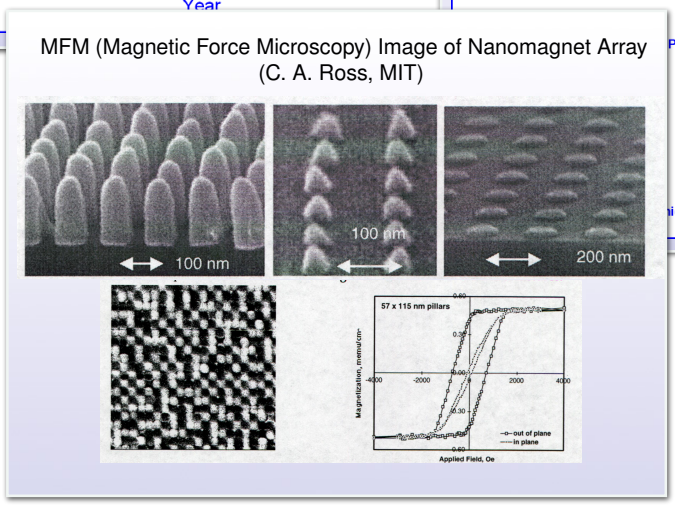
Magnetic permeability / origin of magnetic moments?

Magnetic Diagram





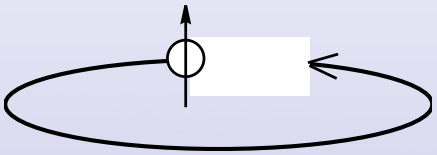




A quantum mechanical view of magnets: Pauli exclusion principle and Coulomb interactions

- Source of magnetic moments

- Magnetic moment: $\mathcal{M} = g\mu_B \mathbf{J}$
  proportional to the angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$
  - Spin moment $\mathbf{S}$
  - Orbital moment $\mathbf{L}$



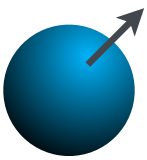
Localized state: atomic state

- Since the rotational symmetry is preserved, it has the quantum eigenstates $|jm\rangle$:

$$\mathbf{J}^2|jm\rangle = j(j+1)|jm\rangle$$

where

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$



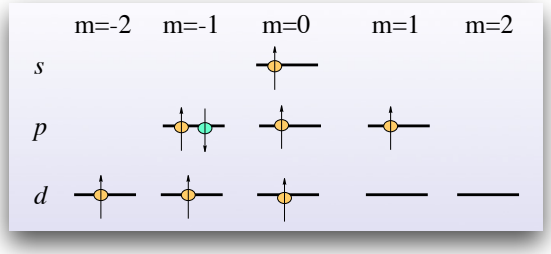
- If the spherical symmetry is broken, e.g., inside a lattice, the orbital moment can be quenched due to the lack of rotational symmetry, i.e.,

$$\langle \mathbf{L} \rangle = 0$$

Hund's rule

1. Maximum total $S = \max S_z$ with $S_z = \sum_i m_{si}$
   Obeying the Pauli exclusion principle
2. Maximum total $L = \max L_z$ with $L_z = \sum_i m_{li}$
   Minimizing the Coulomb interaction energy
3. Spin-orbit interaction:

$$J = \begin{cases} |L+S| & \text{if less than half-filled} \\ |L-S| & \text{if more than half-filled} \end{cases}$$



Exchange energy

- Pauli exclusion principle: anti-symmetric two-particle wavefunction

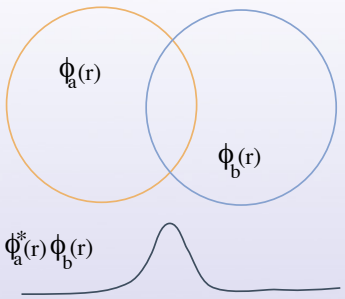
$$|\Psi(\mathbf{r}_1\uparrow;\mathbf{r}_2\uparrow)\rangle = \frac{1}{\sqrt{2}}\left[\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2) - \phi_b(\mathbf{r}_1)\phi_a(\mathbf{r}_2)\right]|\uparrow\rangle|\uparrow\rangle$$

- Coulomb interaction

$$V_C(\mathbf{r}_1 - \mathbf{r}_2) = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

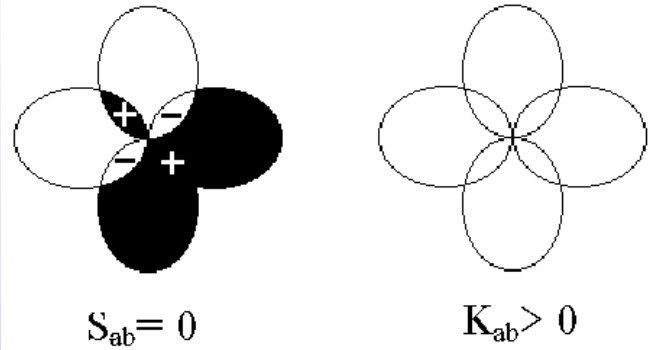
$$\begin{aligned} E_{C2} &= <\Psi(1,2)|V_C|\Psi(1,2)\rangle \\ &= \int d\mathbf{r}_1 d\mathbf{r}_2 V_C(\mathbf{r}_1-\mathbf{r}_2)|\phi_a(\mathbf{r}_1)|^2|\phi_b(\mathbf{r}_2)|^2 - \\ &\quad \int d\mathbf{r}_1 d\mathbf{r}_2 V_C(\mathbf{r}_1-\mathbf{r}_2)\phi_a^*(\mathbf{r}_1)\phi_b^*(\mathbf{r}_2)\phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1) \\ &= U_{ab} - J_{ab} \end{aligned}$$

Exchange density



Gaining more (negative) exchange energy by aligning spins:
Hund's 1st rule

Overlap and Exchange Integrals of the atomic p-orbitals

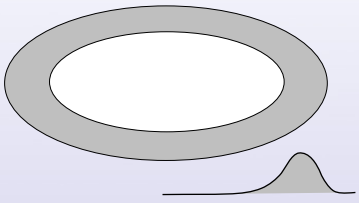


Hund's 2nd rule

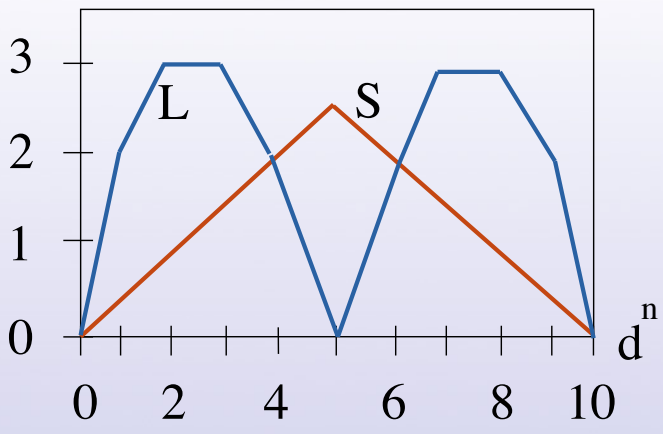
Minimization of Coulomb Energy Term U_{ab}

by letting $\rho(\mathbf{r})$ be separated: Hund's 2nd rule

$$Y_{lm}(\theta,\phi) = (-1)^m Y^*_{l-m}(\theta,\phi)$$



Configuration of 3d Transition Metal Ions



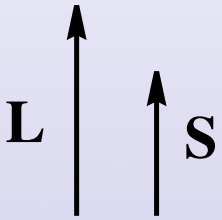
Spin-orbit coupling

determined by the sign of the coupling constant

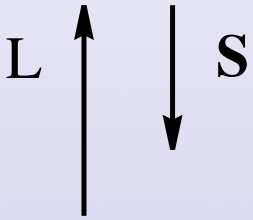
$$\lambda \mathbf{L} \cdot \mathbf{S}$$

$$\lambda \sim -\frac{dV(r)}{dr}$$

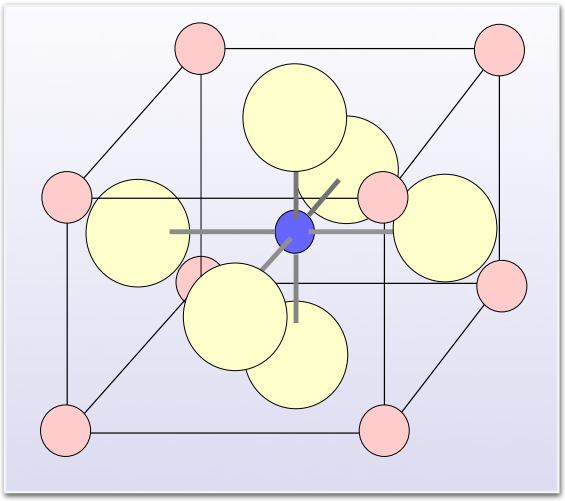
high spin

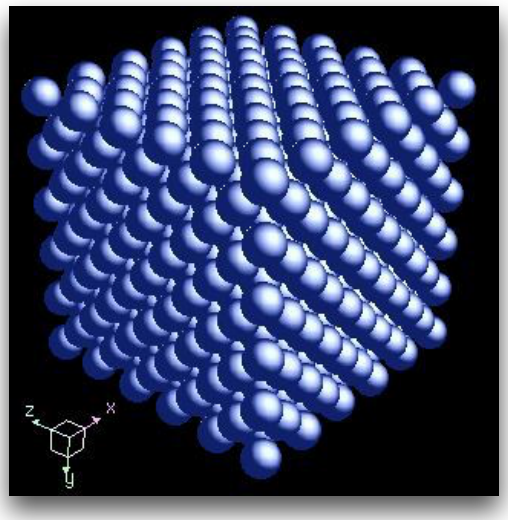


low spin



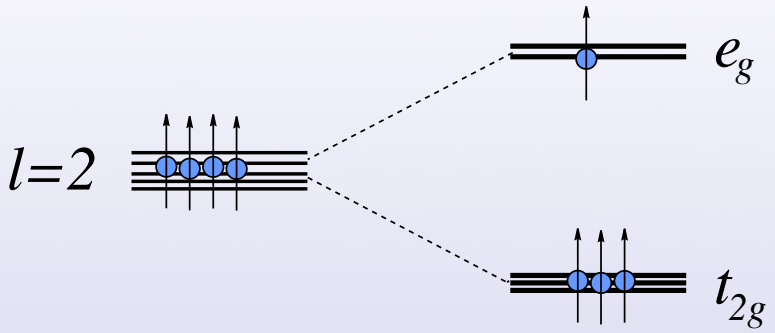
Magnetic moments in solids





Cubic lattice: broken spherical symmetry

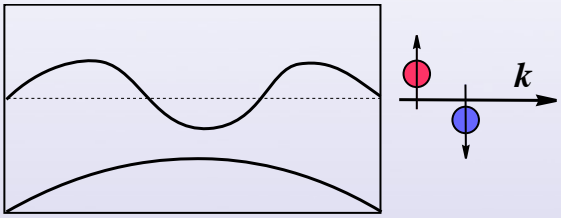
Crystal Field Splitting:



$$|e_g\rangle = \{|x^2 - y^2\rangle, |z^2 - r^2/3\rangle\}$$
$$|t_{2g}\rangle = \{|xy\rangle, |yz\rangle, |zx\rangle\}$$

Delocalized state

- A free electron state such as $|\mathbf{k}\rangle$ may not be an eigenstate of the angular momentum operator $\mathbf{L}$.
- Only $|sm_s\rangle$ may contribute to the magnetic moment.



- Exception: Diamagnetic shielding current in a superconducting state.

Kinetic energy vs Coulomb energy

- Uncertainty Principle:

$$\Delta p \approx \frac{\hbar}{\Delta x}$$

- Kinetic Energy:

$$E_K = \frac{p^2}{2m} \approx \frac{\hbar^2}{2m}\frac{1}{(\Delta x)^2}$$

- Coulomb Exchange Energy:

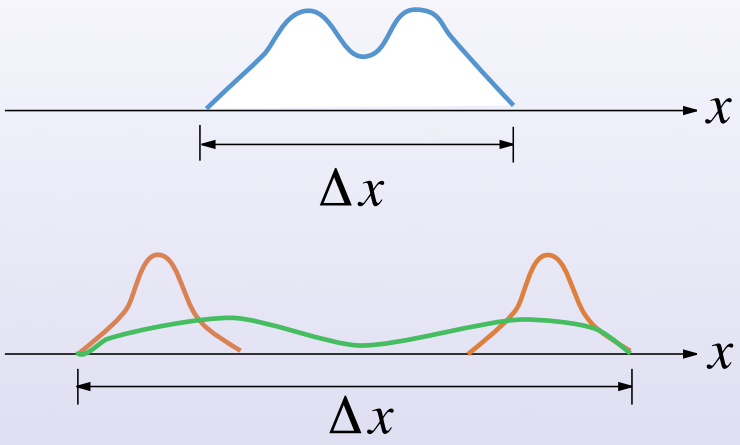
$$E_C \approx -A\frac{e^2}{\Delta x}$$

where $A \sim 0.1$, an order of magnitude smaller than the direct Coulomb interaction energy.

When $\Delta x \gg 1$, the Coulomb energy dominates over the kinetic energy.

$\Rightarrow$ **Wigner solid: frozen localized electrons**

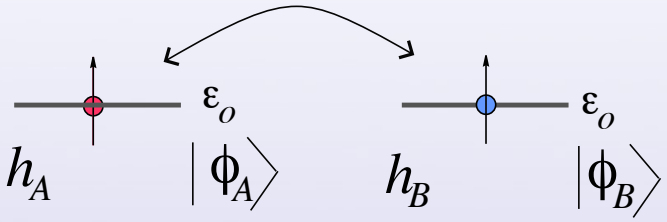
Wigner crystal: metal-insulator transition



Result of the competition between kinetic and Coulomb energy!

Delocalized state: Molecular or Band state

$$t = \langle \phi_A | V_{AB} | \phi_B \rangle$$

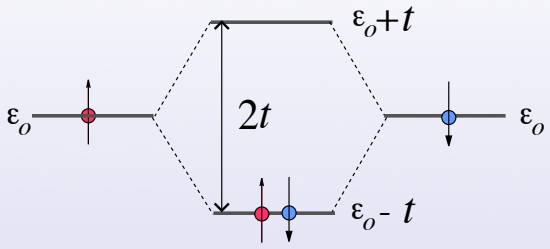


$$\mathcal{H}_o = h_A + h_B + V_{AB}$$

$$\mathcal{H}_o = \begin{pmatrix} \varepsilon_o & t \\ t & \varepsilon_o \end{pmatrix}$$

Single-particle eigenstates and eigenvalues:

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|\phi_A\rangle \pm |\phi_B\rangle) \qquad \varepsilon_\pm = \varepsilon_o \pm t$$

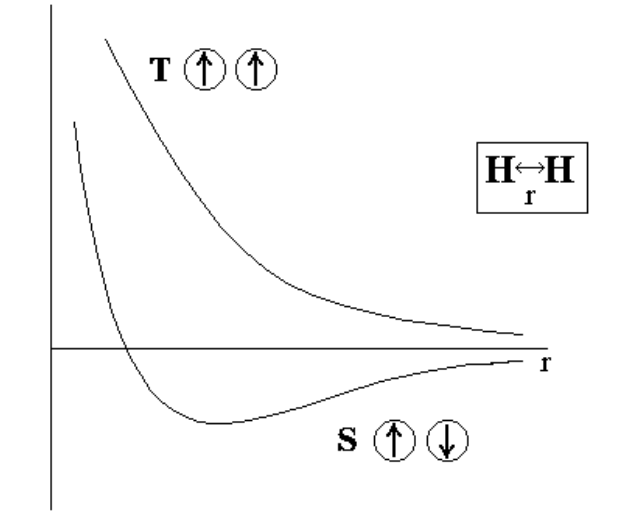


Corresponding two-particle state:

$$\Psi_2\rangle = \frac{1}{\sqrt{2}}[|\psi_+,\uparrow\rangle|\psi_+,\downarrow\rangle - |\psi_+,\downarrow\rangle|\psi_+,\uparrow\rangle]$$

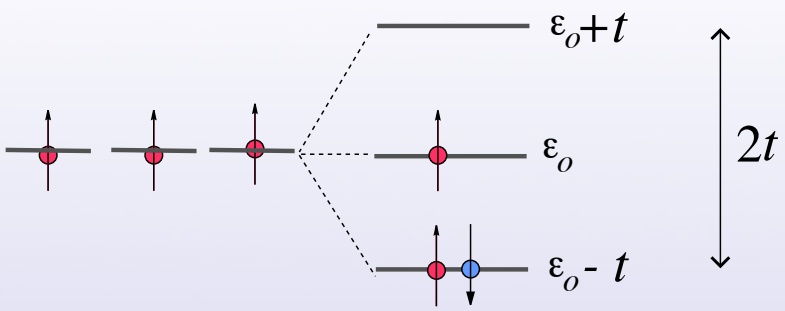
⇒ Spin-singlet ground state with single-particle molecular states $|\psi_\pm\rangle$

Energy Curve for a Hydrogen Molecule

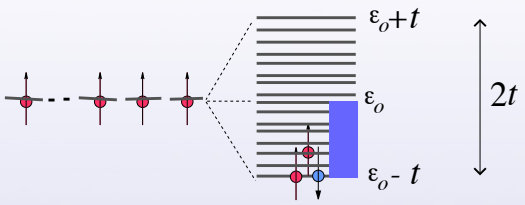


Consider two hydrogen atoms separated by a distance d. What are the ground states of this system in the limits of $d \to 0$ and $d \to \infty$? What is the dominating factor in each limit? Try to make a qualitative argument in describing the physics.
What about a lattice of hydrogen atoms with a lattice constant d? Discuss the possible physical properties of the lattice with varying d from ∞ to 0.

