What is Solid State Physics?

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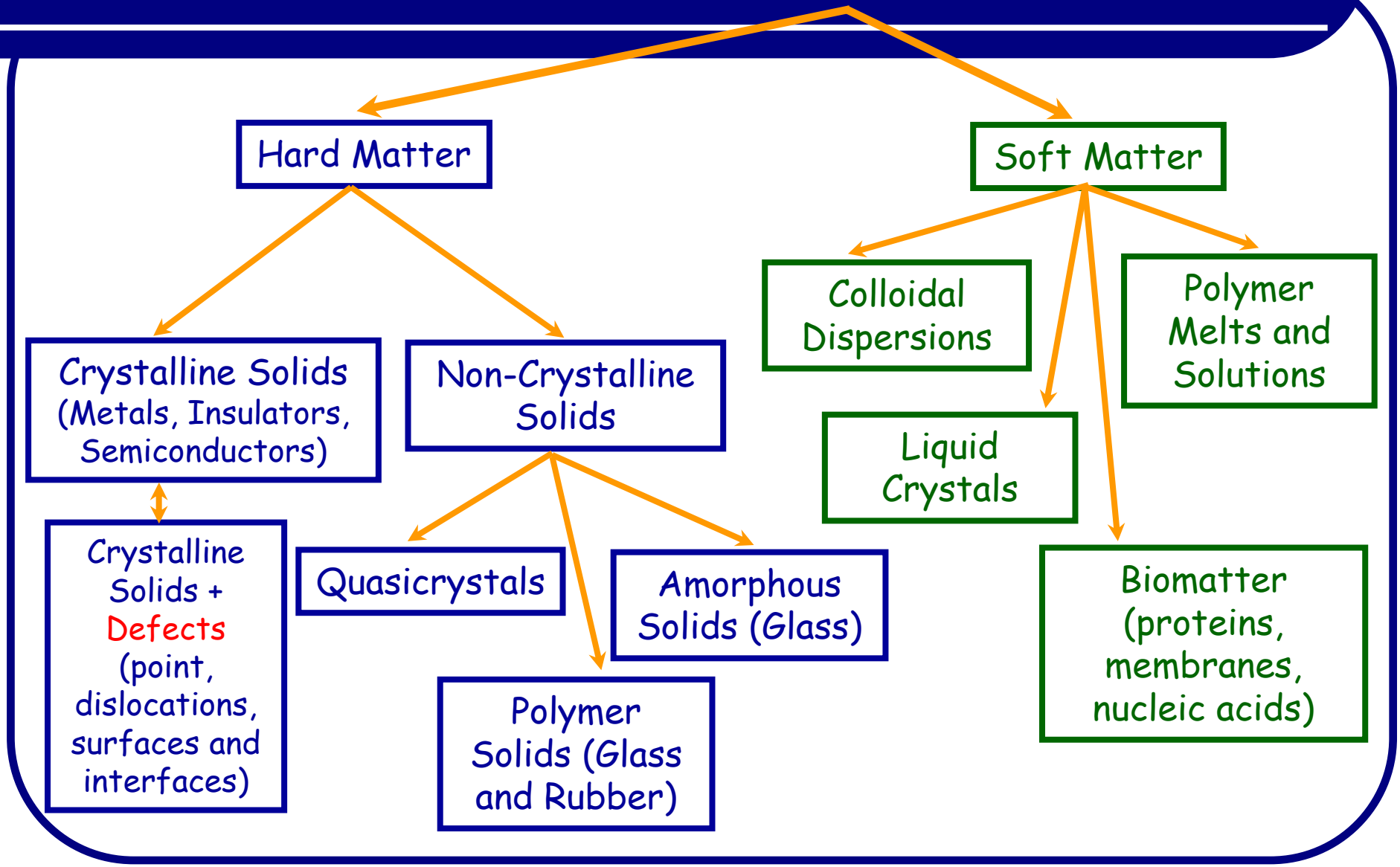
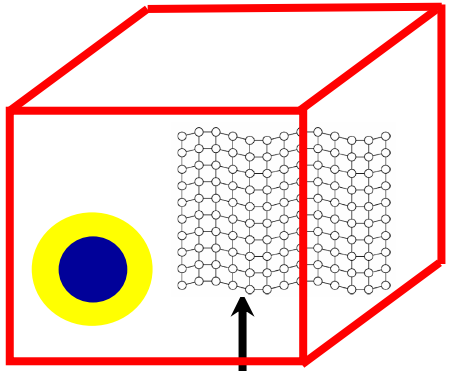
PHYS 624: Introduction to Solid State Physics
http://www.physics.udel.edu/~bnikolic/teaching/phys624/phys624.html

Condensed Matter Systems



Basic Notions of Condensed Matter

❑**Quasiparticles excitations** which look nearly as individual particles as possible - modern condensed matter theory asserts that a **solid crystal is actually a gas of weakly interacting quasiparticles**.



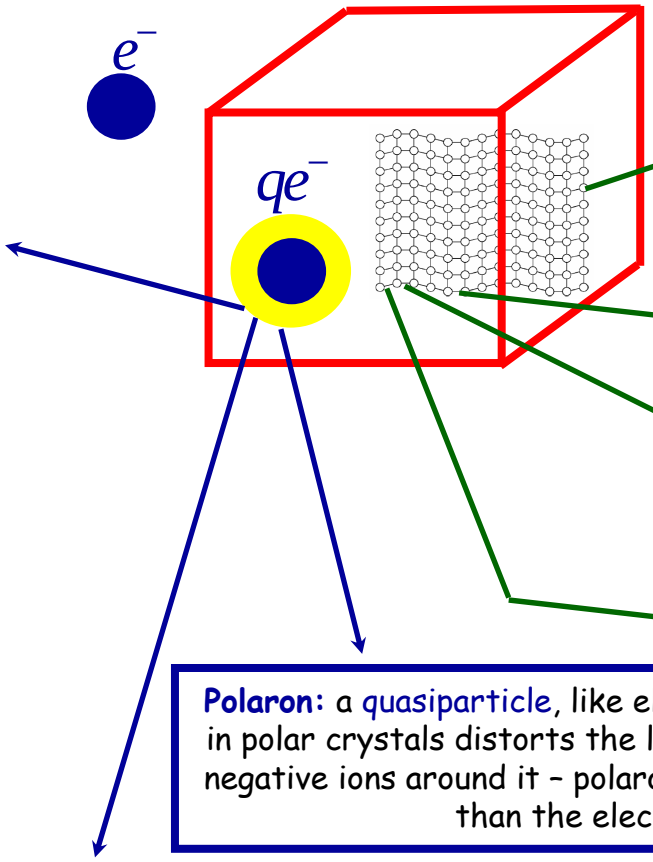
Scalar Bosons (Spin=0)

❑**Broken symmetry, long-range order, and order parameters** → Phases of matter are characterized by the symmetry of their ground (lowest energy) state (Landau, 1937).

❑Phase Transitions between different broken symmetry states: **Classical** (at T>0) and **Quantum** (at T=0).

Quasiparticles vs Collective Excitations

Electron: a quasiparticle consisting of a real electron and the cloud of effective charge of opposite sign due to exchange an correlation effects arising interaction with all other electrons in the system. The electron is a **fermion with spin ½**. The Fermi energy (highest occupied state) is of the order of 5 eV and the Fermi velocity is 10^8 cm/s, so it can be treated like a nonrelativistic particle. The mass of quasiparticle can be substantially different than that of the free electron.



Phonon: This is a collective excitation, corresponding to coherent motion of all the atoms in the solid. It is quantized lattice vibration with a typical energy scale $\hbar\omega \sim 0.1eV$

Exciton: bound state of electron and hole with binding energy $10eV$

Plasmon: longitudinal charge oscillations of the entire electron gas relative to the lattice of ions due to the long-range nature of the Coulomb interaction

Polaron: a quasiparticle, like electron, whose motion in polar crystals distorts the lattice of positive and negative ions around it – polaron has different mass than the electron.

Magnon: collective excitation of the spin degrees of freedom on the crystalline lattice with an energy scale $\hbar\omega \sim 0.001 - 0.1eV$

Hole: a quasiparticle, like the electron, but of opposite charge; it corresponds to the absence of electron for a single-particle state which lies below the Fermi level. The notion of a hole is particularly convenient when the reference state consists of a quasiparticle states that are fully occupied and are separated by an energy gap from the unoccupied state.

Experimental Probes of Condensed Matter Phases and Quasiparticle Dynamics

- **Scattering:** Send neutrons or X-rays into the system with prescribed energy and momentum; measure the energy and momentum of the outgoing neutrons or X-rays.
- **NMR:** Apply static magnetic field B and measure absorption and emission of magnetic radiation at frequencies of the order of $\omega_c = \frac{geB}{m}$.
- **Thermodynamics:** Measure the response of macroscopic variables (energy, volume, etc.) to variations of the temperature, pressure, etc.
- **Transport:** Set up a potential $\nabla\varphi$ or thermal gradient ∇T and measure the electrical or heat current. The gradients can be held constant or made to oscillate at finite frequency.