Three-Sites Molecular States



N-Sites States: Tight-Binding Energy Band

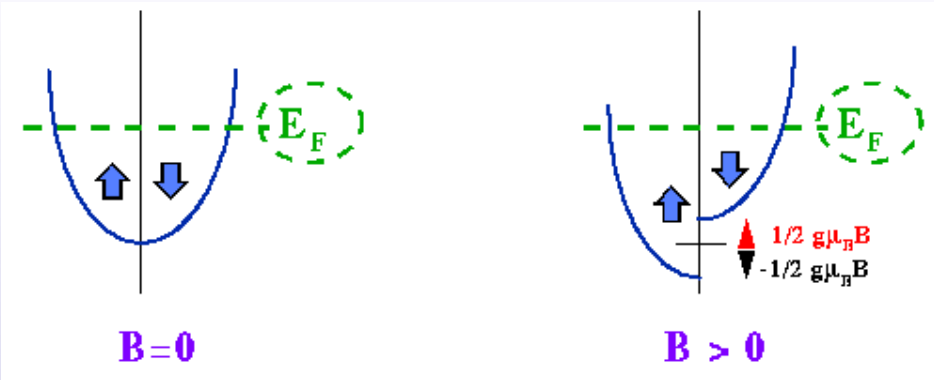


These delocalized molecular state is stable when the Coulomb interaction energy U is **smaller** than the kinetic energy gain $W = 2t$.

$$U = \langle \Psi_2 | V_C(1,2) | \Psi_2 \rangle \approx \int d\mathbf{r}_1 d\mathbf{r}_2 V_C(\mathbf{r}_1 - \mathbf{r}_2)\rho_A(\mathbf{r}_1)\rho_A(\mathbf{r}_2)$$

: on-site Coulomb interaction energy

Pauli paramagnetism



♠ the change of the Density-of-states due to the Zeeman coupling:

$$D(\varepsilon) = \frac{dN(\varepsilon)}{d\varepsilon}$$

Pauli Paramagnetic Susceptibility

$$\Delta N_\uparrow = \int_{-\mu_B B}^{E_F} \frac{1}{2} D(E+\mu_B B) dE - \int_0^{E_F} \frac{1}{2} D(E) dE = \frac{1}{2}\mu_B B D(E_F)$$

$$\Delta N_\downarrow = \int_{\mu_B B}^{E_F} \frac{1}{2} D(E-\mu_B B) dE - \int_0^{E_F} \frac{1}{2} D(E) dE = -\frac{1}{2}\mu_B B D(E_F)$$

$$M = \mu_B(\Delta N_\uparrow - \Delta N_\downarrow) = \mu_B^2 D(E_F) B = \frac{3N\mu_B^2}{2k_B T_F} B \implies \chi_s = \frac{3N\mu_B^2}{2k_B T_F}$$

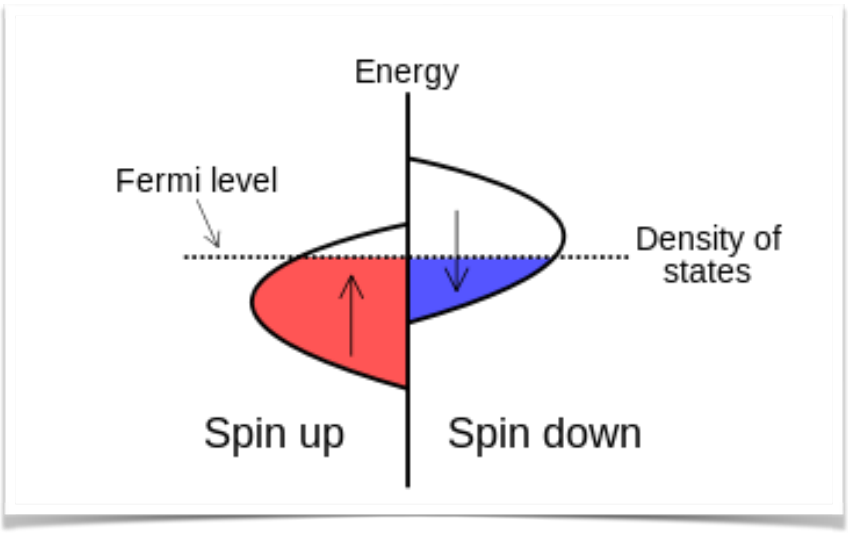
Substracting the Landau diamagnetic contribution $\chi_L = -\frac{N\mu_B^2}{2k_B T_F}$, we have the Pauli Paramagnetic Susceptibility:

$$\chi_P = \frac{N\mu_B^2}{k_B T_F}$$

Effective hamiltonians and phenomenological theory

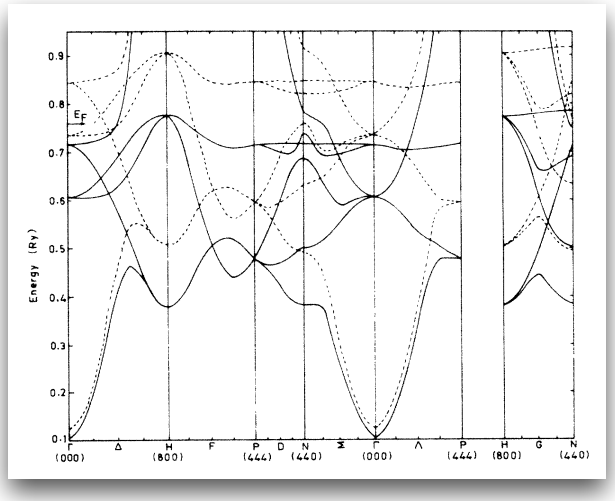
- Stoner theory
- Hubbard model
- Heisenberg model
- Anderson impurity model
- Kondo model

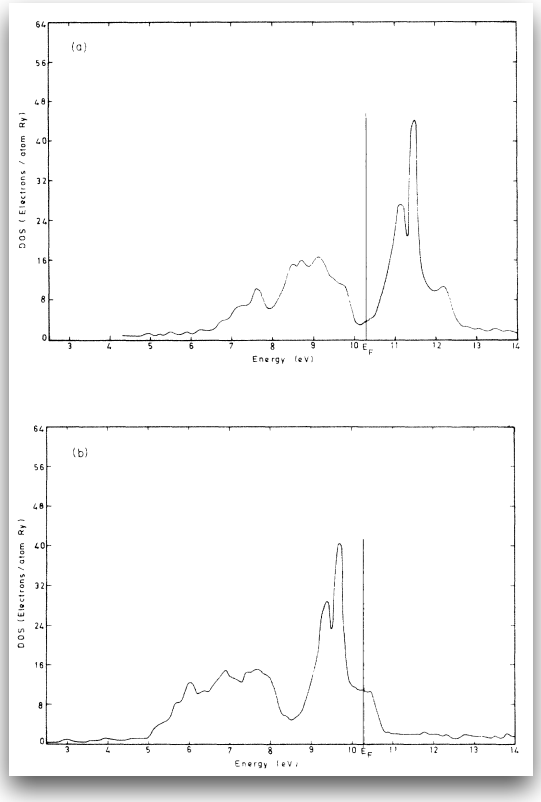
Stoner theory:
How can a metal be a ferromagnet?



https://commons.wikimedia.org/wiki/File:Stoner_model_of_ferromagnetism.svg

Band structure of ferromagnetic Fe metal





http://dx.doi.org/10.1103/PhysRevB.34.2299

Stoner model

Collective Electron Ferromagnetism
Edmund C. Stoner
Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences
Vol. 165, No. 922 (Apr. 14, 1938), pp. 372-414

Stoner model

$$\mathcal{H} = \sum_{\vec{k},s} \epsilon_{\vec{k}}\, \hat{c}^{\dagger}_{\vec{k}s}\, \hat{c}_{\vec{k}s} + U \int d^3r\ \hat{\rho}_{\uparrow}(\vec{r})\,\hat{\rho}_{\downarrow}(\vec{r})$$

kinetic energy

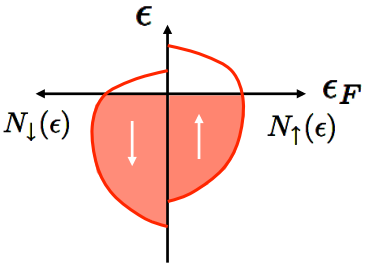
contact interaction
note: exchange hole

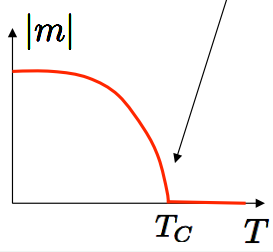
kinetic energy versus exchange energy

mean field treatment $\hat{\rho}_s(\vec{r}) = n_s + [\hat{\rho}_s(\vec{r}) - n_s]$

mean density of electron with spin *s*

spin polarization $m = n_{\uparrow} - n_{\downarrow} \propto |T - T_C|^{1/2}$ ← mean field exponent





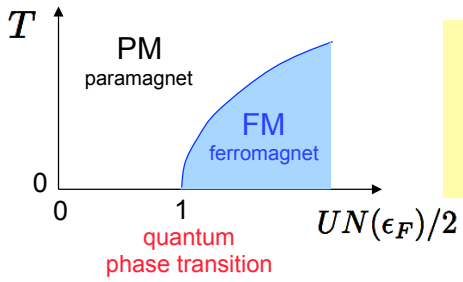
spontaneously broken symmetries

$O(3)$ rotation

$\mathscr{K}$ time reversal

ETH solid state theory lecture by M. Sigrist
http://www.itp.phys.ethz.ch/education/fs14/sst/slides/magnetism.pdf

$$k_B T_C \propto \sqrt{1 - \frac{U_c}{U}} \qquad U_c N(\epsilon_F) = 2 \qquad N(\epsilon) = 2\sum_{\vec{k}} \delta(\epsilon - \epsilon_{\vec{k}})$$

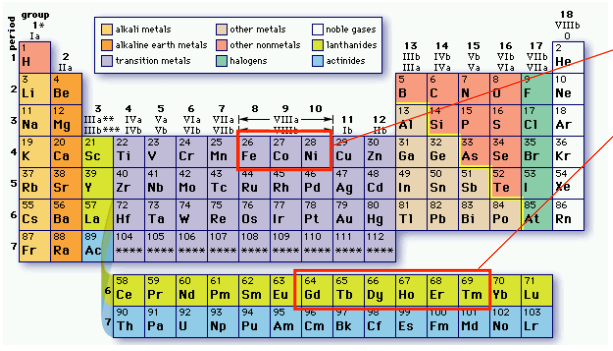


Stoner criterion for FM

$$UN(\epsilon_F) > 2$$

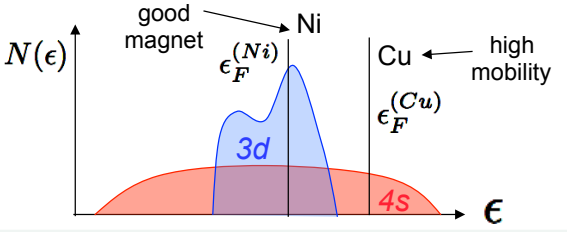
large

$$\frac{\text{exchange energy}}{\text{kinetic energy}}$$



3d-transition metals Fe Co Ni

4f-rare earths Gd Tb Dy Ho Er Tm



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Generalized spin susceptibility

Hamiltonian: system in spatial/time dependent magnetic field

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}} + \mathcal{H}_Z$$

$$\mathcal{H}_0 = \sum_{\vec{k},s} \epsilon_{\vec{k}}\, \hat{c}^\dagger_{\vec{k}\,s}\, \hat{c}_{\vec{k}\,s} \qquad \mathcal{H}_{\text{int}} = U \int d^3r\, \hat{\rho}_\uparrow(\vec{r})\, \hat{\rho}_\downarrow(\vec{r})$$

$$\mathcal{H}_Z = -\frac{g\mu_B}{\hbar} \int d^3r\, \vec{H}(\vec{r},t) \cdot \widehat{\vec{S}}(\vec{r})$$

$$\widehat{\vec{S}}(\vec{r}) = \frac{\hbar}{2} \sum_{s,s'} \hat{\Psi}^\dagger_s(\vec{r})\, \vec{\sigma}_{ss'}\, \hat{\Psi}_{s'}(\vec{r}) = \frac{\hbar}{2} \begin{pmatrix} \hat{\Psi}^\dagger_\uparrow(\vec{r})\hat{\Psi}_\downarrow(\vec{r}) + \hat{\Psi}^\dagger_\downarrow(\vec{r})\hat{\Psi}_\uparrow(\vec{r}) \\ -i\,\hat{\Psi}^\dagger_\uparrow(\vec{r})\hat{\Psi}_\downarrow(\vec{r}) + i\,\hat{\Psi}^\dagger_\downarrow(\vec{r})\hat{\Psi}_\uparrow(\vec{r}) \\ \hat{\Psi}^\dagger_\uparrow(\vec{r})\hat{\Psi}_\uparrow(\vec{r}) - \hat{\Psi}^\dagger_\downarrow(\vec{r})\hat{\Psi}_\downarrow(\vec{r}) \end{pmatrix}$$

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http://www.itp.phys.ethz.ch/education/fs14/sst/slides/magnetism.pdf

$$\mathcal{H}_Z = -\frac{g\mu_B}{\hbar} \int d^3r\, \vec{H}(\vec{r},t) \cdot \widehat{\vec{S}}(\vec{r}) \qquad \vec{H} = \frac{1}{2} H^+(\vec{q},\omega) e^{i\vec{q}\cdot\vec{r} - i\omega t} e^{\eta t} \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}$$

in x-y-direction

$$\mathcal{H}_Z = -\frac{g\mu_B}{\hbar\Omega} \sum_{\vec{k}} H^+(\vec{q},\omega)\, \hat{S}^-_{\vec{k},-\vec{q}}\, e^{-i\omega t + \eta t} + \text{h.c.}$$

with $\widehat{\vec{S}}_{\vec{q}} = \int d^3r\, \widehat{\vec{S}}(\vec{r}) e^{-i\vec{q}\cdot\vec{r}} = \frac{\hbar}{2\Omega} \sum_{\vec{k},s,s'} c^\dagger_{\vec{k},s}\, \vec{\sigma}_{ss'} c_{\vec{k}+\vec{q},s'} = \frac{1}{\Omega} \sum_{\vec{k}} \widehat{\vec{S}}_{\vec{k},\vec{q}}$

first goal

field-induced magnetization:

$$M^+_{\text{ind}} = \frac{\mu_B}{\hbar} \langle S^+_{\text{ind}}(\vec{q},\omega) \rangle$$

equation of motion ($U=0$):

$$i\hbar \frac{\partial}{\partial t} \hat{S}^+_{\vec{k},\vec{q}} = [\hat{S}^+_{\vec{k},\vec{q}}, \mathcal{H}_0 + \mathcal{H}_Z]$$

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http://www.itp.phys.ethz.ch/education/fs14/sst/slides/magnetism.pdf

$$i\hbar\frac{\partial}{\partial t}\hat{S}^{+}_{\vec{k},\vec{q}}(t)_{\vec{k},\vec{q}} = (\epsilon_{\vec{k}+\vec{q}}-\epsilon_{\vec{k}})\hat{S}^{+}_{\vec{k},\vec{q}}(t)+g\hbar\mu_B(\hat{c}^{\dagger}_{\vec{k}+\vec{q}\uparrow}\hat{c}_{\vec{k}+\vec{q}\uparrow}-\hat{c}^{\dagger}_{\vec{k}\downarrow}\hat{c}_{\vec{k}\downarrow})H^{+}(\vec{q},\omega)e^{-i\omega t}$$

linear order: $\langle S^{+}_{\text{ind}}(\vec{q},t)\rangle = \langle S^{+}_{\text{ind}}(\vec{q},\omega)\rangle e^{-i\omega t+\eta t}$

$$(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}} - \hbar\omega + i\hbar\eta)\langle S^{+}_{\vec{k},\vec{q}}\rangle = -g\hbar\mu_B(n_{\vec{k}+\vec{q}\uparrow} - n_{\vec{k}\downarrow})H^{+}(\vec{q},\omega)$$

$$\langle S^{+}_{\text{ind}}(\vec{q},\omega)\rangle = \frac{1}{\Omega}\sum_{\vec{k}}\langle S^{+}_{\vec{k},\vec{q}}\rangle = \frac{\hbar}{\mu_B}\chi_0(\vec{q},\omega)H^{+}(\vec{q},\omega)$$

$$\chi_0(\vec{q},\omega) = -\frac{g\mu_B^2}{\Omega}\sum_{\vec{k}}\frac{n_{\vec{k}+\vec{q}\uparrow} - n_{\vec{k}\downarrow}}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}} - \hbar\omega + i\hbar\eta}$$

analog to Lindhard function

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http://www.itp.phys.ethz.ch/education/fs14/sst/slides/magnetism.pdf

feedback effect through interaction:

$$\mathcal{H}_{\text{int}} = \frac{U}{\Omega}\sum_{\vec{k},\vec{k}',\vec{q}'}\hat{c}^{\dagger}_{\vec{k}+\vec{q}'\uparrow}\hat{c}_{\vec{k}\uparrow}\hat{c}^{\dagger}_{\vec{k}'-\vec{q}'\downarrow}\hat{c}_{\vec{k}'\downarrow} = -\frac{U}{\Omega\hbar^2}\sum_{\vec{q}'}\hat{S}^{+}_{\vec{q}'}\hat{S}^{-}_{-\vec{q}'} + const.$$

approximation

$$-\frac{U}{\hbar^2}\langle S^{+}(\vec{q},\omega)\rangle\hat{S}^{-}_{-\vec{q}} = -\frac{g\mu_B}{\hbar}H^{+}_{\text{ind}}(\vec{q},\omega)\hat{S}^{-}_{-\vec{q}} \quad\Leftarrow\quad H^{+}_{\text{ind}}(\vec{q},\omega) = \frac{U}{g\mu_B\hbar}\langle S^{+}(\vec{q},\omega)\rangle$$

$$\begin{aligned}
M^{+}(\vec{q},\omega) &= \tfrac{\mu_B}{\hbar}\langle S^{+}(\vec{q},\omega)\rangle \\
&= \chi_0(\vec{q},\omega)[H^{+}(\vec{q},\omega) + H^{+}_{\text{ind}}(\vec{q},\omega)] \\
&= \chi_0(\vec{q},\omega)H^{+}(\vec{q},\omega) + \chi_0(\vec{q},\omega)\tfrac{U}{g\mu_B\hbar}\langle S^{+}(\vec{q},\omega)\rangle \\
&= \chi_0(\vec{q},\omega)H^{+}(\vec{q},\omega) + \chi_0(\vec{q},\omega)\tfrac{U}{g\mu_B^2}M^{+}(\vec{q},\omega)
\end{aligned}$$

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http://www.itp.phys.ethz.ch/education/fs14/sst/slides/magnetism.pdf

$$M^+(\vec{q},\omega) = \chi(\vec{q},\omega)H^+(\vec{q},\omega)$$

$$\chi(\vec{q},\omega) = \frac{\chi_0(\vec{q},\omega)}{1 - \frac{U}{2\mu_B^2}\chi_0(\vec{q},\omega)}$$

RPA form of spin susceptibility

spin order instabilities: $1 = \frac{U}{2\mu_B^2}\chi_0(\vec{q},\omega=0)$

Stoner instability: uniform ferromagnet $\vec{q} \to 0$

$$\chi_0(\vec{q},0) = -\frac{2\mu_B^2}{\Omega}\sum_{\vec{k}}\frac{n_{\vec{k}+\vec{q}\uparrow} - n_{\vec{k}\downarrow}}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}} \xrightarrow{\vec{q}\to 0} -\frac{2\mu_B^2}{\Omega}\sum_{\vec{k}}\frac{\partial f(\epsilon_{\vec{k}})}{\partial \epsilon_{\vec{k}}} = \chi_0(T)$$

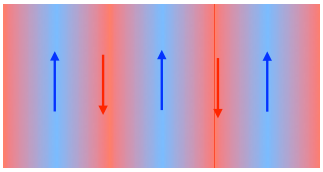
$$1 = \frac{U}{2\mu_B^2}\chi_0 = \frac{UN(\epsilon_F)}{2}\left[1 - \frac{\pi^2}{6}(k_B T_C)^2 \Lambda_1^2\right]$$

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$$1 = \frac{U}{2\mu_B^2}\chi_0(\vec{q},\omega=0)$$

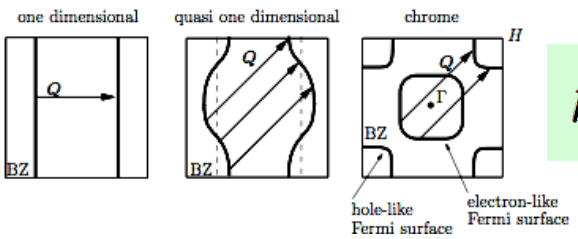
$$\chi(\vec{Q},0) = \max_{\vec{q}}\chi_0(\vec{q},0)$$

spin density wave instability with wavevector $\vec{Q}$



Fermi surface nesting: $\epsilon_{\vec{k}+\vec{Q}} = -\epsilon_{\vec{k}}$

$$\chi_0(\vec{Q};T) \approx \mu_B^2 N(\epsilon_F)\ln\left(\frac{1.14\epsilon_0}{2k_B T}\right)$$

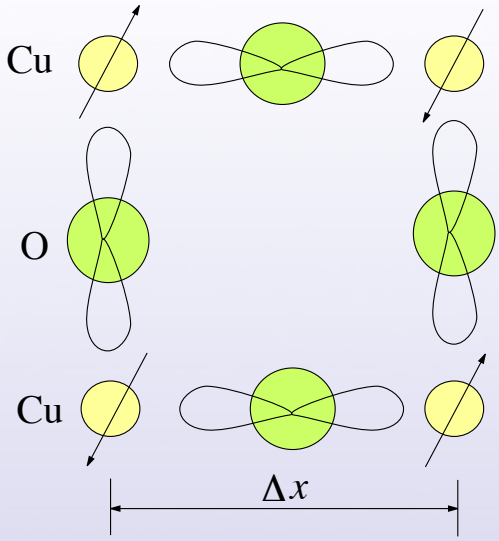


$$k_B T_N = 1.14\epsilon_0 e^{-2/UN(\epsilon_F)}$$

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http://www.itp.phys.ethz.ch/education/fs14/sst/slides/magnetism.pdf

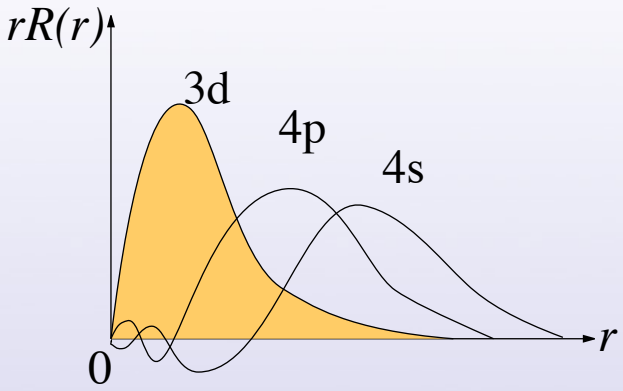
Hubbard model

Transition Metal Oxides



The larger Δx, the smaller t, i.e., $W \implies$ more localized!

Why Transition Metals (TM) and TM Compounds?



$\Rightarrow$ both $3d$ and $4f$ electron wavefunctions are extremely localized:
no node in radial wavefunctions

A Model for the Exchange Interactions in Solids

When $U \gg W$, the localized states of $|\Psi_o\rangle$ becomes stable relative to the band (molecular) state $|\Psi_2\rangle$:

$$|\Psi_o\rangle = \frac{1}{\sqrt{2}}\left[|\phi_\alpha, s_1\rangle|\phi_\beta, s_2\rangle - |\phi_\beta, s_2\rangle|\phi_\alpha, s_1\rangle\right]$$

which is a combination of the localized orbitals $|\phi_{A,B}\rangle$ instead of the molecular states $|\psi_\pm\rangle$.

Here the starting Hamiltonian $\mathcal{H}_o$ include the interaction term of $\hat{U}$:

$$\mathcal{H}_o = h_A + h_B + \hat{U}$$

and the hopping term V_{AB} should be considered as a perturbation.

Two-particle excited states:

$$|\Psi_o(s_1, s_2)\rangle = |\phi_A, s_1\rangle|\phi_B, s_2\rangle$$
$$|\Psi_A(\uparrow,\downarrow)\rangle = |\phi_A, \uparrow\rangle|\phi_A, \downarrow\rangle$$
$$|\Psi_B(\uparrow,\downarrow)\rangle = |\phi_B, \uparrow\rangle|\phi_B, \downarrow\rangle$$

$$\mathcal{H}_o|\Phi_o\rangle = 2\varepsilon_o|\Psi_o\rangle$$
$$\mathcal{H}_o|\Phi_A\rangle = (2\varepsilon_o + U)|\Psi_A\rangle$$
$$\mathcal{H}_o|\Phi_B\rangle = (2\varepsilon_o + U)|\Psi_B\rangle$$

Anti-ferromagnetic Superexchange Interactions

Only remaining degrees of freedom of the ground state $|\Psi_o\rangle$ are

spins!

$$|\Psi_p(s_1, s_2)\rangle = |s_1, s_2\rangle$$

Energy Correction via the Perturbation Theory with $\mathcal{H}_1 = V_{AB}$

- First-order correction:

$$\langle s_1, s_2|\mathcal{H}_1|s_1, s_2\rangle = 0$$

Pauli exclusion prohibits the double occupancy at the same site:

$$|\phi_A, \uparrow\rangle|\phi_A, \uparrow\rangle = 0$$

That is,

$$|\phi_A, s_1\rangle|\phi_A, s_1\rangle = 0$$

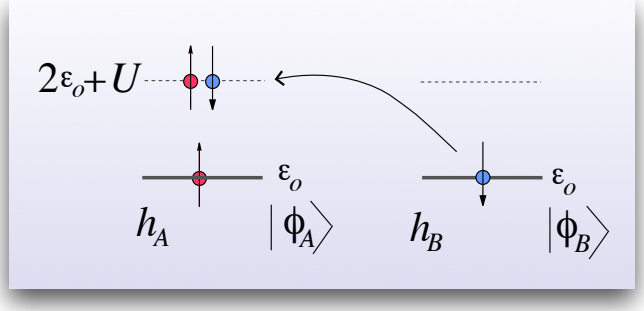
- Second-order correction:

$$\langle\uparrow,\downarrow|\mathcal{H}_1|\Phi_A\rangle = \langle\uparrow,\downarrow|\mathcal{H}_1|\Phi_B\rangle = t$$

$$\langle\uparrow,\uparrow|\mathcal{H}_1|\Phi_A\rangle = \langle\uparrow,\uparrow|\mathcal{H}_1|\Phi_B\rangle = 0$$

$$E^{(2)}_{\uparrow,\uparrow} = -\sum_n{}' \frac{|\langle\uparrow,\uparrow|\mathcal{H}_1|\Phi_n\rangle|^2}{E_n - E_o} = 0$$

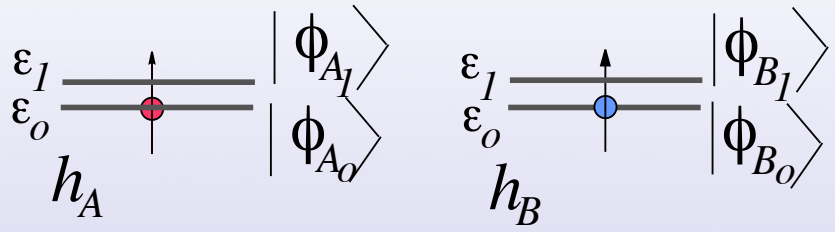
$$E^{(2)}_{\uparrow,\downarrow} = -\sum_n{}' \frac{|\langle\uparrow,\downarrow|\mathcal{H}_1|\Phi_n\rangle|^2}{E_n - E_o} = -\frac{2t^2}{U} = -J_{\mathrm{AF}}$$



$$\mathcal{H}_{\mathrm{eff}} = +J_{\mathrm{AF}}\vec{\sigma}_A \cdot \vec{\sigma}_B$$

Ferromagnetic Superexchange Interactions

What happens if additional degenerate (or almost degenerate) states exist at each atom while $U \gg W$?



Now additional excited states become available:

$$|\Phi_A(\uparrow,\uparrow)\rangle = |\phi_{A_o},\uparrow\rangle|\phi_{A_1},\uparrow\rangle$$

and

$$\langle\Phi_o(\uparrow,\uparrow)|\mathcal{H}_1|\Phi_A(\uparrow,\uparrow)\rangle \neq 0$$

$$\mathcal{H}_o|\Phi_A(\uparrow,\uparrow)\rangle = (\varepsilon_o + \varepsilon_1 + U - J)|\Phi_A(\uparrow,\uparrow)\rangle = E_A(\uparrow,\uparrow)|\Phi_A(\uparrow,\uparrow)\rangle$$

If the exchange energy is larger than the difference $|\varepsilon_o - \varepsilon_1|$, i.e.,

$$J > |\varepsilon_o - \varepsilon_1|$$

we have

$$E_A(\uparrow,\uparrow) < E_A(\uparrow,\downarrow)$$

Therefore,

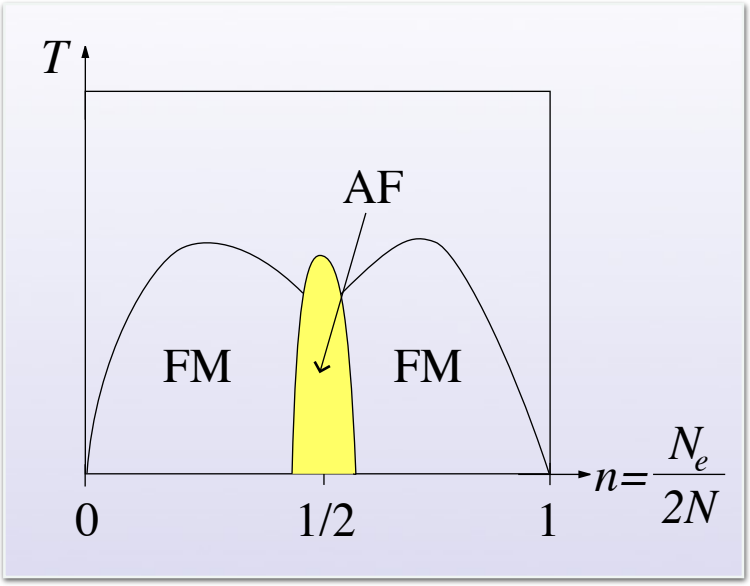
$$E^{(2)}_{\uparrow,\uparrow} = -\sum_n{}' \frac{|\langle\uparrow,\uparrow|\mathcal{H}_1|\Phi_n\rangle|^2}{E_n - E_o} \approx -\frac{2t^2}{U-J} < E^{(2)}_{\uparrow,\downarrow} = -\frac{2t^2}{U}$$

Ferromagnetic Exchange Interaction

$$\mathcal{H}_{\text{eff}} = -|J_{FM}|\vec{\sigma}_A \cdot \vec{\sigma}_B$$

FM Metal and AF Insulator

- depending on band-filling
  controlled by band degeneracy or by doping



Heisenberg model

- A mean field solution

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + g\mu_B \mathbf{H} \cdot \sum_i \mathbf{S}_i$$

Introducing an effective field $\mathbf{H}_{\text{eff}}$,

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + g\mu_B \mathbf{H} \cdot \sum_i \mathbf{S}_i = g\mu_B \sum_i \mathbf{S}_i \cdot \mathbf{H}_{\text{eff}}$$

where the effective mean field

$$\mathbf{H}_{\text{eff}} = \mathbf{H} - \frac{1}{g\mu_B} \sum_j J_{ij} \mathbf{S}_j$$

and the average magnetization

$$\langle \mathbf{S}_i \rangle = \frac{V}{N} \frac{\mathbf{M}}{g\mu_B}$$

$$\mathbf{H}_{\text{eff}} = \mathbf{H} + \lambda \mathbf{M}$$

$$\lambda = \frac{V}{N} \frac{J_o}{(g\mu_B)^2}$$

$$M = -\frac{N}{V} \frac{\partial F}{\partial H} = M_o\left(\frac{H_{\text{eff}}}{T}\right)$$

- For the case of $H = 0$,
  one can fine the magnetization M by solving the equation:

$$M(T) = M_o(\frac{\lambda M}{T})$$

$$\chi_o(T) = \left(\frac{\partial M_o}{\partial H}\right)_{H=0} = \frac{M_o'(0)}{T}$$

  where the Curie's constant is determined to be $C_o = M_o'(0)$.