Quantum Hamiltonian of Condensed Matter Physics

"The general theory of quantum mechanics is now almost complete. The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

P. A. M. Dirac 1929

$$\hat{H} = \underbrace{\sum_{n=1}^{N_N} \frac{\mathbf{P}_n^2}{2M_n}}_{T_N:\ \text{motion of nuclei}} + \underbrace{\frac{e^2}{2}\sum_{n\neq m=1}^{N_N} \frac{Z_n Z_m}{|\mathbf{R}_n - \mathbf{R}_m|}}_{V_{N-N}:\ \text{interaction between nuclei}}$$

Quantization

$$\mathbf{p} \equiv -i\hbar\frac{\partial}{\partial \mathbf{r}}, \quad \mathbf{P} \equiv -i\hbar\frac{\partial}{\partial \mathbf{R}}$$

$$+ \underbrace{\sum_{i=1}^{N_e} \frac{\mathbf{p}_i^2}{2M_i}}_{T_e:\ \text{motion of electrons}} + \underbrace{\frac{e^2}{2}\sum_{i\neq j=1}^{N_e} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}}_{V_{e-e}:\ \text{interaction between electrons}} - \underbrace{e^2\sum_{n=1}^{N_N}\sum_{i=1}^{N_e} \frac{Z_n}{|\mathbf{R}_n - \mathbf{r}_i|}}_{V_{e-N}:\ \text{interaction between electrons and nuclei}}$$

Complexity in Solid State Hamiltonian

Even for chemist, the task of solving the Schrödinger equation for modest multi-electron atoms proves insurmountable without bold approximations.

The problem facing condensed matter physicist is qualitatively more severe:

$$N_N \sim N_e \sim 10^{23}$$

Energy scales: $10^{-2}\,\text{eV} - 10^{4}\,\text{eV}$

CM Theorist is entrapped in the "thermodynamic limit"

The Way Out: Separate Length and Energy Scales

- Energy: $\omega\ ,\ T\ < 1\,eV$
- Time: $\Delta\tau \sim \frac{\hbar}{1eV} \sim \frac{\hbar}{10^{-19}\,J} \sim 10^{-15}\,s$
- Length: $|\,x_i - x_j\,|,\ q^{-1} \gg 1\ \text{Å}$

forget about atom formation + forget about crystal formation

+ Born-Oppenheimer approximation for $\frac{m_e}{m_N} \ll 1$

$$\Downarrow$$

$$\hat{H}_{\text{electronic}} = \hat{T}_e + \hat{V}_{e-I} + \hat{V}_{e-e},\quad \hat{V}_{e-I}(\mathbf{r}+\mathbf{r}_n) = \hat{V}_{e-I}(\mathbf{r}),\ \mathbf{r}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

"Non-Interacting" Electrons in Solids: Band Structure Calculations

- In band structure calculations electron-electron interaction is approximated in such a way that the resulting problem becomes an effective single-particle quantum mechanical problem …

$$\hat{H}_{\text{IE,H,LDA}}(\mathbf{r})\phi_{\mathbf{k}b}^{\text{IE,H,LDA}}(\mathbf{r}) = \varepsilon^{\text{IE,H,LDA}}(\mathbf{k},b)\phi_{\mathbf{k}b}^{\text{IE,H,LDA}}(\mathbf{r})$$

$$\hat{H}_{\text{electronic}} = \hat{T}_e + \hat{V}_{e-I} + \hat{V}_{e-e}$$

$$\hat{H}_{\text{IE}} = \hat{T}_e + \hat{V}_{e-I} = \sum_{i=1}^{N_e} H_{\text{IE}}(\mathbf{r}_i)$$

$$\hat{H}_{\text{Hartree}} = \hat{T}_e + \hat{V}_{e-I} + e^2 \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, \; n(\mathbf{r}) = \sum_{\varepsilon^H(\mathbf{k},b)\le E_F} |\phi_{\mathbf{k}b}^{\text{H}}(\mathbf{r})|^2 = n(\mathbf{r}+\mathbf{r}_n)$$

$$\hat{H}_{\text{LDA}} = \hat{H}_{\text{IE}}(\mathbf{r}) + e^2 \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \frac{\delta E_{\text{xc}}^{\text{LDA}}[n_e]}{\delta n(\mathbf{r})}, \quad E_{\text{xc}}^{\text{LDA}}[n_e] = \int d\mathbf{r}\, n(\mathbf{r}) e_{\text{xc}}^{\text{LDA}}(n(\mathbf{r}))$$

From Many-Body Problem to Density Functional Theory (and its LDA approximation)

- "Classical" Schrödinger equation approach:

$$V(\mathbf{r}) \overset{SE}{\Rightarrow} \Psi(\mathbf{r}_1,\ldots,\mathbf{r}_{N_e}) \overset{\langle\Psi|\ldots|\Psi\rangle}{\Rightarrow} \text{average of observables}$$

- Example: **Particle density**

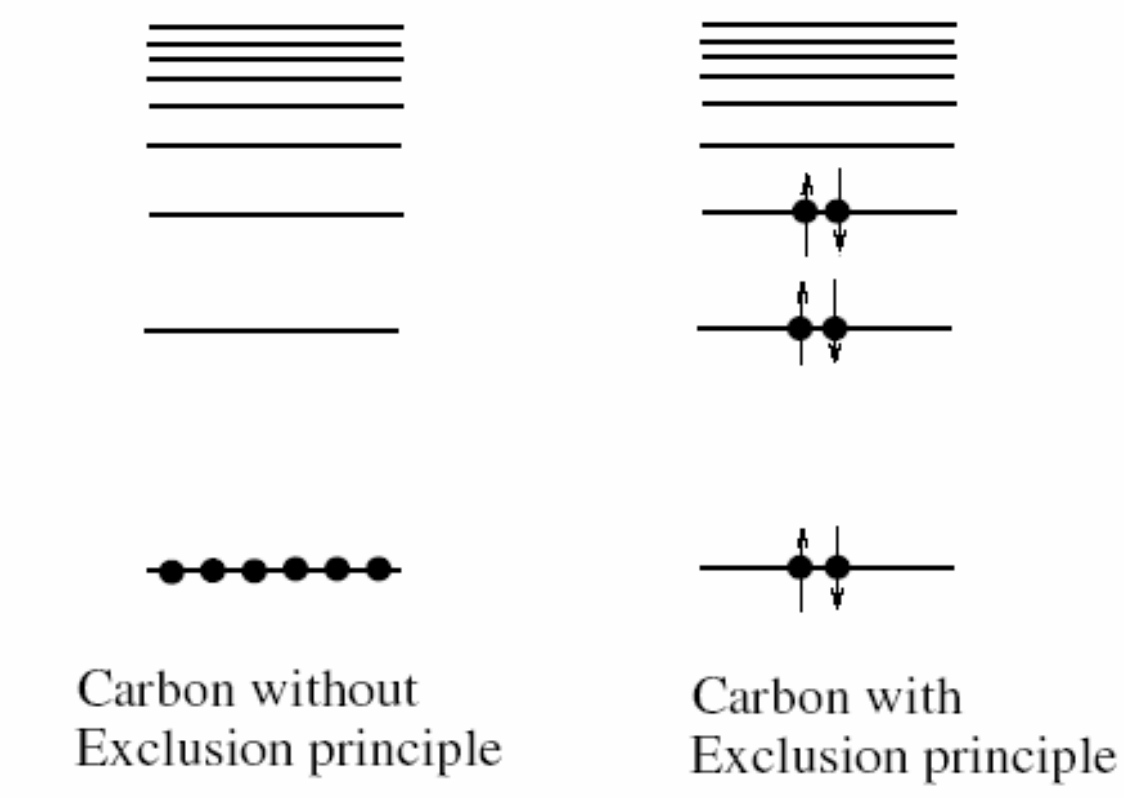
$$n(\mathbf{r}) = N\int d\mathbf{r}_2 \int d\mathbf{r}_3 \cdots \int d\mathbf{r}_N \Psi^*(\mathbf{r},\ldots,\mathbf{r}_{N_e})\Psi(\mathbf{r},\ldots,\mathbf{r}_{N_e})$$

- DFT approach (Kohn-Hohenberg):

$$n_0(\mathbf{r}) \Rightarrow \Psi_0(\mathbf{r}_1,\ldots,\mathbf{r}_{N_e}) \Rightarrow V(\mathbf{r})$$

$$\Psi_0(\mathbf{r}_1,\ldots,\mathbf{r}_{N_e}) \equiv \Psi_0[n_0(\mathbf{r})]$$

Pauli Exclusion Principle for Atoms



Carbon without Exclusion principle

Carbon with Exclusion principle

Without the exclusion principle all electrons would occupy the same atomic orbital.
There would be no chemistry, no life!

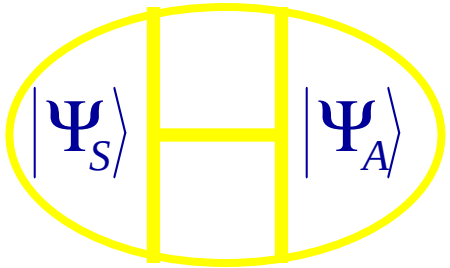
Many-Body Wave Function of Fermions

"It is with a heavy heart, I have decided that Fermi-Dirac, and not Einstein is the correct statistics, and I have decided to write a short note on paramagnetism." W. Pauli in a letter to Schrödinger (1925).

- All electrons in the Universe are **identical** → two physical situations that differ only by interchange of identical particles are indistinguishable!

$$P_{ij}\Psi(x_1,\ldots,x_i,\ldots,x_j,\ldots,x_n) = P_{ij}\Psi(x_1,\ldots,x_j,\ldots,x_i,\ldots,x_n)$$

$$\hat{P}_{ij}\hat{H} = \hat{H}\hat{P}_{ij} \leftarrow \langle\Psi|\hat{A}|\Psi\rangle = \langle\Psi|\hat{P}_{ij}^{\dagger}\hat{A}\hat{P}|\Psi\rangle \Leftrightarrow \hat{P}_{ij}\hat{A} = \hat{A}\hat{P}$$



$$\hat{P}_\alpha|\Psi_S\rangle = |\Psi_S\rangle, \quad \hat{P}_\alpha|\Psi_A\rangle = \begin{cases} +|\Psi_A\rangle, \hat{P}_\alpha \text{ is even} \\ -|\Psi_A\rangle, \hat{P}_\alpha \text{ is odd} \end{cases}$$

$$\hat{P}_\alpha\hat{A}|\Psi\rangle = \hat{A}|\Psi\rangle, \quad \hat{A} = \frac{1}{N!}\sum_\alpha \varepsilon_\alpha \hat{P}_\alpha$$

Pauli Exclusion Principle for Hartree-Fock or Kohn-Scham Quasiparticles

"There is no one fact in the physical world which has greater impact on the way things are, than the Pauli exclusion principle." I. Duck and E. C. G. Sudarshan, "Pauli and the Spin-Statistics Theorem" (World Scientific, Singapore, 1998).

- Two identical fermions **cannot occupy** the same quantum-mechanical state:

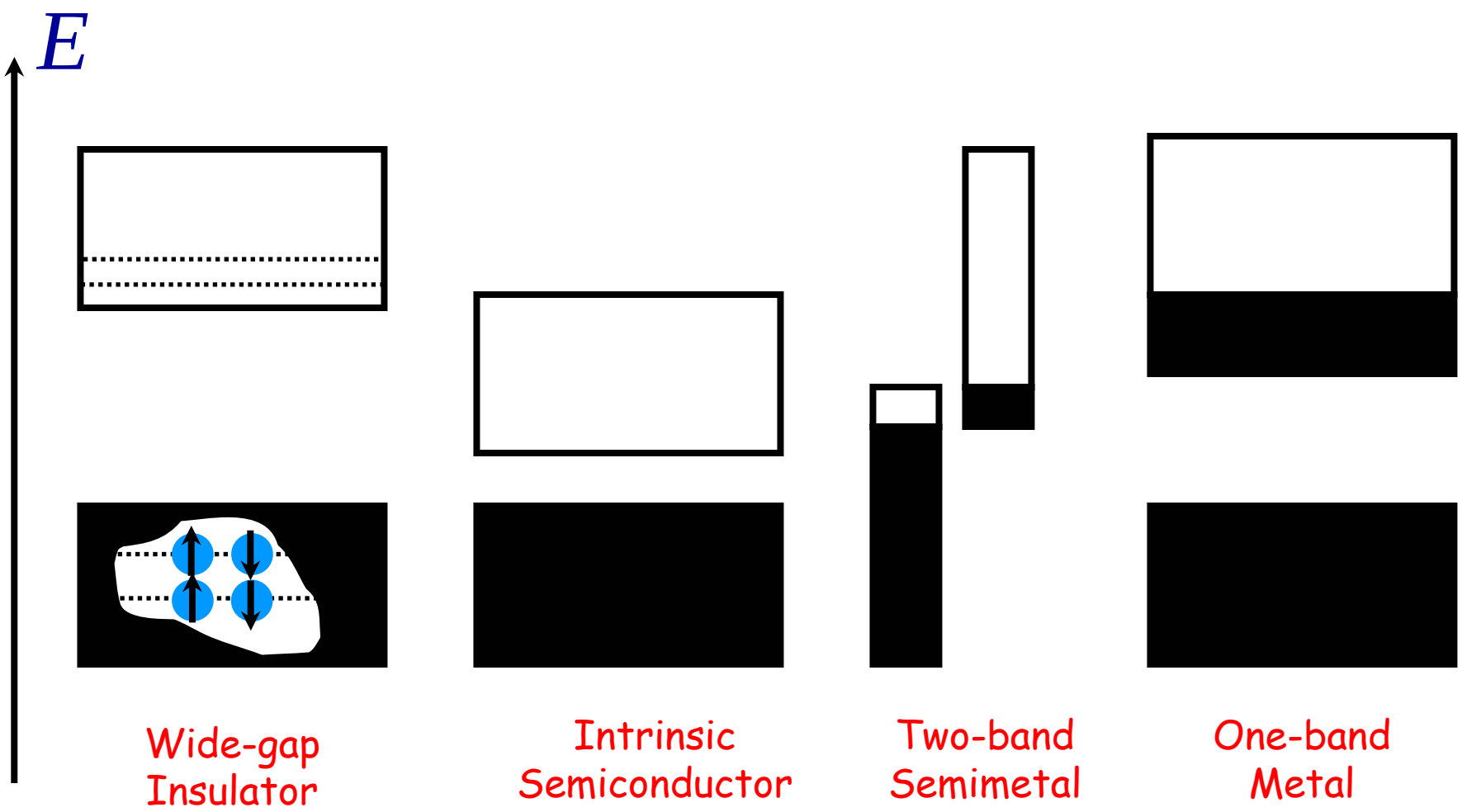
$$\hat{H} = \hat{h}_1 + \hat{h}_2 + \ldots + \hat{h}_N$$

$$\hat{h}_i \left| \phi_i \right\rangle = e_i \left| \phi_i \right\rangle \Rightarrow \hat{H} \left| \Phi_{1,2,\ldots,N_e} \right\rangle = E_{1,2,\ldots,N_e} \left| \Phi_{1,2,\ldots,N_e} \right\rangle$$

$$E_{1,2,\ldots,N_e} = e_1 + e_2 + \ldots + e_{N_e}$$

$$\left| \Phi_{1,2,\ldots,N_e} \right\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(1) & \cdots & \phi_{N_e}(1) \\ \vdots & \ddots & \vdots \\ \phi_1(N_e) & \cdots & \phi_{N_e}(N_e) \end{vmatrix} \Rightarrow n_{\mathbf{k}\sigma} = \frac{1}{e^{(\varepsilon_{\mathbf{k}\sigma} - \mu)/k_B T} + 1}$$

Energy Bands and Rigid Band Filling



Electron-Electron Interactions in Metals

❑**Bloch theory of electrons in metals:** completely independent particles (e.g., even more sophisticated Hartree-Fock fails badly because dynamic correlations cancel miraculously exchange effects).

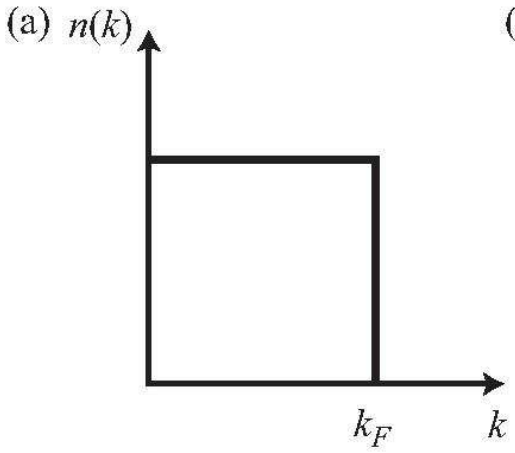
❑Why is long-range **strong** (of the order of kinetic energy) Coulomb interaction marginal in metals?

1. In system with itinerant electrons, Coulomb interaction is very effectively screened on the length scale of k_F^{-1} .
2. In the presence of Fermi surface the scattering rate between electrons with energy $E_F + \hbar\omega$ vanishes proportional to ω^2 since the Pauli principle strongly reduces the number of scattering channels that are compatible with energy and momentum conservations – Landau "quasielectrons" live very long!

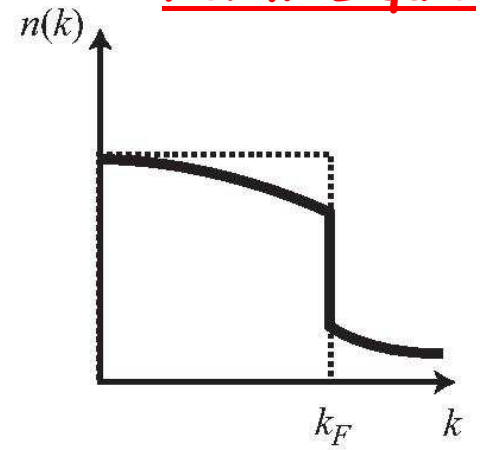
DFT (and LDA) only describes an equivalent one-electron substitute system with the same ground-state energy and electron density. Altough we may expect that the ground-state properties are reasonably described, the wave functions and excitation energies (band structures) may be used only if the prerequisites of the Landau Fermi Liquid theory are fulfilled.