- For the case of $H \neq 0$,

$$\chi = \frac{\partial M}{\partial H} = \frac{\partial M_o}{\partial H_{\text{eff}}}\frac{\partial H_{\text{eff}}}{\partial H} = \chi_o(1 + \lambda\chi)$$

$$\chi = \frac{\chi_o}{1 - \lambda\chi_o} = \frac{C_o}{T - T_c}$$

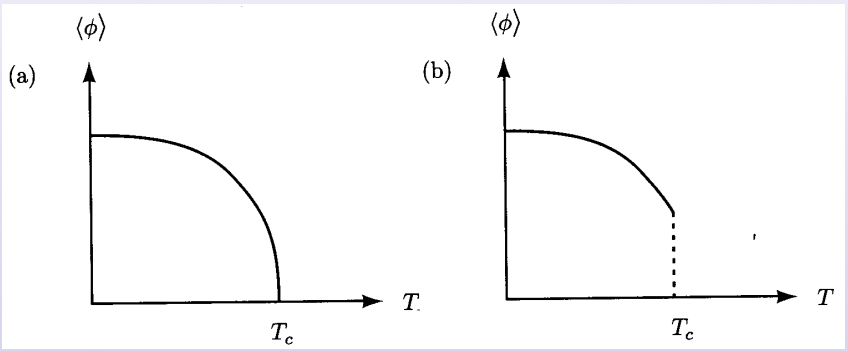
  where the critical temperature T_c becomes

$$T_c = \frac{N}{V}\frac{(g\mu_B)^2}{3k_B}S(S+1)\lambda = \frac{S(S+1)}{3k_B}J_o$$

Order Parameters: Description of Phase Transition

	$T > T_c$	$T < T_c$	Symmetry
Supercondutor	$\psi_s(\mathbf{r}) = 0$	$\psi_s(\mathbf{r}) \neq 0$	$U(1)$
Magnets	$\mathbf{M}_s(\mathbf{r}) = 0$	$\mathbf{M}_s(\mathbf{r}) \neq 0$	$O(3)$
Ferroelectrics	$\mathbf{P}_s(\mathbf{r}) = 0$	$\mathbf{P}_s(\mathbf{r}) \neq 0$	$O(3)$
Liquid/Gas-Solid	$\rho(\mathbf{G}) = 0$ for $\mathbf{G} \neq 0$	$\rho(\mathbf{G}) \neq 0$ for $\mathbf{G} \neq 0$	$\mathcal{T}_{\mathbf{R}}$
Order-disorder	$\eta = 0$	$\eta \neq 0$	Z_2

$$\eta = \langle n_A \rangle_A - \langle n_B \rangle_A$$



Bragg-Williams Theory

Consider the Ising model with the spin $\sigma = |\uparrow\rangle$ or $|\downarrow\rangle$. The order parameter $m = \langle\sigma\rangle$ is the average of the spin:

$$m = (N_\uparrow - N_\downarrow)/N$$

- Entropy S:

$$S = \ln C^N_{N_\uparrow} = \ln C^N_{N(1+m)/2}$$

$$\frac{S}{N} = s(m) = \ln 2 - \frac{1}{2}(1+m)\ln(1+m) - \frac{1}{2}(1-m)\ln(1-m)$$

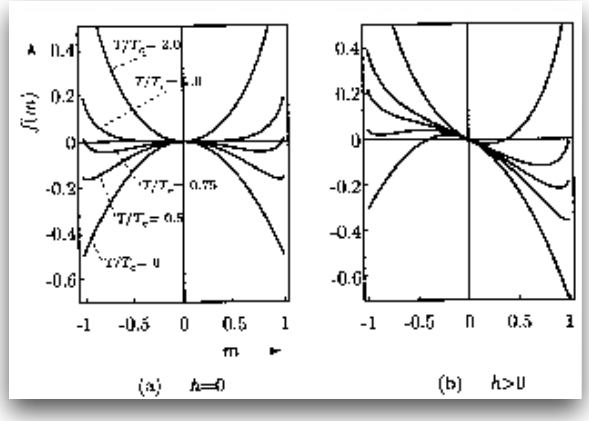
- Average Energy E:

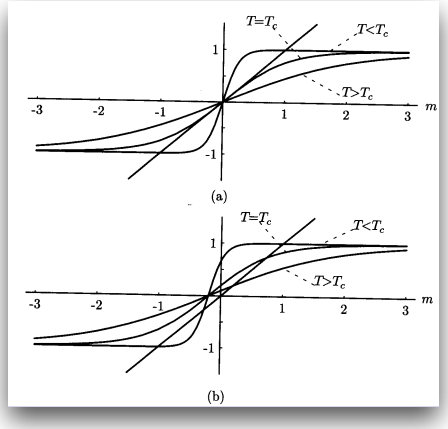
$$E = -J\sum_{\langle ij\rangle} m^2 = -\frac{1}{2}JNzm^2$$

where z is the number of nearest neighbor sites.

- Bragg-Williams free energy $f(T,m)$:

$$f(T,m) = (E - TS)/N = -\frac{1}{2}Jzm^2 + \frac{1}{2}T[(1+m)\ln(1+m) + (1-m)\ln(1-m)] - T\ln 2$$





- The equation of state under an external field h:

$$\frac{\partial f}{\partial m} = -zJm + \frac{1}{2}T\ln[(1+m)/(1-m)] = h$$

$$-zJm + T\tanh^{-1} m = h$$

$$\therefore m = \tanh[(h + T_c m)/T]$$

Note that $h_{\text{eff}} = h + T_c m$.

- Mean field solutions for $h = 0$:
  - near $T \approx 0$:

$$m = \tanh(T_c m/T) \approx 1 - 2e^{-2zJ/T}$$

  - near $T \to T_c^-$:

$$m \approx (T_c/T)m - \frac{1}{3}(T_c/T)^3 m^3 \approx (T_c/T)m - \frac{1}{3}m^3$$

$$m = \pm[3(T_c - T)/T]^{1/2}$$

Ginzburg-Landau Functional

Free energy near T_c

$$s(m) = \ln 2 - \frac{1}{2}m^2 - \frac{1}{12}m^4 + ...$$

$$f(m) = \frac{1}{2}(T - T_c)m^2 + \frac{1}{12}m^4 - T\ln 2 + ...$$

where $T_c = zJ$

Assuming $\phi(\mathbf{r})$ as a local order parameter,

$$F = \int d\mathbf{r} f(T, \phi(\mathbf{r})) + \int d\mathbf{r} \frac{1}{2} c |\nabla\phi(\mathbf{r})|^2$$

where f can be expanded by

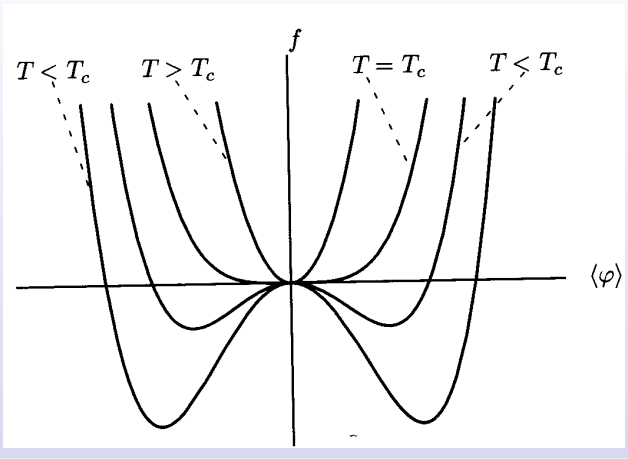
$$f(T, \phi) = \frac{1}{2}r\phi^2 - w\phi^3 + u\phi^4 + ...$$

where $r = a(T - T_c)$

Symmetry properties of the free energy functional F!

Second-Order Phase Transition

$$f(T, \phi) = \frac{1}{2}r\phi^2 + u\phi^4$$



The equation of state:

$$r\phi + 4u\phi^3 = h$$

- For $h = 0$,

$$\phi = \begin{cases} 0 & \text{if } T > T_c \\ \pm(-r/4u)^{1/2} & \text{if } T < T_c \end{cases}$$

$\phi \sim (T_c - T)^\beta$ where $\beta = 1/2$.

- Susceptibility χ

$$[r + 12u\phi^2]\frac{\partial\phi}{\partial h} = 1$$

$$\chi = \frac{\partial\phi}{\partial h} = \begin{cases} 1/r & \text{if} T > T_c \\ 1/(2|r|) & \text{if} T < T_c \end{cases}$$

$$\chi \sim |T - T_c|^{-\gamma}$$

with $\gamma = 1$.

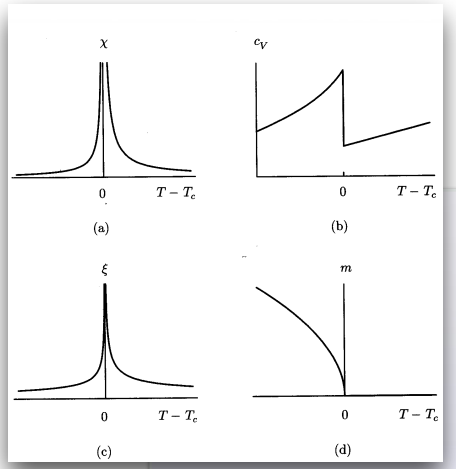
- Free energy density f

$$f = \begin{cases} 0 & \text{if} T > T_c \\ -r^2/(16u) & \text{if} T < T_c \end{cases}$$

- Specific heat c_v

$$c_v = -T\frac{\partial^2 f}{\partial T^2} = \begin{cases} 0 & \text{if} T > T_c \\ Ta^2/(8u) & \text{if} T < T_c \end{cases}$$

correlation length



$$\chi^{-1}(\mathbf{r},\mathbf{r}') = \frac{\delta^2 F}{\delta\phi(\mathbf{r})\delta\phi(\mathbf{r}')} = (r + 12u\phi^2 - c\nabla^2)\delta(\mathbf{r}-\mathbf{r}')$$

$$\chi(\mathbf{q}) = \frac{1}{r + 12u\phi^2 + cq^2}$$

$$\chi(\mathbf{q}) = \frac{\chi}{1+(q\xi)^2} = \frac{1}{c}\frac{\xi^2}{1+(q\xi)^2}$$

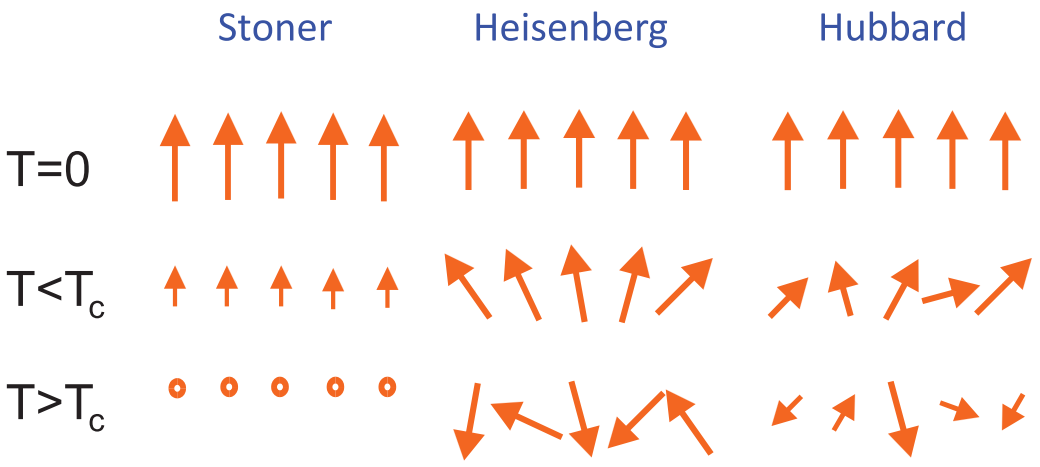
where

$$\xi = c^{1/2}[r + 12u\phi^2]^{-1/2} = \begin{cases} (c/r)^{1/2} & \text{if} T > T_c \\ c^{1/2}/(-2r)^{1/2} & \text{if} T < T_c \end{cases}$$

and the correlation length $\xi \sim |T - T_c|^{-\nu}$ with $\nu = 1/2$.

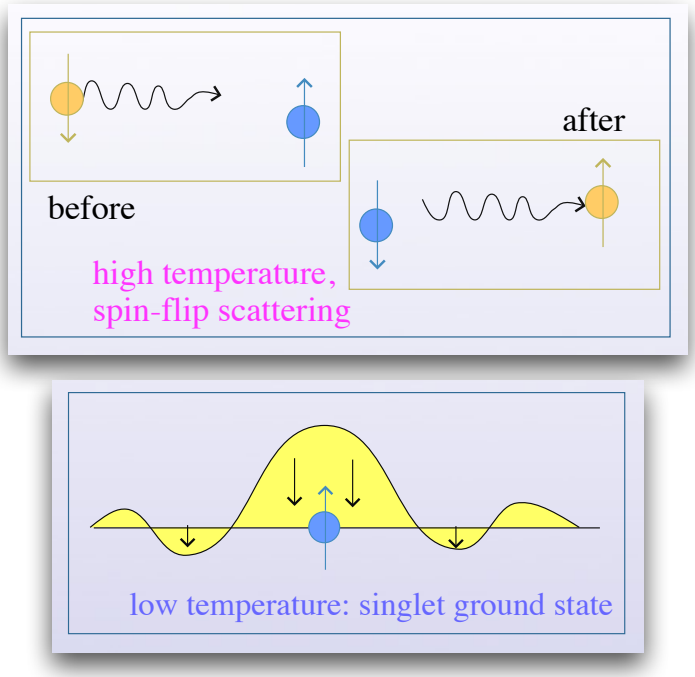
$$\xi_0 = \left(\frac{c}{r(T=0)}\right)^{1/2} = \left(\frac{c}{aT_c}\right)^{1/2}$$

Stoner vs Heisenberg vs Hubbard models



Anderson impurity model

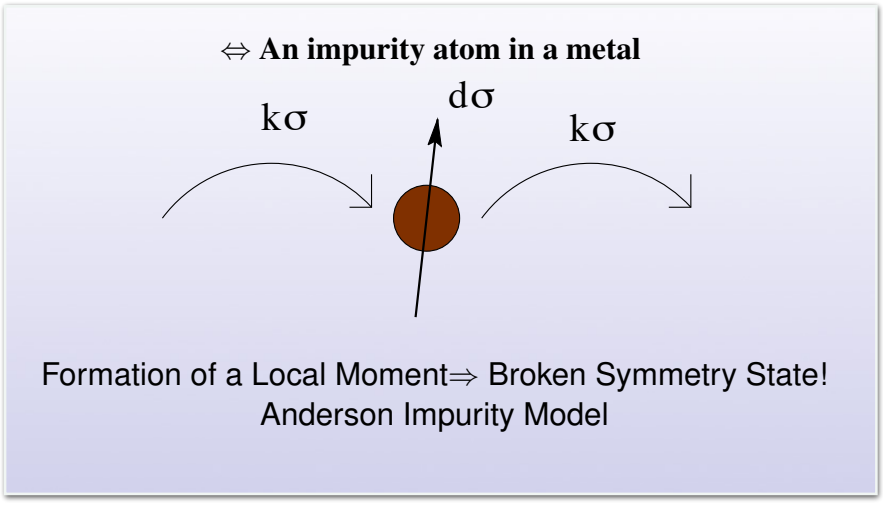
- Magnetic impurity in a metal



Formation of local magnetic moment in metals

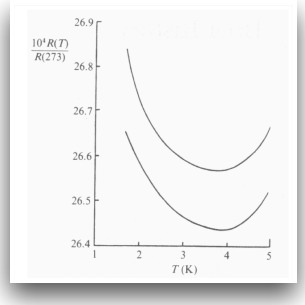
- How does the magnetic moment of a magnetic impurity survive in a metallic environment?
- How does it affect the properties of the host metal?