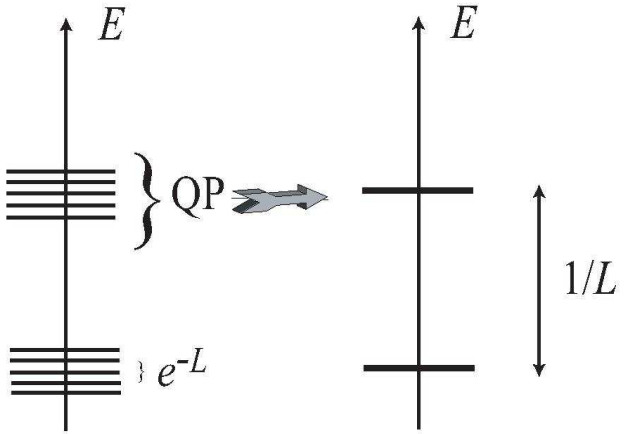
Real Free Electrons vs. Landau Quasielectrons

Fermi Gas

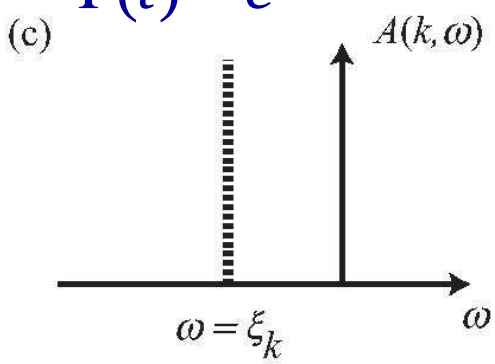


Fermi Liquid

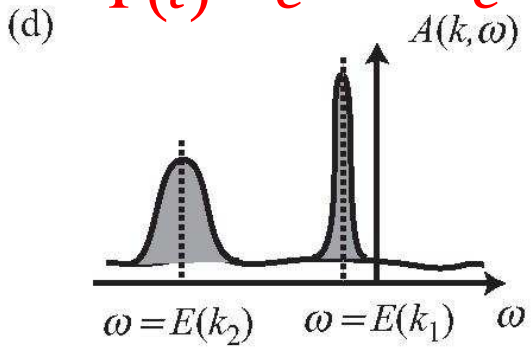




$$\Psi(t) \sim e^{-iE(k)t/\hbar}$$



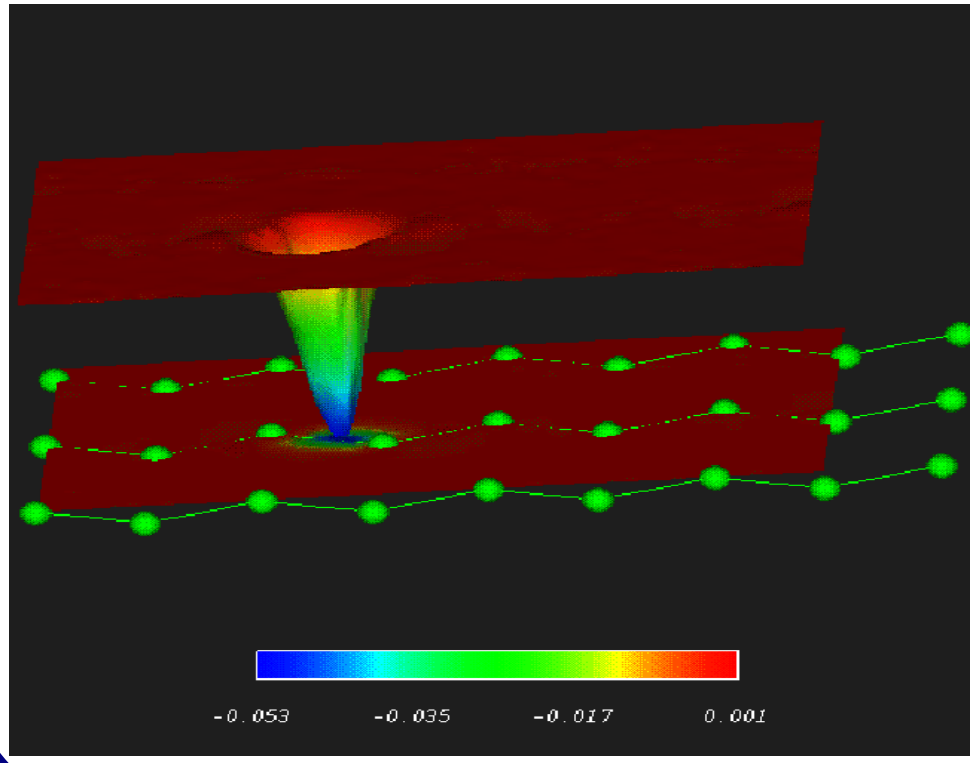
$$\Psi(t) \sim e^{-iE(k)t/\hbar} e^{-t/\tau}$$

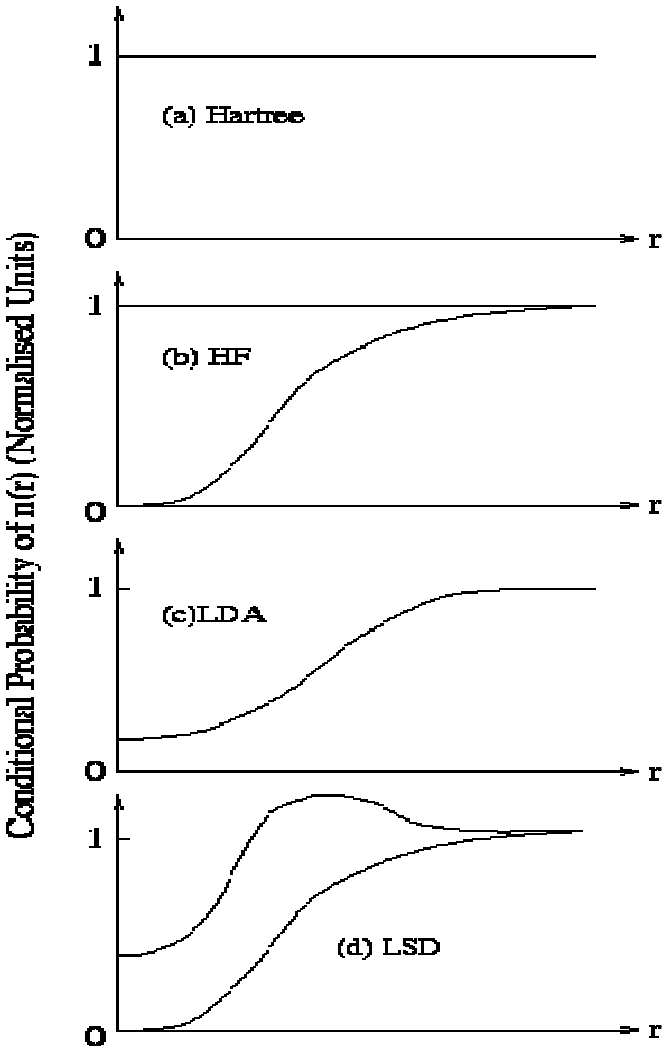


A quasiparticle state is in fact made of very large number of exact eigenstatates of the interacting system. The separation of these states is exponentially small in the system size and thus irrelevant physically for reasonable systems. The cluster of all these states form the quasiparticle with its average enery and lifetime (= inverse of the energy broadening).

Exchange-Correlation Hole

- Surrounding every electron in a solid there's an exclusion zone, called the exchange-correlation hole, into which other electrons rarely venture. This is the hole around an electron near the centre of a bond in silicon.





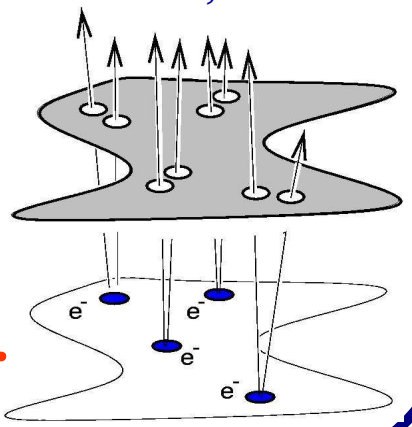
From Weakly to Strongly Correlated Electrons

- Exchange and Correlation in 3D gas of noninteracting fermions:

$$g_{\sigma,\sigma}(\mathbf{r},\mathbf{r}') = -\left[\frac{3n}{2}\frac{\sin x - x\cos x}{x^3}\right]^2$$

$$g_{\sigma,-\sigma}(\mathbf{r},\mathbf{r}') = 0, \quad x = k_F\,|\mathbf{r}-\mathbf{r}'|$$