A localized state coupled to delocalized states?

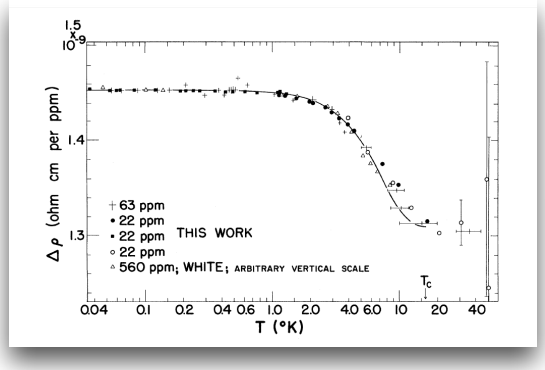


Puzzles:
Resistivity of copper, gold, silver and many other metals with small amount of magnetic impurities at low temperatures.

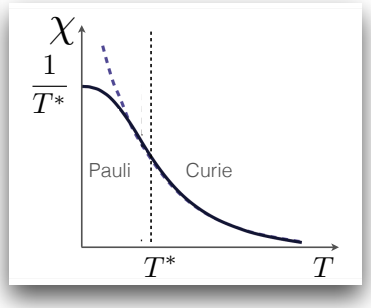
Resistance minimum?



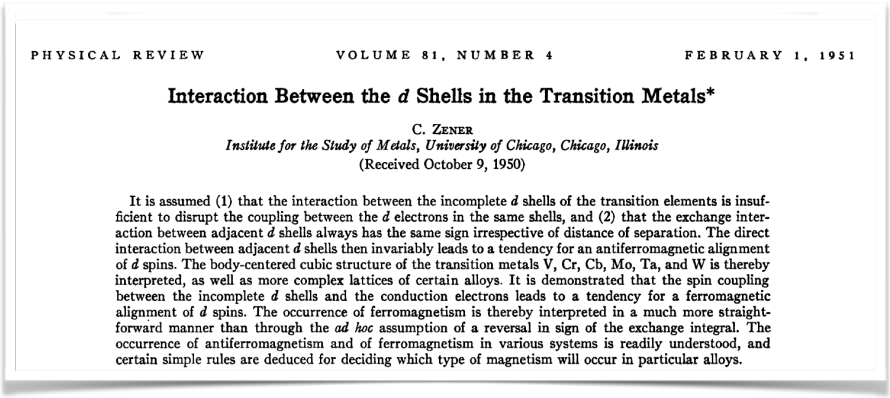
Logarithmic behavior as $T \to 0$?



Magnetic susceptibility?



An early phenomenological theory: identifying magnetic moment as a source of puzzles



PHYSICAL REVIEW VOLUME 81, NUMBER 4 FEBRUARY 1, 1951

Interaction Between the *d* Shells in the Transition Metals*

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(Received October 9, 1950)

It is assumed (1) that the interaction between the incomplete *d* shells of the transition elements is insufficient to disrupt the coupling between the *d* electrons in the same shells, and (2) that the exchange interaction between adjacent *d* shells always has the same sign irrespective of distance of separation. The direct interaction between adjacent *d* shells then invariably leads to a tendency for an antiferromagnetic alignment of *d* spins. The body-centered cubic structure of the transition metals V, Cr, Cb, Mo, Ta, and W is thereby interpreted, as well as more complex lattices of certain alloys. It is demonstrated that the spin coupling between the incomplete *d* shells and the conduction electrons leads to a tendency for a ferromagnetic alignment of *d* spins. The occurrence of ferromagnetism is thereby interpreted in a much more straightforward manner than through the *ad hoc* assumption of a reversal in sign of the exchange integral. The occurrence of antiferromagnetism and of ferromagnetism in various systems is readily understood, and certain simple rules are deduced for deciding which type of magnetism will occur in particular alloys.

$$\sum_{k\sigma} \varepsilon_k n_{k\sigma} + J\vec{S}.\vec{s}$$

Owen, Browne, Knight and Kittel, Phys. Rev. 102, 1501 (1956).
K. Yosida, Phys. Rev. 106, 893 (1957),
and others

Anderson impurity model (AIM)

$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_{\sigma} \varepsilon_d n_{d\sigma}$$
$$+ \sum_{k,\sigma} V_{kd}(a^\dagger_{k\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{k\sigma}) + U n_{d\uparrow} n_{d\downarrow}$$

Hartree-Fock solution of AIM

$$U n_{d\uparrow} n_{d\downarrow} \rightarrow U n_{d\uparrow} \langle n_{d\downarrow} \rangle + U \langle n_{d\uparrow} \rangle n_{d\downarrow} - U \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle$$

$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_{\sigma} E_{d\sigma} n_{d\sigma}$$
$$+ \sum_{k,\sigma} V_{kd}(a^\dagger_{k\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{k\sigma})$$

$E_{d\sigma} = \varepsilon_d + U \langle n_{d-\sigma} \rangle$ effective level

$$G^r_\sigma(\omega) = \frac{1}{\omega - \varepsilon_d - U\langle n_{d-\sigma}\rangle - \Sigma^r(\omega)}$$

$$\Sigma^r(\omega) = \sum_k \frac{|V_k|^2}{\omega - \varepsilon_k + i\eta}$$

P. W. Anderson, Phys. Rev. **124**, 41(1961)

Hartree-Fock solution of AIM

$$\langle n_{d-\sigma}\rangle = -\frac{1}{\pi}\int d\omega Im G^r_{-\sigma}(\omega) f_{FD}(\omega)$$

$$G^r_\sigma(\omega) = \frac{1}{\omega - \varepsilon_d - U\langle n_{d-\sigma}\rangle - \Sigma^r(\omega)}$$

$$\Sigma^r(\omega) = \sum_k \frac{|V_k|^2}{\omega - \varepsilon_k + i\eta} = \int \rho(\epsilon)\frac{|V(\epsilon)|^2}{\omega - \epsilon + i\eta}$$

P. W. Anderson, Phys. Rev. **124**, 41(1961)

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Hartree-Fock solution of AIM

$$\Sigma^r(\omega) = \sum_k \frac{|V_k|^2}{\omega - \varepsilon_k + i\eta} = \int \rho(\epsilon)\frac{|V(\epsilon)|^2}{\omega - \epsilon + i\eta}$$

$$\int \rho(\epsilon)\frac{|V(\epsilon)|^2}{\omega - \epsilon + i\eta} = P\int \rho(\epsilon)\frac{|V(\epsilon)|^2}{\omega - \epsilon} - i\pi\delta(\omega)|V(\omega)|^2$$

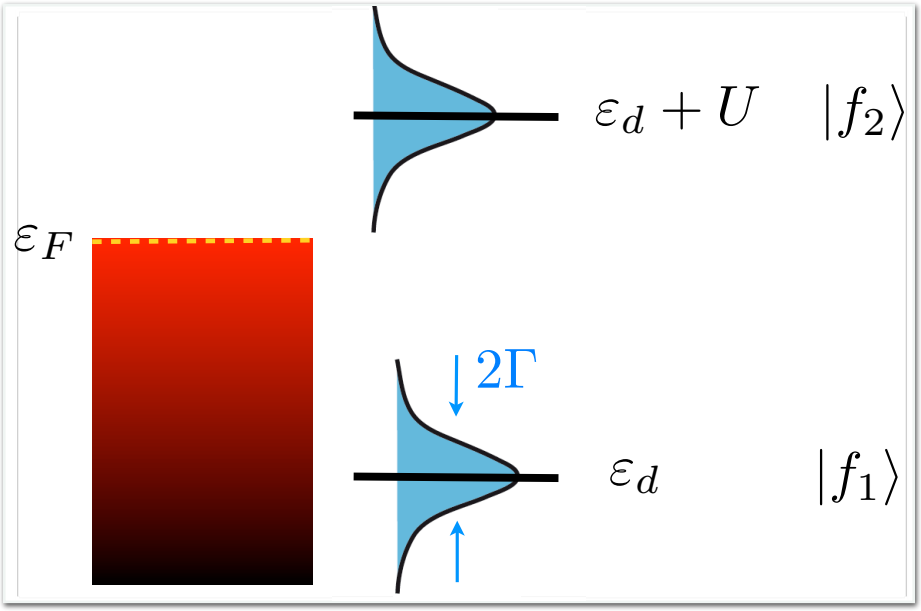
level shift width

$$\Sigma^r(\omega) \approx \frac{\Gamma}{\pi}\int_{-D}^{D}\frac{1}{\omega - \epsilon} - i\Gamma = -\frac{\Gamma}{\pi} ln\left|\frac{D+\omega}{D-\omega}\right| - i\Gamma$$

P. W. Anderson, Phys. Rev. **124**, 41(1961)

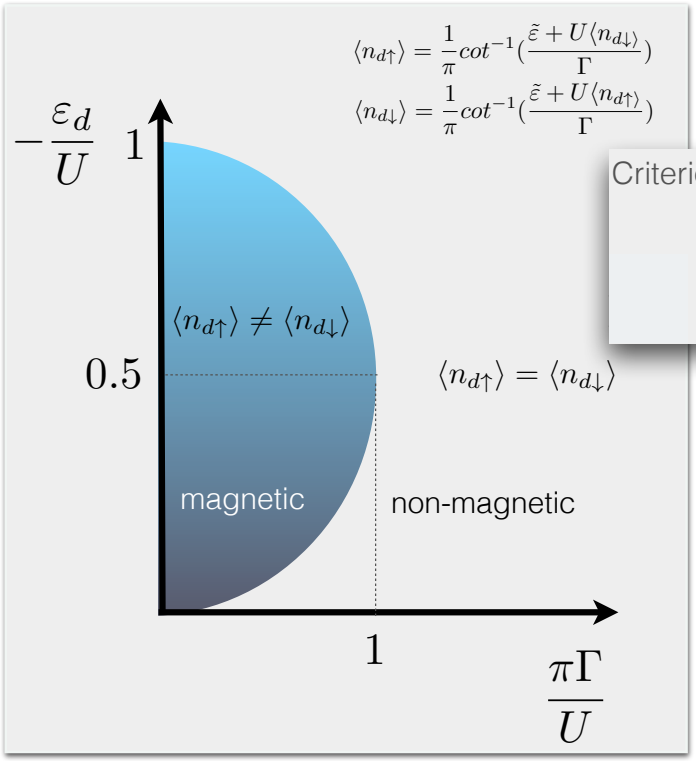
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Impurity levels of AIM



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Self-consistent "broken symmetry" solutions



Criterion for local moment formation at half-filling

$$\frac{\pi\Gamma}{U} < 1$$

$$U\rho(\varepsilon_F) > 1$$

Similar to Stoner's criterion for ferromagnetism

$$\langle n_{d\sigma}\rangle = -\frac{1}{\pi}\int d\omega Im G^r_\sigma(\omega) f_{FD}(\omega)$$

$$\langle n_{d\sigma}\rangle \approx \int_{-\infty}^{0} \frac{d\omega}{2\pi} \frac{2\Gamma}{(\omega - \tilde{\varepsilon} - U\langle n_{d-\sigma}\rangle)^2 + \Gamma^2}$$

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Phase shift by impurity scattering

$$G^{\sigma}_{kk'} = \frac{\delta_{kk'}}{\omega - \varepsilon_k + i\eta} + \frac{V_k}{\omega - \varepsilon_k + i\eta} G^r_{\sigma}(\omega) \frac{V^*_{k'}}{\omega - \varepsilon_{k'} + i\eta}$$

T-matrix

$$T^{\sigma}_{kk'}(\omega) = V_k G^r_{\sigma}(\omega) V^*_{k'} \sim e^{2i\delta^{\sigma}(\omega)} - 1$$

$$ImT^{\sigma}_{kk}(\omega) = -\pi |V_k|^2 \rho^{\sigma}(\omega)$$

Phase shift induced by the impurity

$$\delta^{\sigma}(\omega) = cot^{-1}\left(\frac{\varepsilon_d + U\langle n_{d-\sigma}\rangle - \omega}{\Gamma}\right)$$

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Phase shift by impurity scattering

$$\delta^{\sigma}(\omega) = cot^{-1}\left(\frac{\varepsilon_d + U\langle n_{d-\sigma}\rangle - \omega}{\Gamma}\right)$$

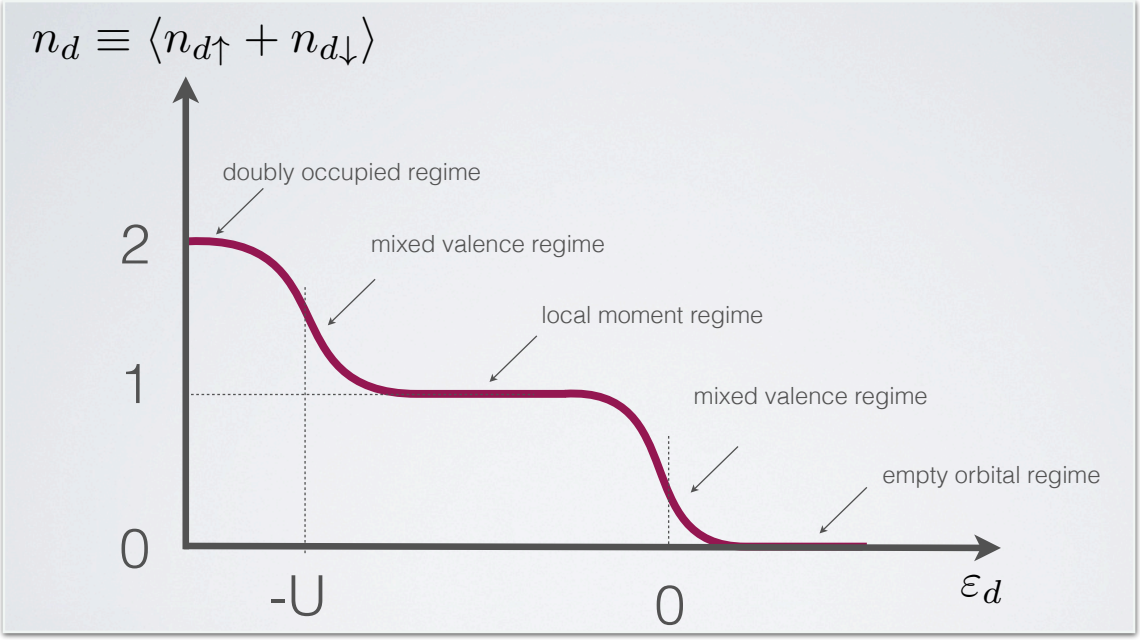
$$\langle n_{d\downarrow}\rangle = \frac{1}{\pi} cot^{-1}\left(\frac{\tilde{\varepsilon} + U\langle n_{d\uparrow}\rangle}{\Gamma}\right) = \frac{\delta^{\downarrow}(0)}{\pi}$$

$$\langle n_{d\uparrow}\rangle = \frac{1}{\pi} cot^{-1}\left(\frac{\tilde{\varepsilon} + U\langle n_{d\downarrow}\rangle}{\Gamma}\right) = \frac{\delta^{\uparrow}(0)}{\pi}$$

Friedel's sum rule that relates the occupancy of the impurity site and the phase shifts of conduction electrons at the Fermi energy scattering on the impurity. This phase shift arises solely from non-spin flip scattering. The role of spin-flip scattering will become evident in the Kondo regime.