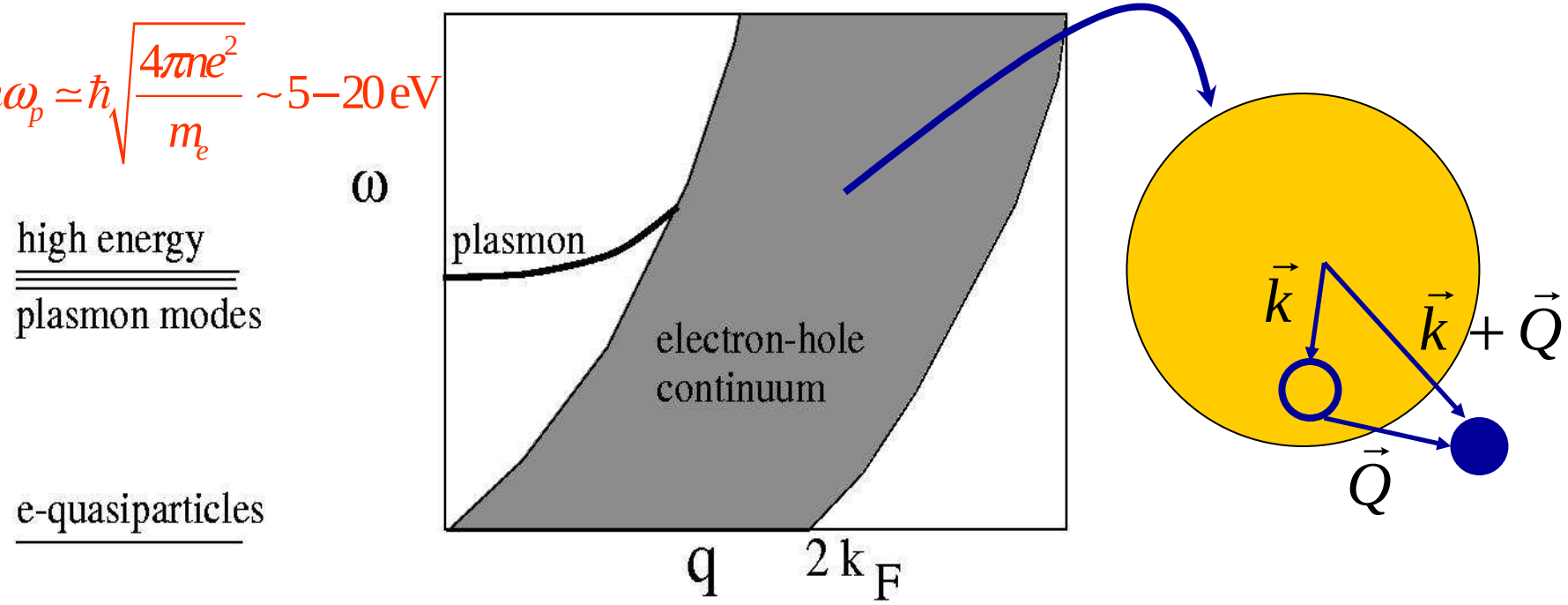
- Correlated Electron System: $g_{\sigma,-\sigma}(\mathbf{r},\mathbf{r}') \neq 0$
- Strongly Correlated Electron System: $g_{\sigma,\sigma}(\mathbf{r},\mathbf{r}') \sim g_{\sigma,-\sigma}(\mathbf{r},\mathbf{r}')$
- Example of novel strongly correlated matter



Fractional Quantum Hall Effect

Survival of Long-Range Coulomb Interaction: Collective Excitations

$$\hbar\omega_p \simeq \hbar\sqrt{\frac{4\pi n e^2}{m_e}} \sim 5-20\,\text{eV}$$



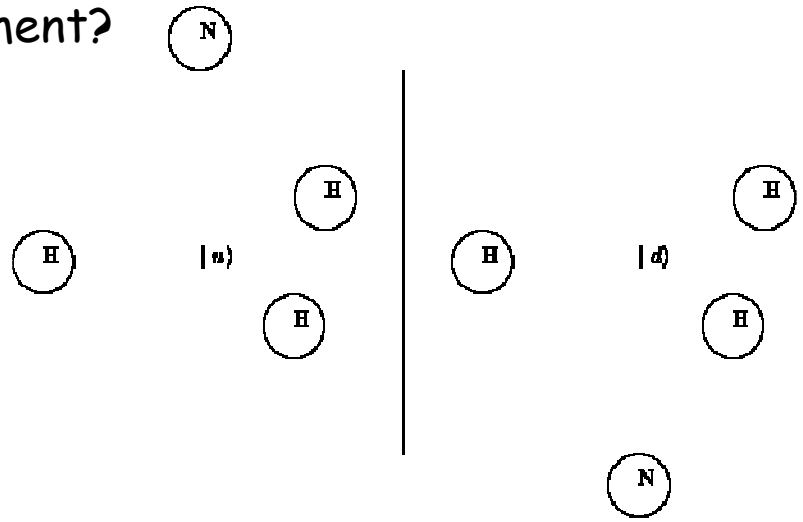
- Bohm and Pines (1953): separate strongly interacting gas into two independent sets of excitations (progenitor of the idea of renormalization!)

high energy → plasmon
low energy → electron-hole pairs

Breaking the Symmetry

QUESTION: In QM we learn that the ground state must have the symmetry of the Hamiltonian - so there can't be a dipole moment (interactions between ions and electrons have no preferred direction in space). On the other hand, ammonia molecule obviously has dipole moment?

RESOLUTION: The ammonia molecule ground state is a superposition of states, so as to recover the symmetry of the Hamiltonian. However, at short time-scale molecule can be trapped in one of the states (due to large potential barrier for tunneling between the states), and we measure non-zero dipole moment.



QUESTION: What about larger molecules (> 10 atoms) which have definite three-dimensional structures which break the symmetry of the Hamiltonian?

RESOLUTION: We cannot understand the structure of molecules starting from Quantum Mechanics of elementary particles - we need additional theoretical ideas (**emergent phenomena**)!

Broken Symmetries and Phases of Matter

- Phases of matter often exhibit much less symmetry than underlying microscopic equations.
- **Example:** Water exhibits full translational and rotational symmetry of Newton's or Schrödinger's equations; Ice, however, is only invariant under the discrete translational and rotational group of its crystal lattice → translational and rotational symmetry of the microscopic equations have been spontaneously broken!
- Order Parameter Paradigm (L. D. Landau, 1940s): Development of phases in a material can be described by the emergence of an "order parameter" (which fluctuates strongly at the critical point):

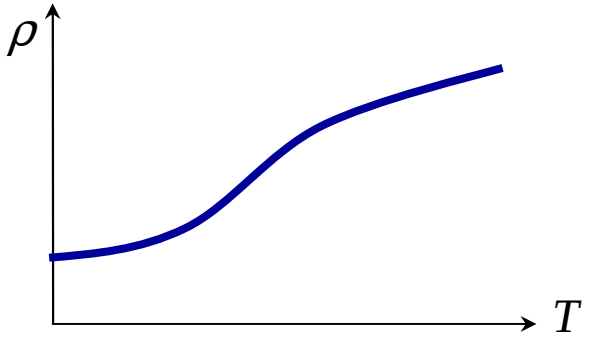
$$M, \quad \Psi(\mathbf{r}) = \sqrt{\rho_s}\, e^{i\varphi}, \quad \rho_{\text{typical}}(\omega, \mathbf{r})$$

Crystalline Hard Condensed Matter Phases

- Positive ions arrange to break translational and rotational symmetry – it is energetically favorable to break the symmetry in the same way in different parts of the system → because of broken symmetries the solids are rigid (i.e., **solid**) and exhibit **long-range order**.
- In crystalline solids discrete subgroups of the translational and rotational group are preserved

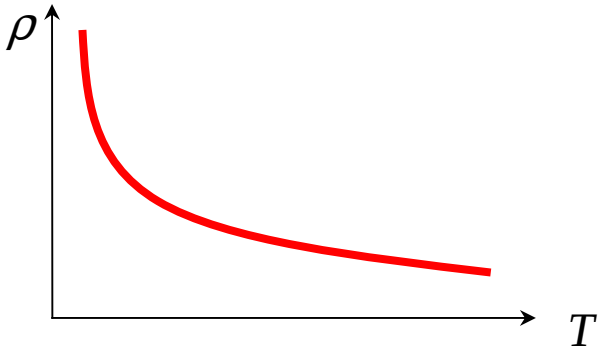
metals

$$T \to 0 \Rightarrow \sigma \neq 0$$



insulators

$$T \to 0 \Rightarrow \sigma \to 0$$



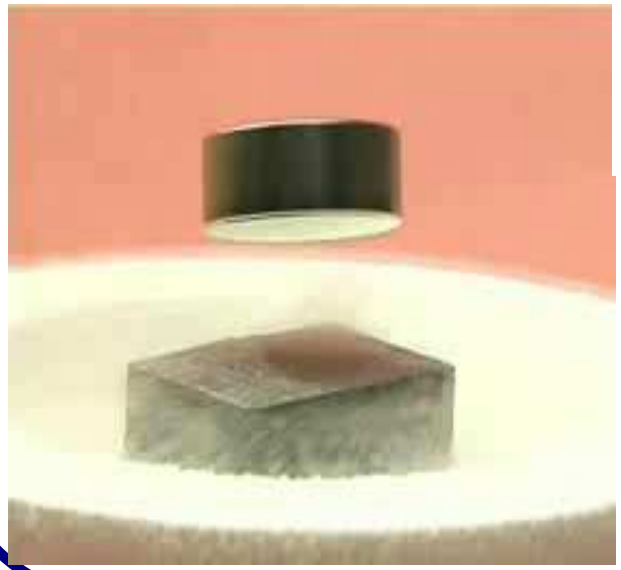
Broken Symmetry States of Metals

Broken U(1)

Superconductors

$$T < T_c \Rightarrow \sigma \to \infty$$

+ Meissner effect

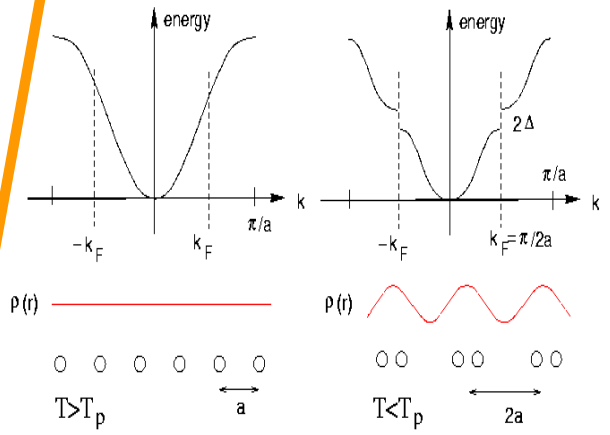


Above a critical temperature, T_c, superconductors are typically normal metals, but not very good conductors. Below T_c, resistivity is zero and the material is a perfect diamagnet. Pure metals, like Pb, Ta, Sn are superconductors, while Cu, Ag, or Au are not.

Material	T_c (K)	Year
Hg	4.1	1911
Pb	7.2	1913
Nb	9.2	1930
$NbN_{0.96}$	15.2	1950
Nb_3Sn	18.1	1954
$Nb_3(Al_{3/4}Ge_{1/4})$	20-21	1966
Nb_3Ga	20.3	1971
Nb_3Ge	23.2	1973
$Ba_xLa_{5-x}Cu_5O_y$	30-35	1986
$YBa_2Cu_3O_{7-\delta}$	95	1987
$Bi_2Sr_2Ca_2Cu_3O_{10}$	110	1988
$Tl_2Ba_2Ca_2Cu_3O_{10}$	125	1988
$HgBa_2Ca_2Cu_3O_{8+\delta}$	133	1993
$HgBa_2Ca_2Cu_3O_{8+\delta}$ at 25 GPa	155	1993
$HgBa_2Ca_2Cu_3O_{8+\delta}$ at 30 GPa	164	1994

Highly Anisotropic

Charge-Density Wave



Spin-Density Wave

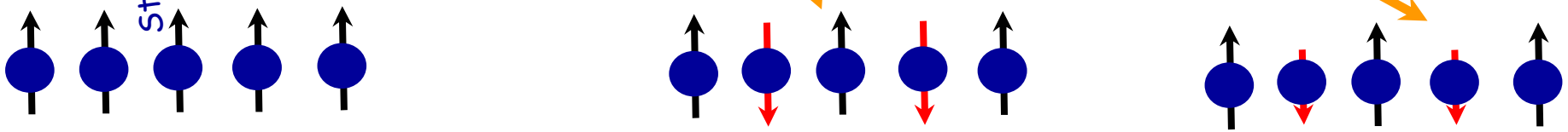
Broken Spin Rotational Symmetry of Metals and Insulators

Stoner Itinerant Electron Magnetism

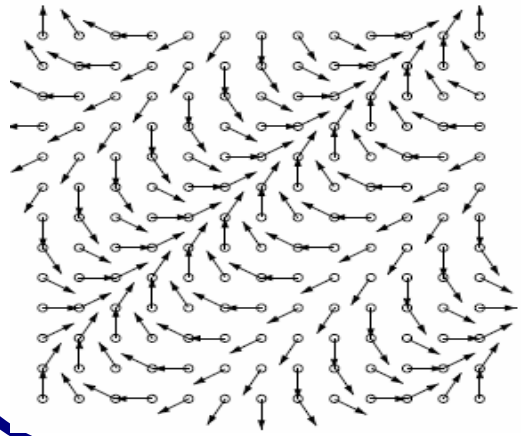
Heisenberg Magnets

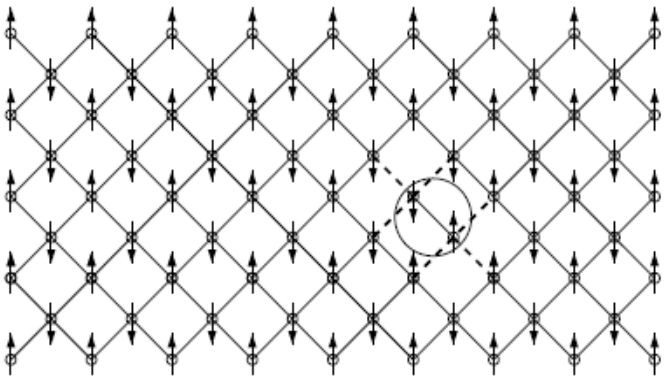
Antiferromagnets

Ferrimagnets



Ground state symmetry determines the properties of collective excitations – Spin waves (Magnons)

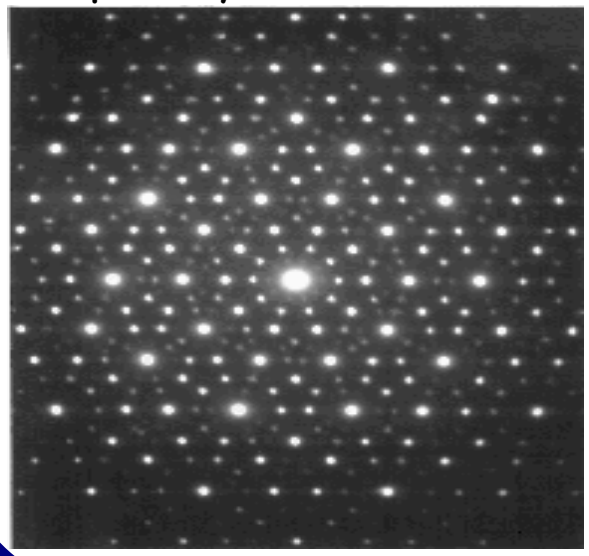


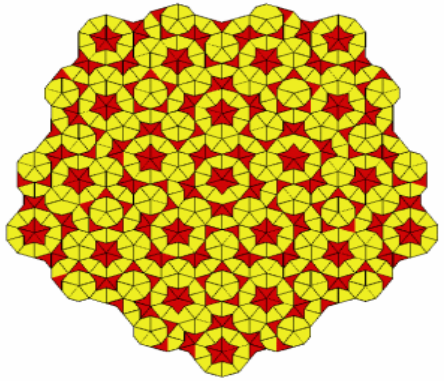


Non-Crystalline Hard CM Phases: Quasicrystals

❑Among the most well known consequences of periodicity is the fact that the only rotational symmetries that are possible are 2-, 3-, 4-, and 6-fold rotations $\Rightarrow$ Five-fold rotations (and any n-fold rotation for $n>6$) are incompatible with periodicity.

❑Quasicrystals =quasiperiodic crystals [D. Shechtman, I. Blech, D. Gratias, and J.W. Cahn, "Metalic phase with with long-range orientational order and no translational symmetry," Phys. Rev. Lett. **53**, 1951 (1984)]: Translational order completely broken; rotational symmetry broken to 5-fold discrete subgroup.

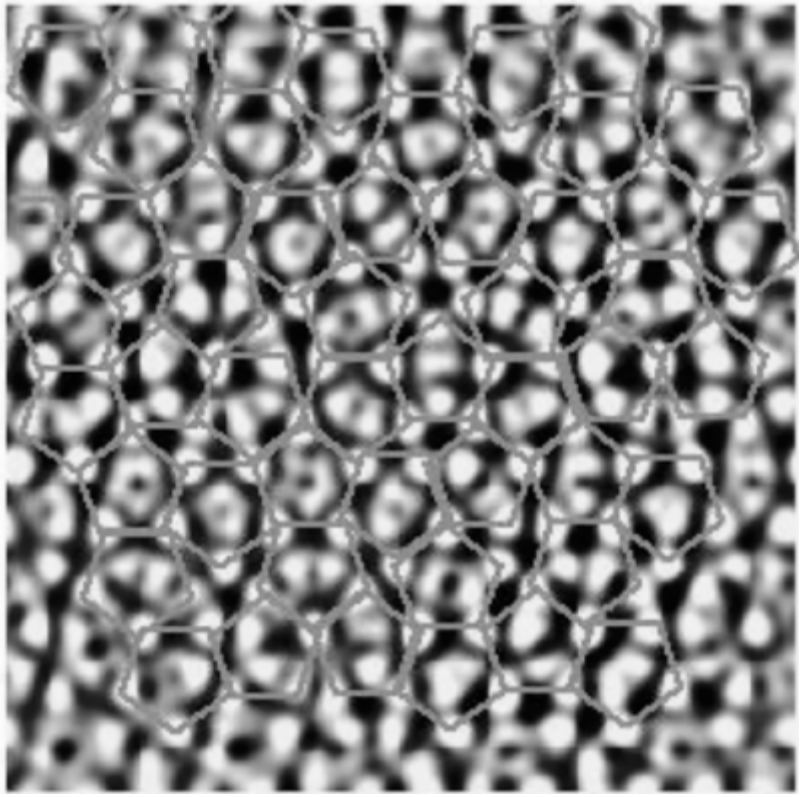




❑Penrose tile is a 2D example of a quasicrystal: There is perfect long-range order and no periodicity in the normal sense.

❑Quasicrystals posses unique physical properties: even though they are all alloys of two or three metals they are very poor conductors of electricity and of heat.