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Anderson impurity model



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Kondo model

Quenching of local moments: Kondo's calculation

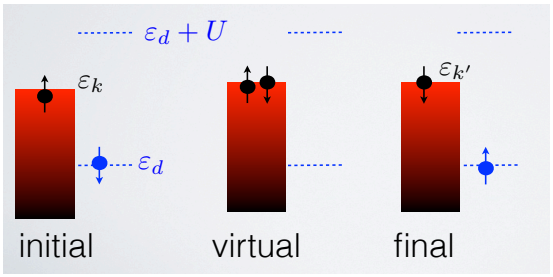
$$H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_\sigma \varepsilon_d n_{d\sigma} + \sum_{k,\sigma} V_{kd}(a^\dagger_{k\sigma} a_{d\sigma} + a^\dagger_{d\sigma} a_{k\sigma}) + U n_{d\uparrow} n_{d\downarrow}$$

$$\Rightarrow \quad H = \sum_{k\sigma} \varepsilon_k n_{k\sigma} + J\vec{S}.\vec{s}$$

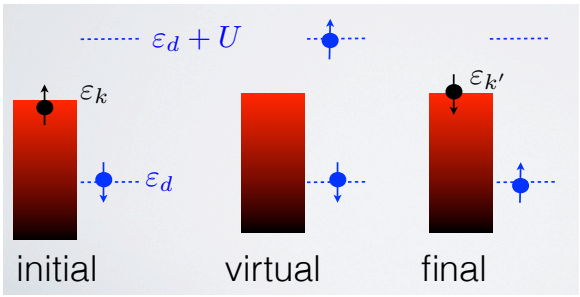
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Spin-flip scattering process …

$$T_{k\uparrow,d\downarrow\to k'\downarrow,d\uparrow} \sim -V_{kd}\frac{1}{\varepsilon_d}V^*_{k'd}$$



$$T_{k\uparrow,d\downarrow\to k'\downarrow,d\uparrow} \sim -V_{kd}\frac{1}{-\varepsilon_d - U}V^*_{k'd}$$



$$J_{kk'} = 2V_{kd}V^*_{k'd}\left(\frac{1}{\varepsilon_k - \varepsilon_d - U} + \frac{1}{\varepsilon_d - \varepsilon_{k'}}\right)$$

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Schrieffer-Wolff transformation

$$\tilde{H} = e^S H e^{-S}$$

$$S = \sum_{k\sigma} \frac{V_k}{\varepsilon_k - \varepsilon_d - U} n_{-\sigma}(c^\dagger_{k\sigma} d_\sigma - d^\dagger_\sigma c_{k\sigma}) + \frac{V_k}{\varepsilon_k - \varepsilon_d}(1 - n_{-\sigma})(c^\dagger_{k\sigma} d_\sigma - d^\dagger_\sigma c_{k\sigma})$$

$$J_{eff} = 2|V_{kd}|^2\left(\frac{1}{\varepsilon_d} - \frac{1}{\varepsilon_d + U}\right) = \frac{2\Gamma}{\pi}\left(\frac{1}{\varepsilon_d} - \frac{1}{\varepsilon_d + U}\right)$$

$$H_K = \sum_{k,\sigma} \varepsilon_k n_{k,\sigma} - \sum_{k,k'} \frac{J_{kk'}}{\hbar^2}(\Psi^\dagger_{k'} S \Psi_k).(\Psi^\dagger_d S \Psi_d)$$

$$\Psi_k = \begin{pmatrix} a_{k\uparrow} \\ a_{k\downarrow} \end{pmatrix} \quad \Psi_d = \begin{pmatrix} a_{d\uparrow} \\ a_{d\downarrow} \end{pmatrix}$$

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Kondo's contribution to resistivity

$$\sigma = \frac{ne^2}{m}\tau(k_F)$$

$$\frac{1}{\tau(k)} = \sum_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'}(1 - cos\theta)\delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'})$$

$$W_{\mathbf{k}\mathbf{k}'} = \frac{2\pi N_{imp}}{\hbar}|T_{\mathbf{k}\mathbf{k}'}|^2$$

$$H = \sum_{\mathbf{k},\mathbf{k}'} J_{\mathbf{k}\mathbf{k}'}(S^+ a^\dagger_{\mathbf{k},\downarrow} a_{\mathbf{k}',\uparrow} + S^- a^\dagger_{\mathbf{k},\uparrow} a_{\mathbf{k}',\downarrow} + S^z(a^\dagger_{\mathbf{k},\uparrow} a_{\mathbf{k}',\uparrow} - a^\dagger_{\mathbf{k},\downarrow} a_{\mathbf{k}',\downarrow}))$$

$$|T_{\mathbf{k}\mathbf{k}'}|^2 = |J_{\mathbf{k}\mathbf{k}'}|^2(2S_z^2 + S^+S^- + S^-S^+)$$

$$W_{\mathbf{k}\mathbf{k}'} = \frac{2\pi N_{imp}}{\hbar}|T_{\mathbf{k}\mathbf{k}'}|^2 = \frac{2\pi N_{imp}}{\hbar}\frac{J^2}{N_s^2}(2S_z^2 + S^+S^- + S^-S$$

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1st order contribution

$$H = \sum_{\mathbf{k},\mathbf{k}'} J_{\mathbf{k}\mathbf{k}'}(S^+ a^\dagger_{\mathbf{k},\downarrow} a_{\mathbf{k}',\uparrow} + S^- a^\dagger_{\mathbf{k},\uparrow} a_{\mathbf{k}',\downarrow} + S^z(a^\dagger_{\mathbf{k},\uparrow} a_{\mathbf{k}',\uparrow} - a^\dagger_{\mathbf{k},\downarrow} a_{\mathbf{k}',\downarrow}))$$

$$|T_{\mathbf{k}\mathbf{k}'}|^2 = |J_{\mathbf{k}\mathbf{k}'}|^2(2S_z^2 + S^+S^- + S^-S^+)$$

$$W_{\mathbf{k}\mathbf{k}'} = \frac{2\pi N_{imp}}{\hbar}|T_{\mathbf{k}\mathbf{k}'}|^2 = \frac{2\pi N_{imp}}{\hbar}\frac{J^2}{N_s^2}(2S_z^2 + S^+S^- + S^-S^+)$$

$$\frac{1}{\tau(k)} = \sum_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'}(1 - cos\theta)\delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'})$$

$$\frac{1}{\tau(k_F)} = \frac{3\pi c_{imp} n J^2}{2\varepsilon_F \hbar}S(S+1)$$

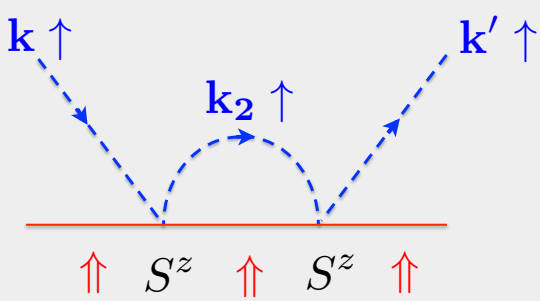
$$c_{imp} = \frac{N_{imp}}{N_s} \qquad n = \frac{p_F^3}{3\pi^2\hbar^3}$$

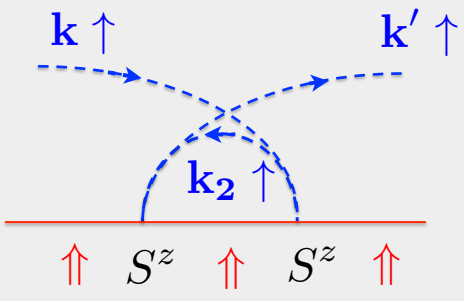
ICMM-CSIC Lecture by Ramon Aguado
http://www.icmm.csic.es/emergence/Kondoeffect-Aguado1.pdf

2nd order corrections

$$\langle \mathbf{k},\sigma|T|\mathbf{k}',\sigma'\rangle_{(2)} = \langle \mathbf{k},\sigma|H\frac{1}{\varepsilon - H_0 + i\eta}H|\mathbf{k}',\sigma'\rangle$$

Longitudinal terms





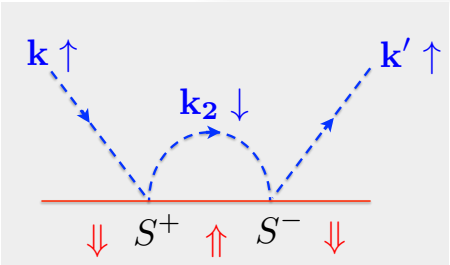
$$J^2\sum_{\mathbf{k_2}} S^zS^z\frac{(1-f(\varepsilon_{\mathbf{k_2}}))}{(\varepsilon-\varepsilon_{\mathbf{k_2}}+i\eta)} + J^2\sum_{\mathbf{k_2}} S^zS^z\frac{f(\varepsilon_{\mathbf{k_2}})}{(\varepsilon-\varepsilon_{\mathbf{k_2}}+i\eta)}$$

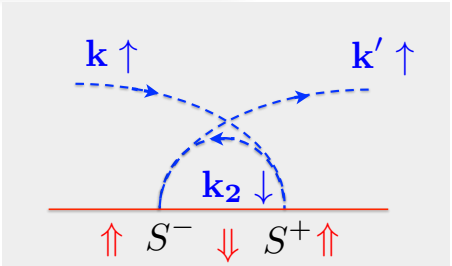
ICMM-CSIC Lecture by Ramon Aguado
http://www.icmm.csic.es/emergence/Kondoeffect-Aguado1.pdf

2nd order corrections

Transverse terms

$$J^2\sum_{\mathbf{k}_1,\mathbf{k}_1',\mathbf{k}_2,\mathbf{k}_2'}\langle \mathbf{k}',\uparrow|S^-a^\dagger_{\mathbf{k}_1\uparrow}a_{\mathbf{k}_1'\downarrow}\frac{1}{\varepsilon-H_0+i\eta}S^+a^\dagger_{\mathbf{k}_2\downarrow}a_{\mathbf{k}_2'\uparrow}|\mathbf{k},\uparrow\rangle$$





$$J^2\sum_{\mathbf{k_2}} S^-S^+\frac{(1-f(\varepsilon_{\mathbf{k_2}}))}{(\varepsilon-\varepsilon_{\mathbf{k_2}}+i\eta)} + J^2\sum_{\mathbf{k_2}} S^+S^-\frac{f(\varepsilon_{\mathbf{k_2}})}{(\varepsilon-\varepsilon_{\mathbf{k_2}}+i\eta)}$$

ICMM-CSIC Lecture by Ramon Aguado
http://www.icmm.csic.es/emergence/Kondoeffect-Aguado1.pdf

2nd order corrections

↦ logarithmic divergence

$$\frac{1}{\tau(p)} = \frac{3\pi c_{imp} n J^2}{2\varepsilon_F \hbar} S(S+1)(1 + \frac{4J}{N_s}\sum_{\mathbf{p}'} \frac{f(\varepsilon_{\mathbf{p}'}) - \frac{1}{2}}{\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}'}})$$

$$\sum_{\mathbf{p}'} \frac{f(\varepsilon_{\mathbf{p}'}) - \frac{1}{2}}{\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}'}} = \int d\varepsilon \rho(\varepsilon) \frac{f(\varepsilon) - \frac{1}{2}}{\varepsilon_{\mathbf{p}} - \varepsilon} = \frac{1}{2}\rho(0) \int_{-D}^{D} d\varepsilon \frac{tanh(\frac{\varepsilon}{2k_B T})}{\varepsilon - \varepsilon_{\mathbf{p}}}$$

$$\varepsilon_{\mathbf{p}} << k_B T \rightarrow \approx \rho(0) \int_{k_B T}^{D} \frac{d\varepsilon}{\varepsilon} = \rho(0) ln \frac{D}{k_B T}$$

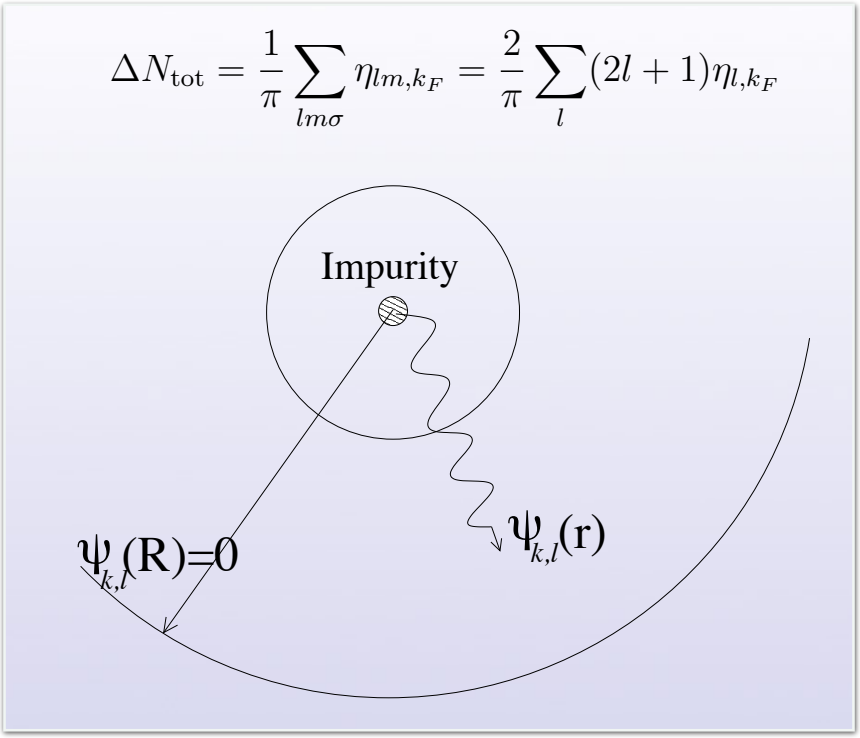
$$R = \frac{3\pi c_{imp} m J^2}{2e^2 \hbar \varepsilon_F} S(S+1)(1 - 4J\rho(0) ln \frac{k_B T}{D})$$

Resistivity diverges as T→ 0!

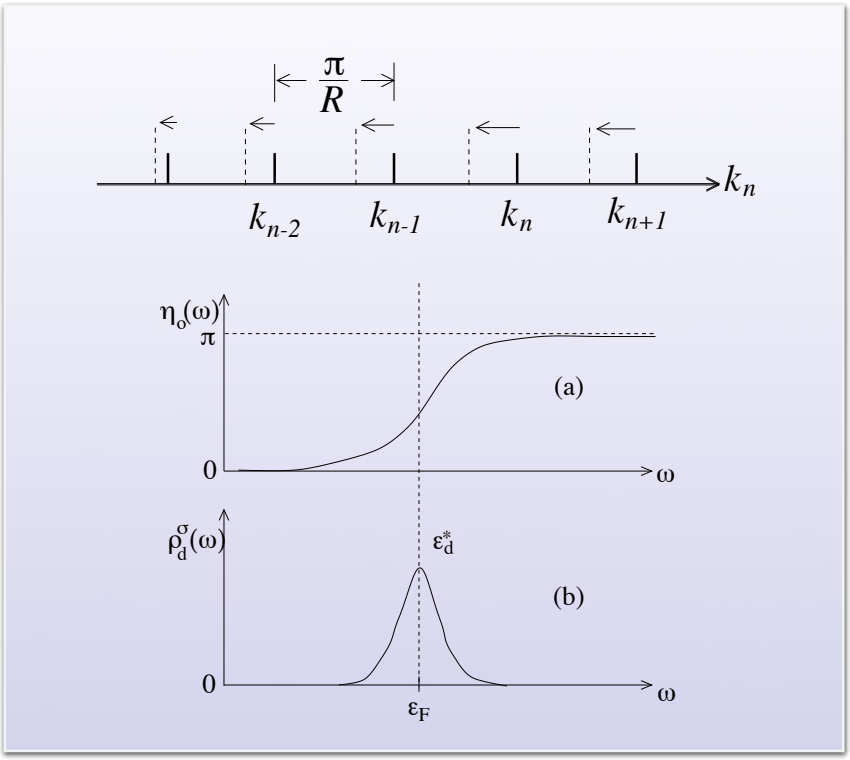
ICMM-CSIC Lecture by Ramon Aguado
http://www.icmm.csic.es/emergence/Kondoeffect-Aguado1.pdf

Friedel Sum Rule

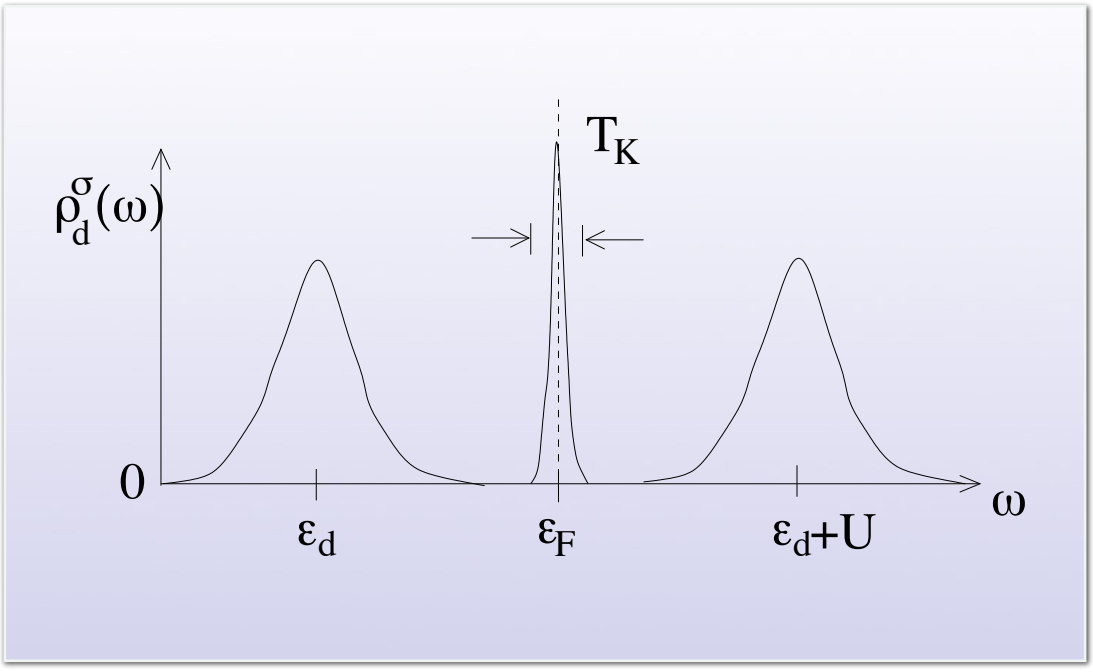
$$\Delta N_{\text{tot}} = \frac{1}{\pi}\sum_{lm\sigma} \eta_{lm,k_F} = \frac{2}{\pi}\sum_{l}(2l+1)\eta_{l,k_F}$$



Scattering Phase Shift and Change of Density-of-State



Kondo Resonance



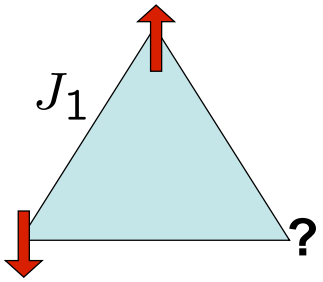
Kondo effect

- Spin-flip scattering between the free electrons of a metal and the local moment of a magnetic impurity ➡ Kondo effect.
- Highly correlated ground state where the conduction electrons form a spin-polarized “cloud” around the magnetic impurity.
- Below “Kondo temperature”, ➡ a narrow resonance at the Fermi energy: Kondo resonance.