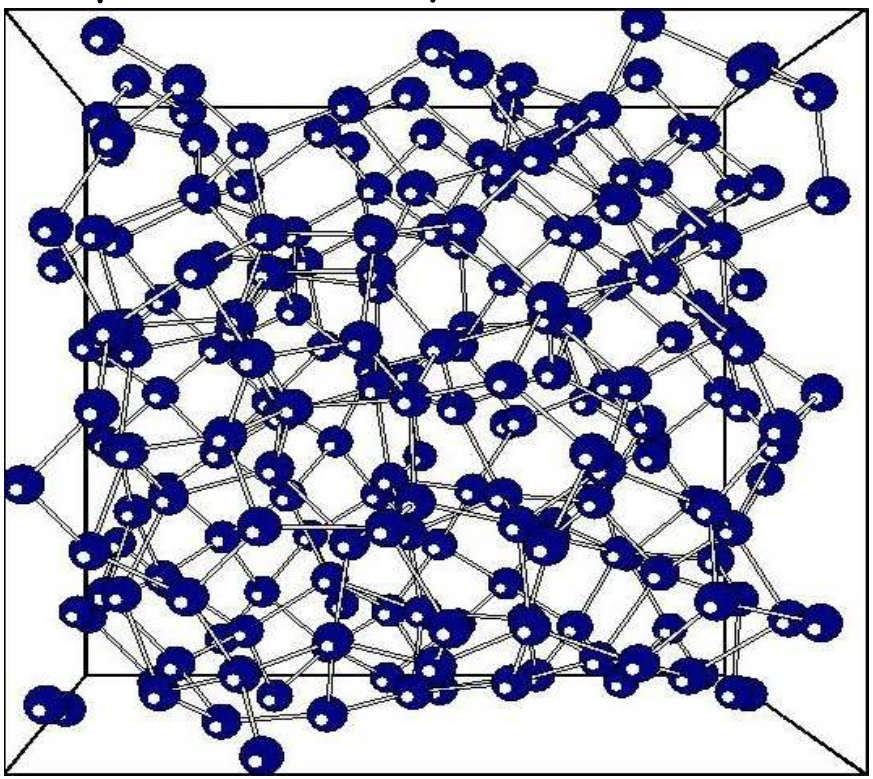
Imaging Quasicrystals via STM



Scanning tunneling microscope image of a 10 nm^2 quasicrystal of AlPdMn with a Penrose tiling overlaid [Ledieu et al., Phys. Rev. B **66**, 184207 (2002)]

Non-Crystalline Hard CM Phases: Glasses

❑Glasses: rigid but random arrangement of atoms; in fact, they are "non-equilibrium phase" – effectively they look more like a frozen "snapshot" of a liquid.

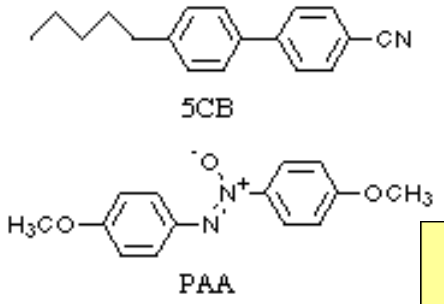


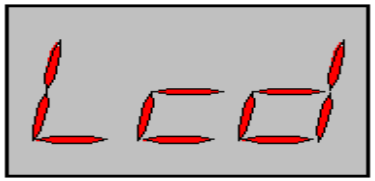
❑**Example:** Amorphous Silicon.

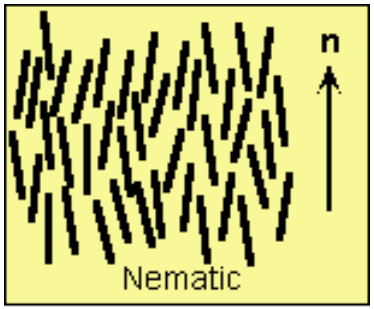
❑The structural glassy materials arise when a liquid is cooled to an amorphous solid fast enough to prevent crystallization, which would otherwise occur if the time had been sufficient for the sample to reach true equilibrium at each temperature. Thus, "frozen" **supercooled liquids** (which have enormous viscosity that prevents any large-scale flow on human time scales) form a glassy state of matter that is substantially different from crystals: it is disordered and only metastable thermodynamically. Moreover, the essential physics of nonequilibrium glassy state (leading to rapid increase in response time, and phenomena like aging, rejuvenation, memory effects, …) is the prototype of **a slow nonexponential relaxation** found in diverse physical systems: spin glasses, disordered insulators (Coulomb glass), magnets, superconductors, proteins, colloidal suspensions, granular assemblies, …

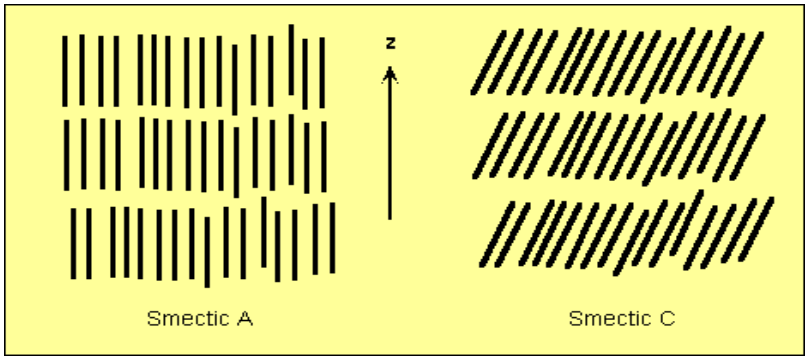
Soft Condensed Matter Phases

- Liquids (full translational and rotational group preserved) vs. Solids (preserve only a discrete subgroups).
- Liquid crystalline phase – translational and rotational symmetry is broken to a combination of discrete and continuous subgroups:









- Polymers – extremely long molecules that can exist in solution or a chemical reaction can take place which cross-links them, thereby forming a gel.

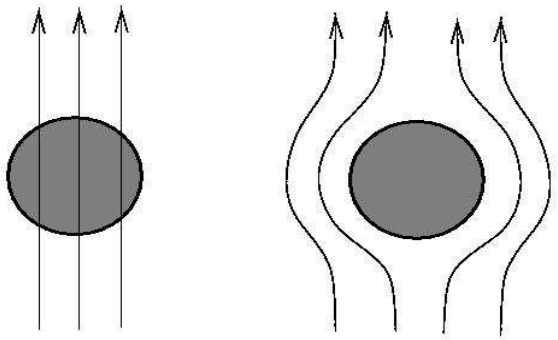
Broken Symmetries and Rigidity

- Phase of a Cooper pair develops a rigidity →it costs energy to bend phase → superflow of particles is directly proportional to gradient of phase:

$$U(x) \sim \frac{1}{2}\rho_s \left[\nabla \phi(x)\right]^2 \Rightarrow \; j_s = \rho_s \nabla \phi_s$$

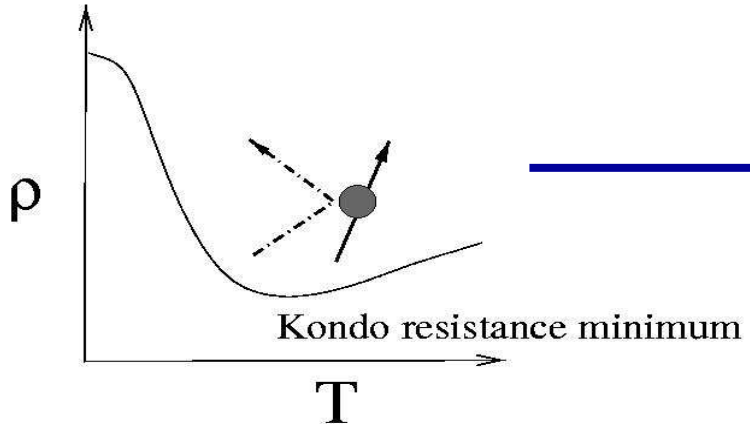
Phase	Broken Symmetry	Rigidity/Superflow
crystal	translation	Momentum (sheer stress)
superfluid	gauge	matter
superconductivity	EM gauge	charge
F- and AF-magnetism	spin rotation	spin (x-y magnets only)
nematic liquid crystal	rotation	angular momentum
?	Time translation	Energy?

High Energy Physics: Lessons from Low Energy Experiments



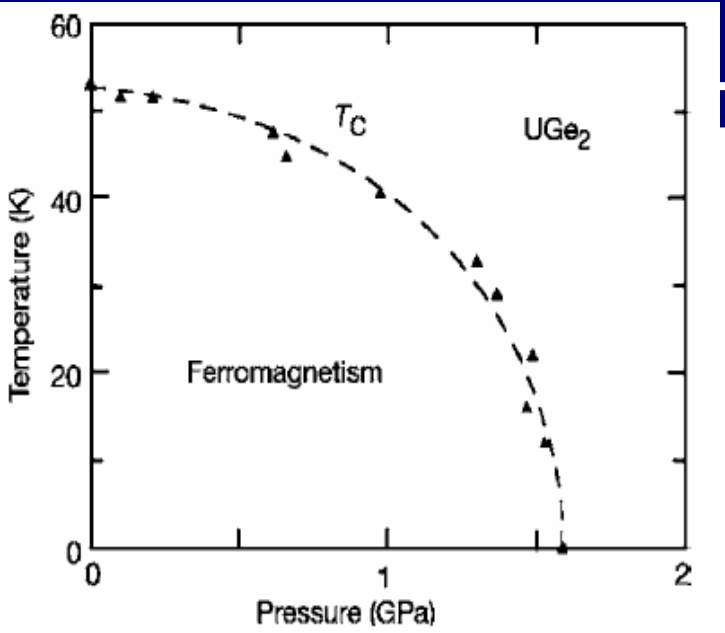
Meissner Effect

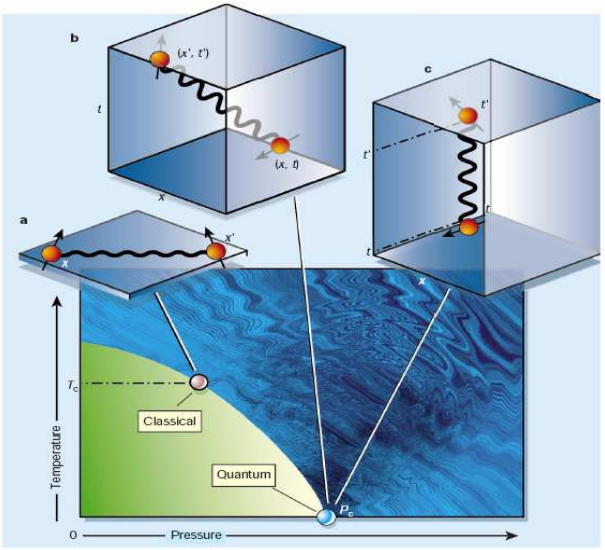
Anderson Higgs Mechanism

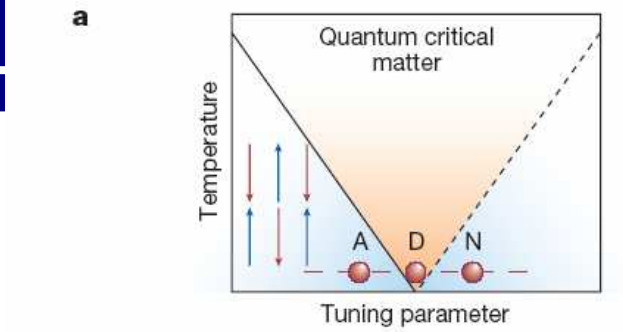


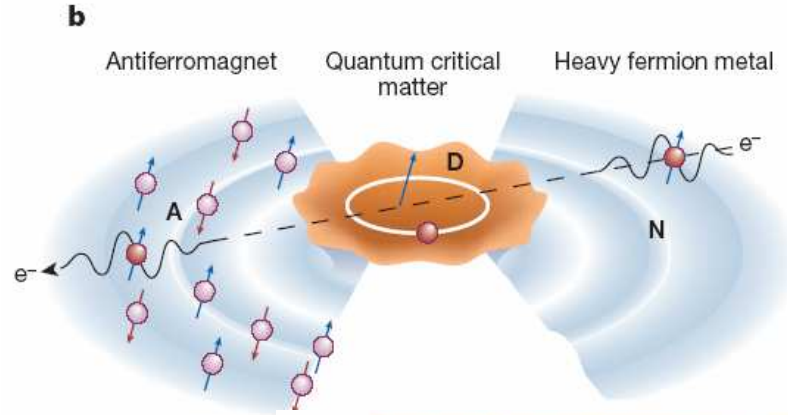
Asymptotic Freedom in the Physics of Quark Confinement

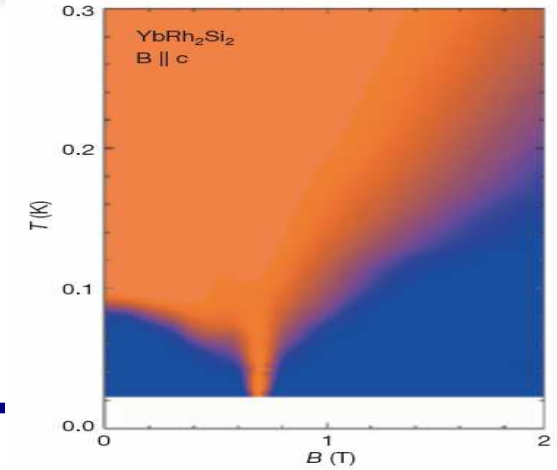
Quantum Critical Matter



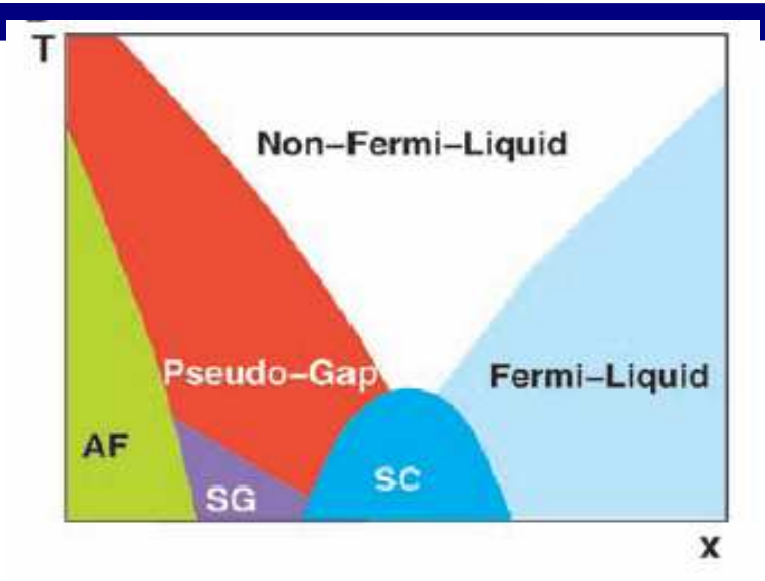


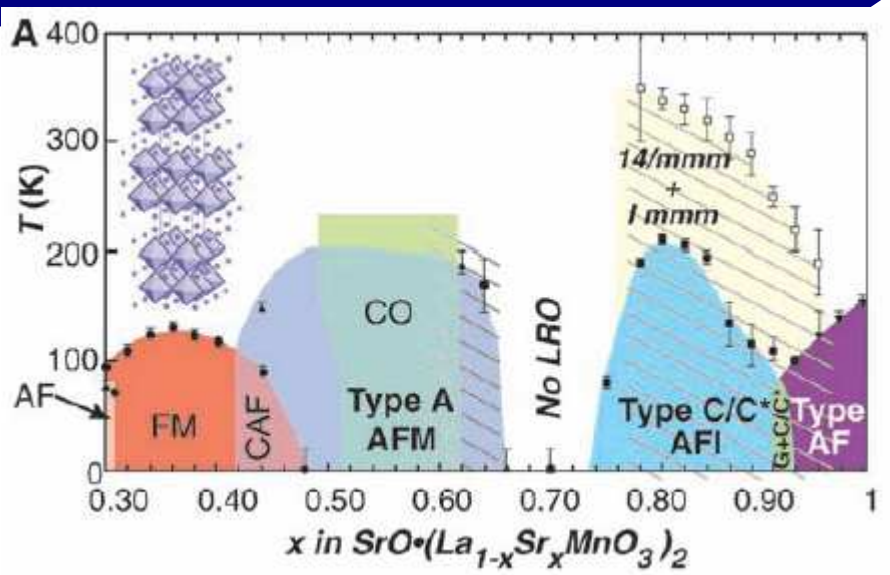


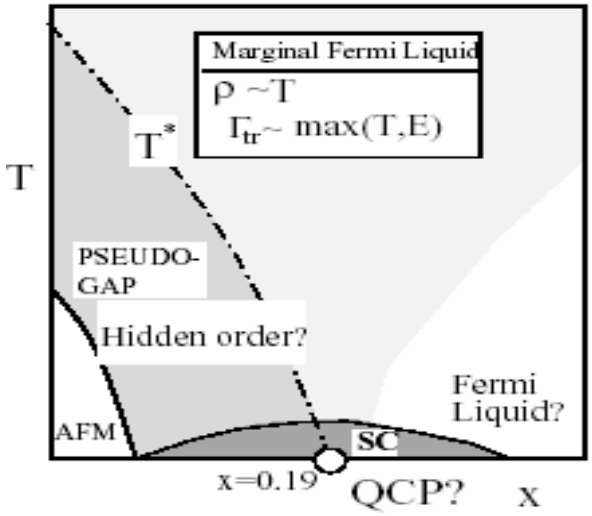


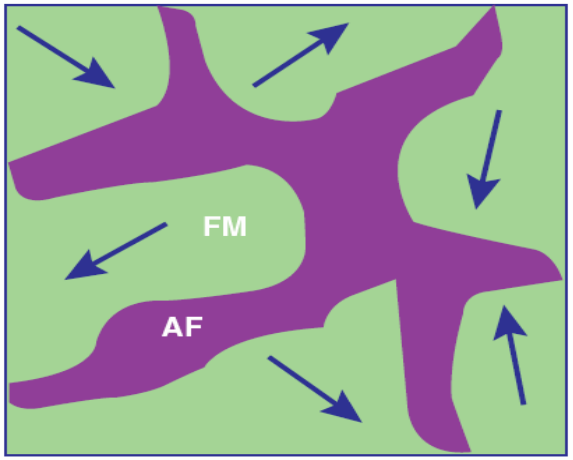


Complexity and Quantum Criticality in Transition Metal Oxides **Strongly Correlated** Materials









Complexity and Diversity of Crystalline Phases