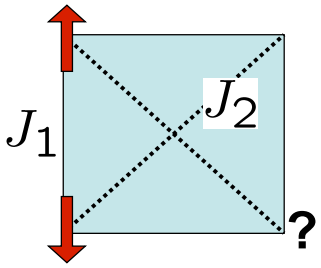
Non-collinear magnetic ordering

- frustration: lattice symmetry and interactions
- spin-orbit coupling

frustration



Topological origin



Extended range interaction

$$E[\{\mathbf{S}_i\}] = \tfrac{1}{2}\textstyle\sum_i \sum_r J(\mathbf{r})\mathbf{S}_i \cdot \mathbf{S}_{i+r}$$

By Fourrier transform:

$$E = \tfrac{1}{2}\textstyle\sum_k J(\mathbf{k})\mathbf{S}_k \cdot \mathbf{S}_{-k}$$

⇒ Minimize J(k)

"Frustrated Spin Systems", Ed. H.T. Diep (World Scientific 2004)
"Introduction to Frustrated Magnetism", Eds. C. Lacroix, P. Mendels, F. Mila, Springer Series in Solid-State Sciences 164 (Springer 2011)

Sprial ordering

Assume $J(\mathbf{k})$ minimized for $k = k_0$

⇓

$\mathbf{S}_\mathbf{k} = 0$ for all k's except $\mathbf{k} = \mathbf{k}_0$

⇓

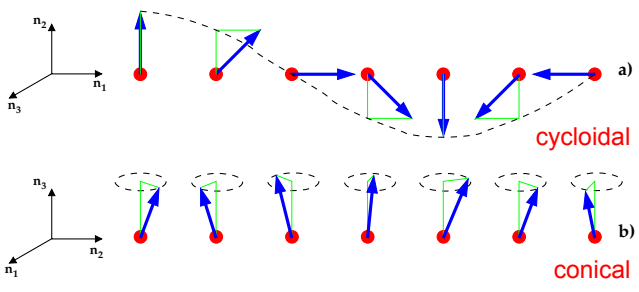
$$\mathbf{S}_i = \frac{1}{\sqrt{N}}(\mathbf{S}_{\mathbf{k}_0} e^{i\mathbf{k}_0 \cdot \mathbf{r}_i} + H.C.)$$

constraint $|\mathbf{S}_i| = 1$

⇓

$$\mathbf{S}_i = (\cos(\mathbf{k}_0 . \mathbf{r}_i), \sin(\mathbf{k}_0 . \mathbf{r}_i), 0)$$

Spiral configuration (non-collinear – coplanar)

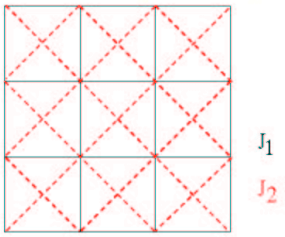


L.M. Sandratskii, Adv. Phys. **47**, 91 (1998)

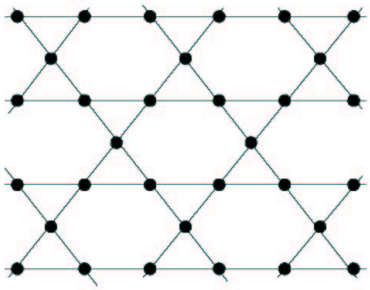
2d frustrated magnets

Lattices with AF frustrating interactions

Melzi et al., PRB **85**, 1318 (2000)



frustrated square lattice (S=1/2): Li_2VOSiO_4



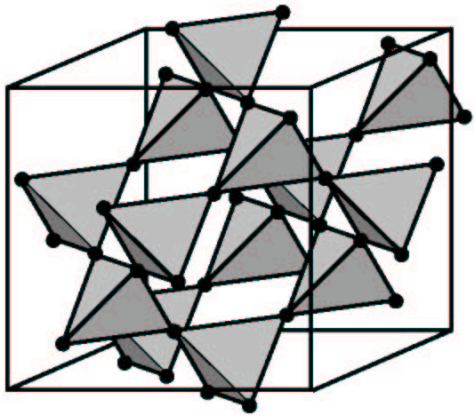
Kagome lattice like $SrCr_{9-x}Ga_{3+x}O_{19}$ (S=3/2)

Ramirez et al., PRL **64** ('90)

Broholm et al., PRL **65** ('90)

3d frustrated magnets

pyrochlores and spinels



Transition metal oxides

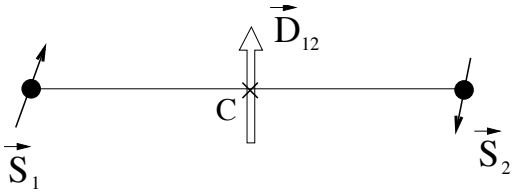
- $ZnCr_2O_4$ spinel
- $A_2Ti_2O_7$ titanates

Ramirez et al., PRL 89, 067202 (2002)

-no ordering down to low temperatures

Dzyaloshinskii-Moriya interaction

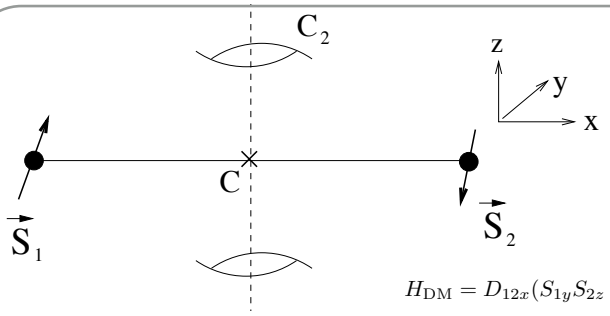
$$H_{\mathrm{DM}} = \mathbf{D}_{12} \cdot (\mathbf{S}_1 \times \mathbf{S}_2)$$



If C is an inversion center i of the crystal,

$$\mathbf{S}_1 \times \mathbf{S}_2 \xrightarrow{i} \mathbf{S}_2 \times \mathbf{S}_1 = -\mathbf{S}_1 \times \mathbf{S}_2.$$

H is only invariant if $\mathbf{D}_{12}= 0$.



a two-fold rotation axis C_2 through C perpendicular to the bond.

$$S_{1x} \xleftrightarrow{C_2} -S_{2x},$$
$$S_{1y} \xleftrightarrow{C_2} -S_{2y},$$
$$S_{1z} \xleftrightarrow{C_2} +S_{2z}.$$

$$H_{\mathrm{DM}} = D_{12x}(S_{1y}S_{2z} - S_{1z}S_{2y}) + D_{12y}(S_{1z}S_{2x} - S_{1x}S_{2z}) + D_{12z}(S_{1x}S_{2y} - S_{1y}S_{2x}).$$

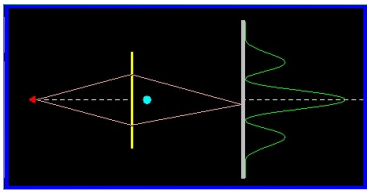
Thus H is invariant only if $D_{12z} = 0$.

Berry phase and topological effects

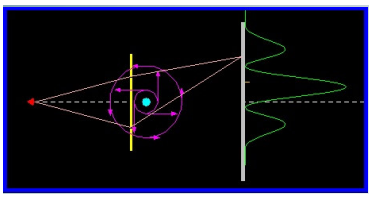
- Spins and geometric phases
- quantum spin Hall effect

Spins and geometric phases

- Geometric phases in Physics
- Aharonov-Bohm effect …



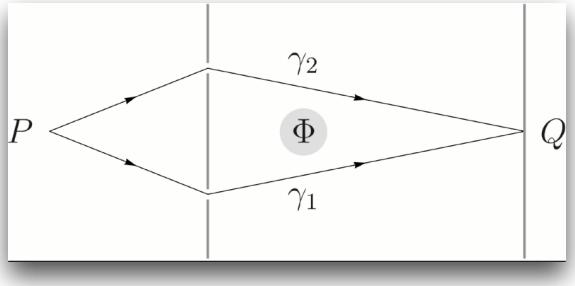
$\Phi_B = 0$



$\Phi_B \neq 0$

Question:
geometric or topological effect?

$$\Phi_B = (\gamma_1 - \gamma_2)/(e/\hbar) = \oint_{C_{1-2}} \mathbf{A} \cdot d\mathbf{l}$$



$$\psi_Q = \psi_1 + \psi_2 = e^{-i\gamma_1}\phi_1\left(1 + (\phi_2/\phi_1)e^{i(e/\hbar)\Phi_B}\right)$$

Fiber bundles, connection, curvature, … and topology

- Holonomy: $\Delta\phi_C = \phi(s_2) - \phi(s_1)$
- Connection: $\mathbf{A}(\mathbf{r})$

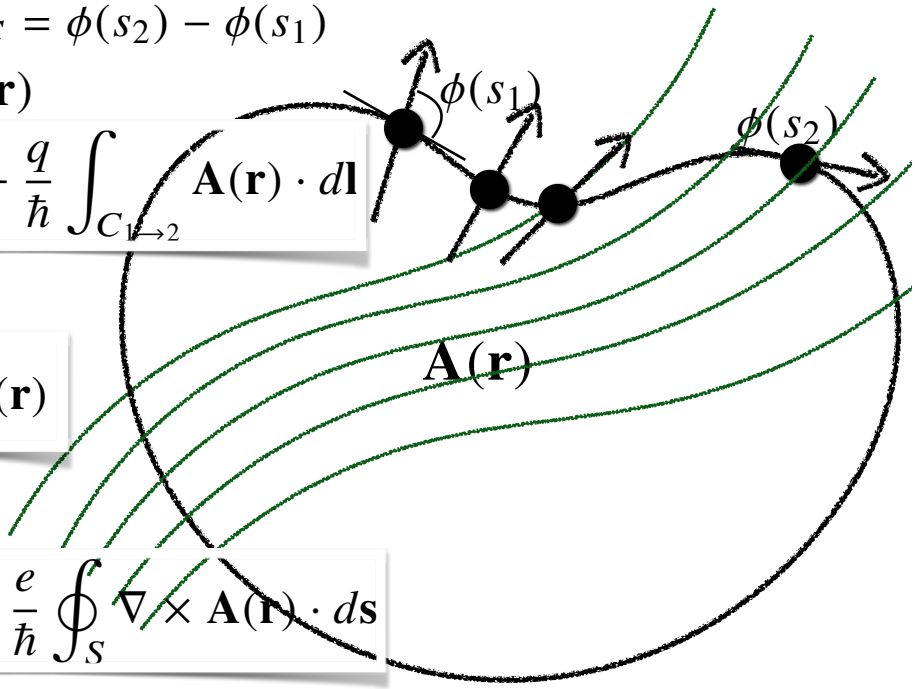
$$\Delta\phi_C = \phi_2 - \phi_1 + \frac{q}{\hbar}\int_{C_{1\to 2}} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{l}$$

- Curvature: $\mathcal{F}_{\mu\nu}$

$$\vec{\mathcal{F}} = \frac{e}{\hbar}\nabla \times \mathbf{A}(\mathbf{r})$$

- Topology

$$C = \oint_S \vec{\mathcal{F}} \cdot d\mathbf{s} = \frac{e}{\hbar}\oint_S \nabla \times \mathbf{A}(\mathbf{r}) \cdot d\mathbf{s}$$



Anholonomy in quantum mechanics:

Berry phase

slow variables

$$\mathcal{H}(\mathbf{r},\mathbf{p};\mathbf{R},\mathbf{P})$$

fast variables

$$|\psi(t)\rangle = e^{i\gamma_n(\mathbf{R})} e^{-i/\hbar \int_0^t dt\ e_n(\mathbf{R}(t))} |n;\mathbf{R}\rangle$$

$$\dot{\gamma}_n(t) = i\langle n|\dot{n}\rangle$$

$$\gamma_n(C) = i\oint_C \left\langle n|\frac{\partial n}{\partial \mathbf{R}}\right\rangle \cdot d\mathbf{R} = \oint_C \mathbf{A}\cdot d\mathbf{R}$$

$$\mathbf{A}(\mathbf{R}) = i\left\langle n|\frac{\partial n}{\partial \mathbf{R}}\right\rangle \Leftarrow \text{Berry connection}$$

$$\gamma_n(C) = i\int_S \left\langle \frac{\partial n}{\partial \mathbf{R}}|\times|\frac{\partial n}{\partial \mathbf{R}}\right\rangle \cdot d^2\mathbf{R} = \int_S \vec{\mathcal{F}}\cdot d^2\mathbf{R}$$

$$\vec{\mathcal{F}}(\mathbf{R}) = \nabla_{\mathbf{R}}\times\mathbf{A}(\mathbf{R}) \Leftarrow \text{Berry curvature}$$

Quantum Hall effect:

Dynamics of Bloch electrons in an electric field

$$H(\boldsymbol{q}) = e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} H e^{i\boldsymbol{q}\cdot\boldsymbol{r}} = \frac{(\hat{\boldsymbol{p}}+\hbar\boldsymbol{q})^2}{2m} + V(\boldsymbol{r}) \qquad u_{n\boldsymbol{q}}(\boldsymbol{r}) = e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\psi_{n\boldsymbol{q}}(\boldsymbol{r})$$

$$v_n(\boldsymbol{q}) = \frac{\partial\varepsilon_n(\boldsymbol{q})}{\hbar\partial\boldsymbol{q}} \qquad u_{n\boldsymbol{q}}(\boldsymbol{r}+\boldsymbol{a}) = u_{n\boldsymbol{q}}(\boldsymbol{r})$$

$$H(t) = \frac{[\hat{\boldsymbol{p}}+e\boldsymbol{A}(t)]^2}{2m} + V(\boldsymbol{r}) \qquad \boldsymbol{v}_n(\boldsymbol{k}) = \frac{\partial\varepsilon_n(\boldsymbol{k})}{\hbar\partial\boldsymbol{k}} - \frac{e}{\hbar}\boldsymbol{E}\times\boldsymbol{\Omega}_n(\boldsymbol{k})$$

$$H(\boldsymbol{q},t) = H(\boldsymbol{q}+\frac{e}{\hbar}\boldsymbol{A}(t)) \qquad \boldsymbol{\Omega}_n(\boldsymbol{k}) = i\langle\boldsymbol{\nabla}_{\boldsymbol{k}}u_n(\boldsymbol{k})|\times|\boldsymbol{\nabla}_{\boldsymbol{k}}u_n(\boldsymbol{k})\rangle$$

$$\boldsymbol{k} = \boldsymbol{q} + \frac{e}{\hbar}\boldsymbol{A}(t)$$

$$\dot{\boldsymbol{k}} = -\frac{e}{\hbar}\boldsymbol{E}$$

Hall conductivity $\sigma_{xy} = \frac{e^2}{\hbar}\int_{\mathrm{BZ}}\frac{d^2k}{(2\pi)^2}\Omega_{k_xk_y}$

$$\dot{\boldsymbol{r}} = \frac{\partial\varepsilon_M(\boldsymbol{k})}{\hbar\partial\boldsymbol{k}} - \dot{\boldsymbol{k}}\times\boldsymbol{\Omega}(\boldsymbol{k})$$

$$\hbar\dot{\boldsymbol{k}} = -e\boldsymbol{E} - e\dot{\boldsymbol{r}}\times\boldsymbol{B}\ .$$

$$\sigma_{xy} = n\frac{e^2}{h}$$

Anomalous Hall effect:

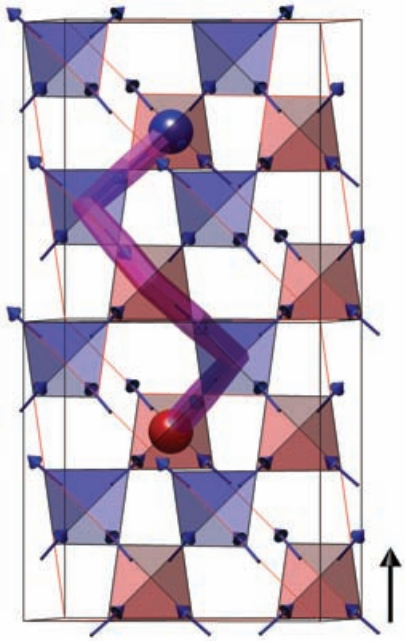
"unquantized" version of quantum Hall effect

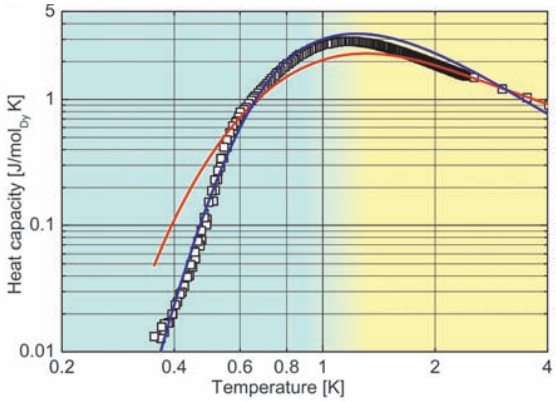
$$\sigma_{xy} = \frac{e^2}{\hbar} \int \frac{d\boldsymbol{k}}{(2\pi)^d} f(\varepsilon_{\boldsymbol{k}}) \Omega_{k_x k_y}$$

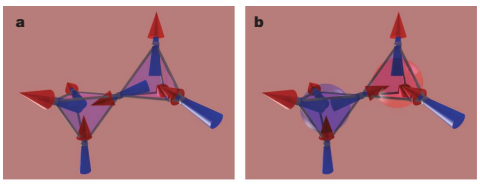
$$H = \frac{\hbar^2 k^2}{2m} + \lambda(\boldsymbol{k} \times \boldsymbol{\sigma}) \cdot \boldsymbol{e}_z - \Delta\sigma_z$$

$$\Omega_{\pm} = \mp \frac{\lambda^2 \Delta}{2(\lambda^2 k^2 + \Delta^2)^{3/2}}$$

Spin ice crystals

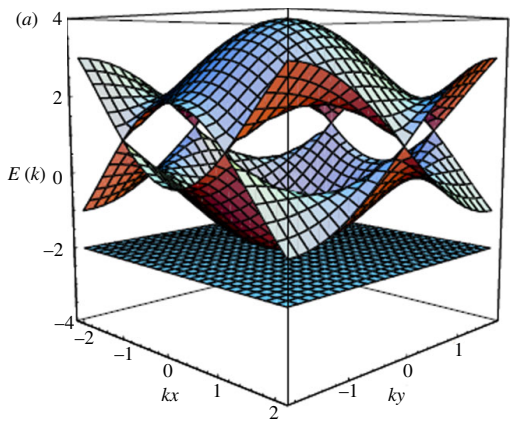






D. J. P. Morris et al., "Dirac Strings and Magnetic Monopoles in the Spin Ice Dy2Ti2O7", Science 326, 411 (2009).

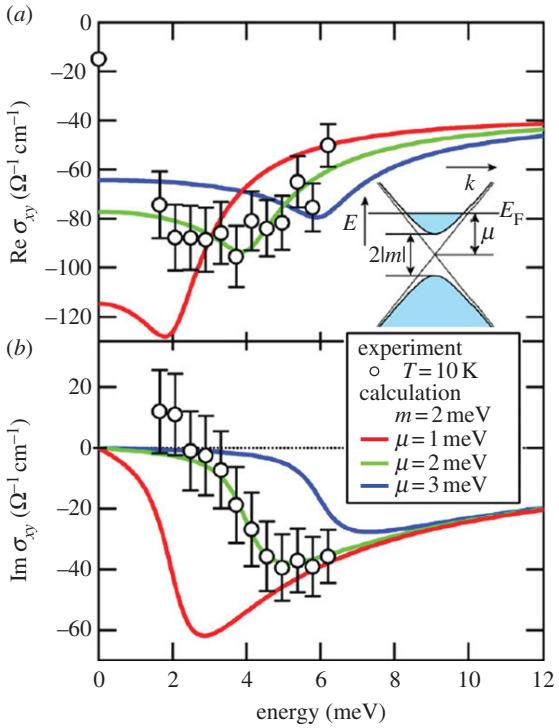
Monopoles in momentum space of $SrRuO_3$



$$H = k_x\sigma_x + k_y\sigma_y + m\sigma_z$$

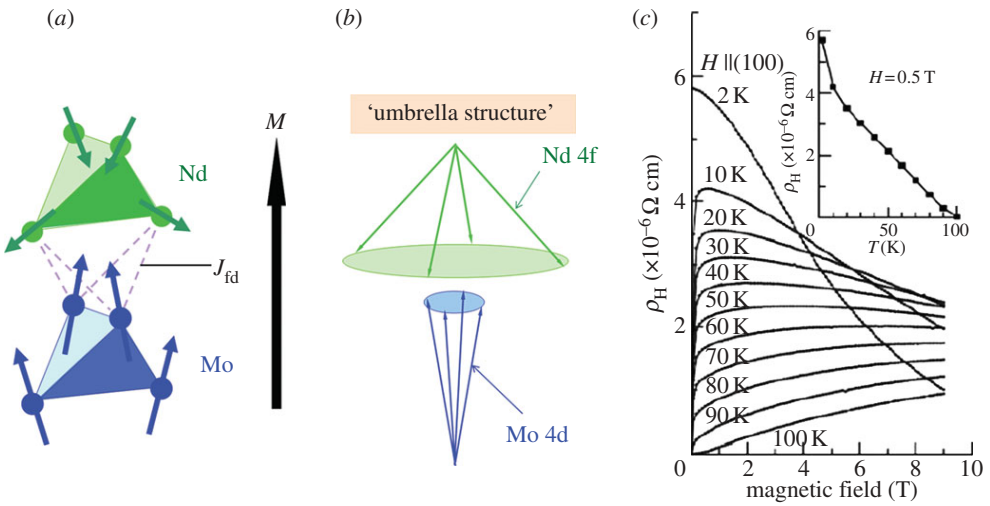
$$\sigma_{xy} = \frac{e^2}{2h}\mathrm{sign}(m)$$

$$\mathbf{b}_n(\mathbf{k}) = \pm\frac{\mathbf{k}}{2|\mathbf{k}|^3}$$



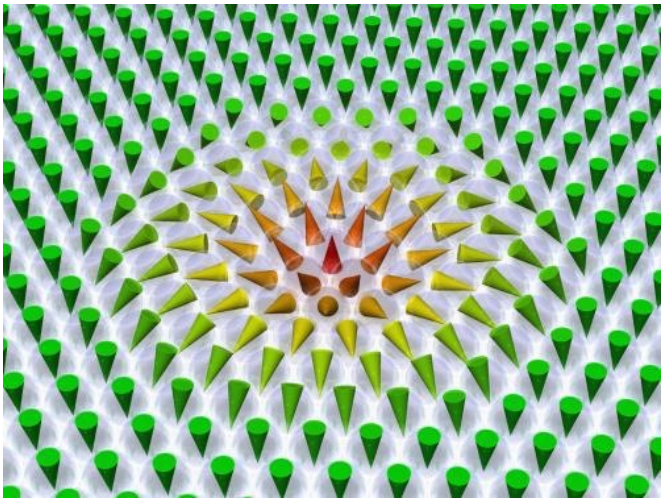
N.Nagaosa, X.Z. Yu and Y. Tokura, "Gauge fields in real and momentum spaces in magnets: monopoles and skyrmions", Phil. Trans. R. Soc. A 370, 58065819 (2012)

Anomalous Hall effect in $Nd_2Mo_2O_7$



N.Nagaosa, X.Z. Yu and Y. Tokura, "Gauge fields in real and momentum spaces in magnets: monopoles and skyrmions", Phil. Trans. R. Soc. A 370, 58065819 (2012)

Skyrmion



Effective electromagnetic fields

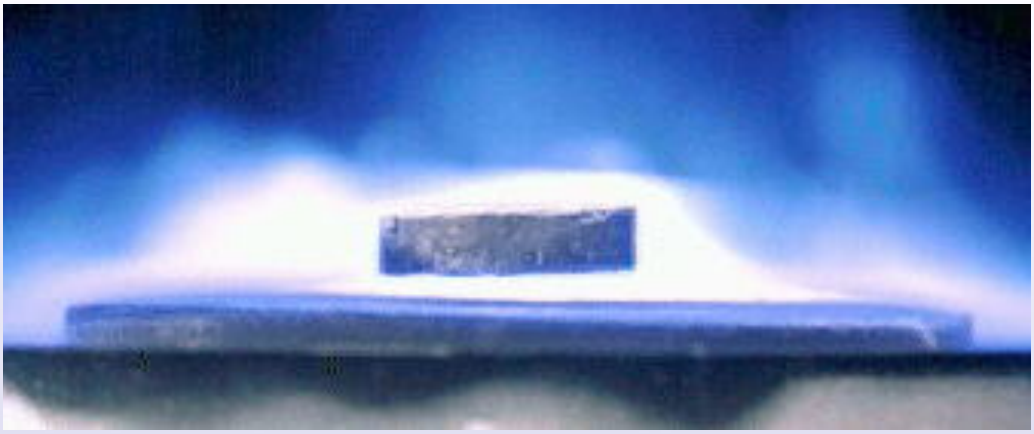
$$e_i = -\partial_i a_0 - \frac{1}{c}\dot{a}_i = \frac{\hbar}{2e}(\mathbf{n}\cdot\partial_i\mathbf{n}\times\dot{\mathbf{n}})$$

$$h_i = [\nabla\times\mathbf{a}]_i = \frac{\hbar c}{2e}\delta_{iz}(\mathbf{n}\cdot\partial_x\mathbf{n}\times\partial_y\mathbf{n})$$

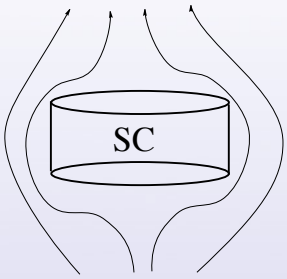
N.Nagaosa, X.Z. Yu and Y. Tokura, "Gauge fields in real and momentum spaces in magnets: monopoles and skyrmions", Phil. Trans. R. Soc. A 370, 58065819 (2012)

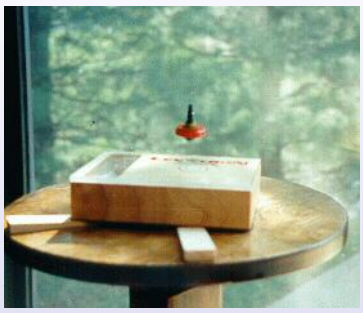
Magnetism and superconductivity

Levitating magnetic bar on a superconducting bed



Perfect diamagnetism: superconductivity





- Inside the superconductor:

$$\mathbf{B} = 0$$

- Supercurrent induced by the current of Cooper pair electrons:

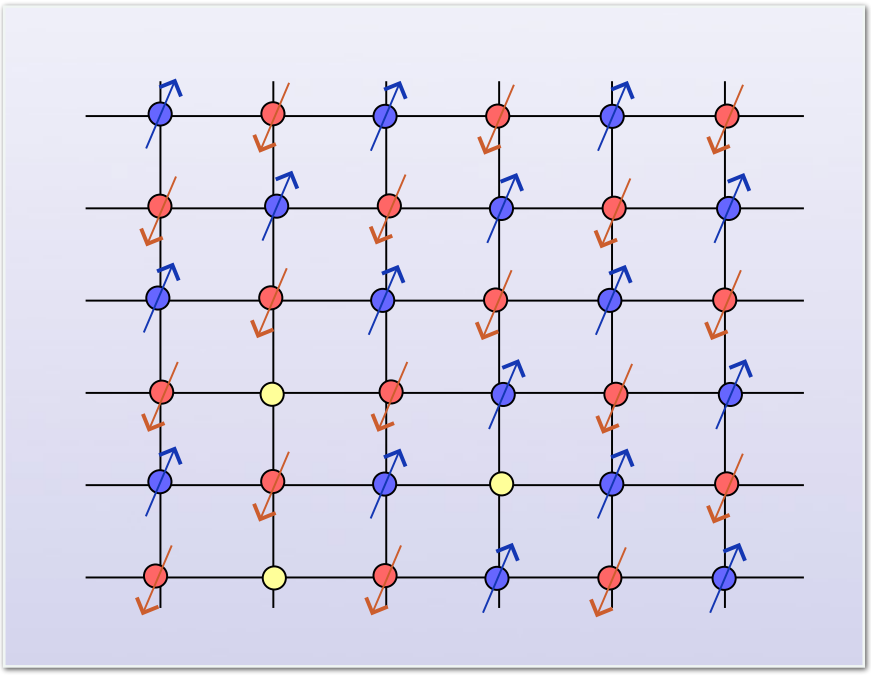
$$\mathbf{J}_s(\mathbf{r}) = \Lambda \cdot \mathbf{A}(\mathbf{r})$$

Meisner effect

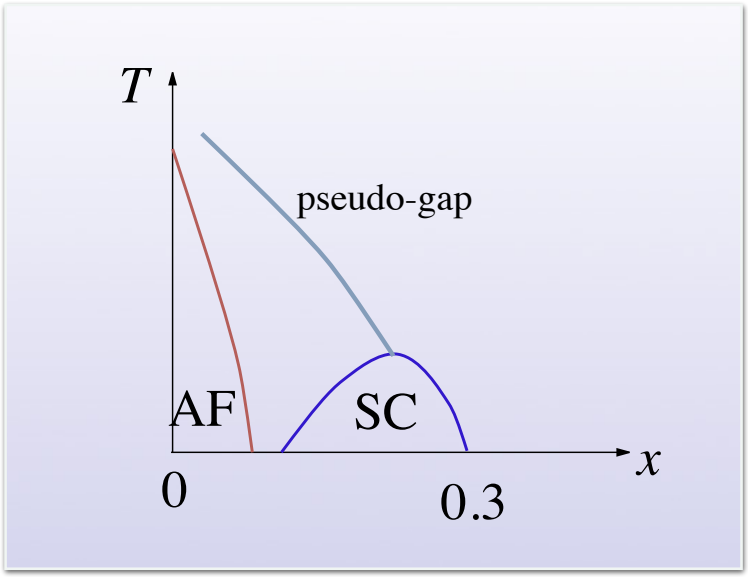


What happens when the half-filled AF insulator is being doped?

↦ High Tc superconductivity?



Phase Diagram of High Tc Superconductors: Doped Cu-oxides Systems



Anti-ferromagnetic Spin Correlation vs. BCS State

- Spin-order Ground State of an Anti-Ferromagnet:

$$|\Psi_{\rm AF}\rangle = \prod_i c^+_{(2i)\uparrow} c^+_{(2i+1)\downarrow}|O\rangle$$

- BCS State of a Superconductor:

$$|\Psi_{\rm BCS}\rangle = \prod_k (u_k + v_k c^+_{k\uparrow} c^+_{-k\downarrow})|O\rangle$$

- t-J Model for the High T_c Superconductivity:

$$\mathcal{H}_{\rm eff} = -\sum_{\langle ij\rangle\sigma} c^+_{i\sigma} c_{j\sigma} + J\sum_{\langle ij\rangle} \mathbf{s}_i \cdot \mathbf{s}_j$$

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