

Center for
Electronic Correlations and Magnetism
University of Augsburg

Theory of correlated fermionic condensed matter

5. Common concepts in correlated Fermi systems

XIV. Training Course in the Physics of Strongly Correlated Systems
Salerno, October 9, 2009

Dieter Vollhardt

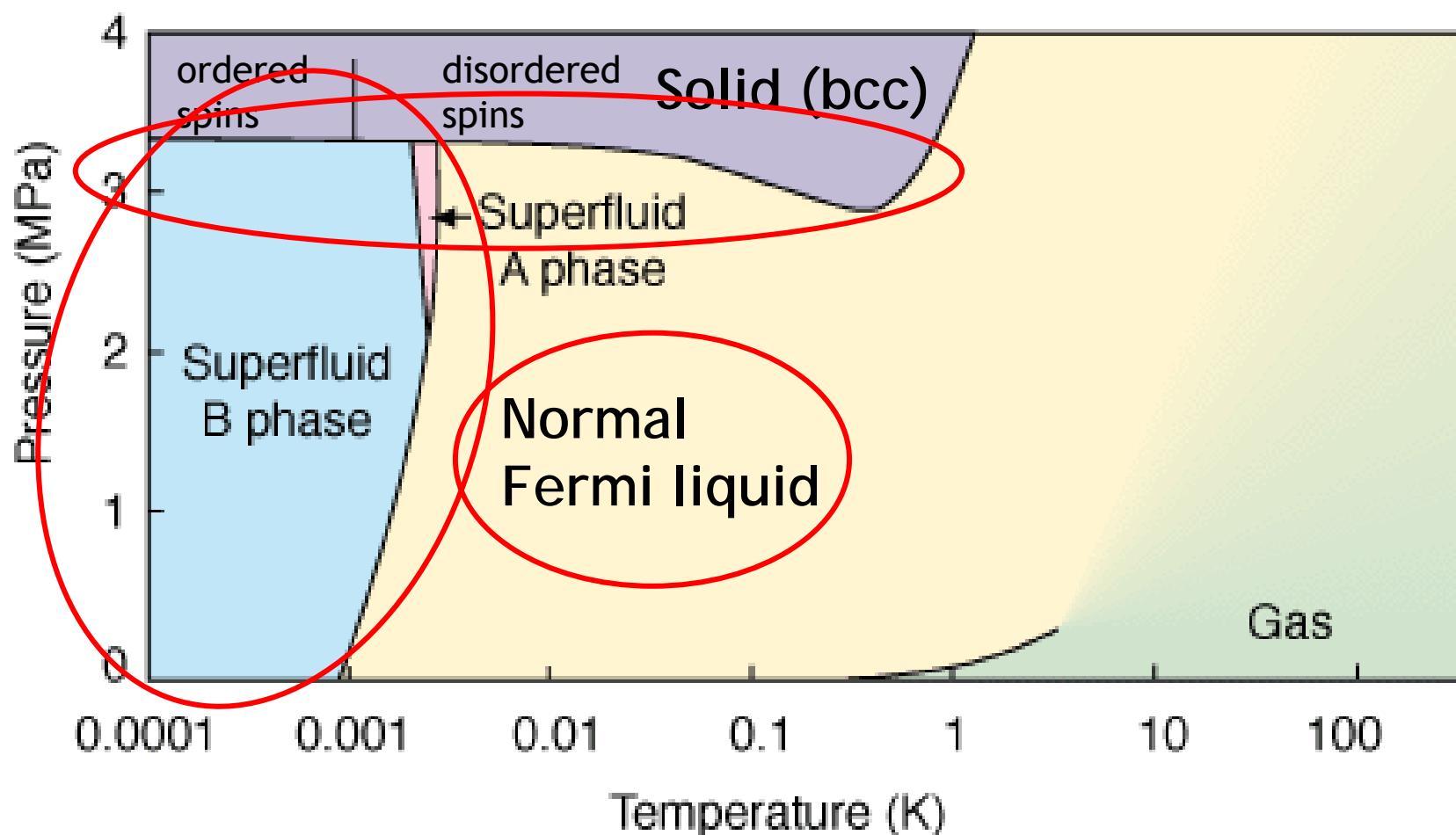
Supported by Deutsche Forschungsgemeinschaft through SFB 484

Outline:

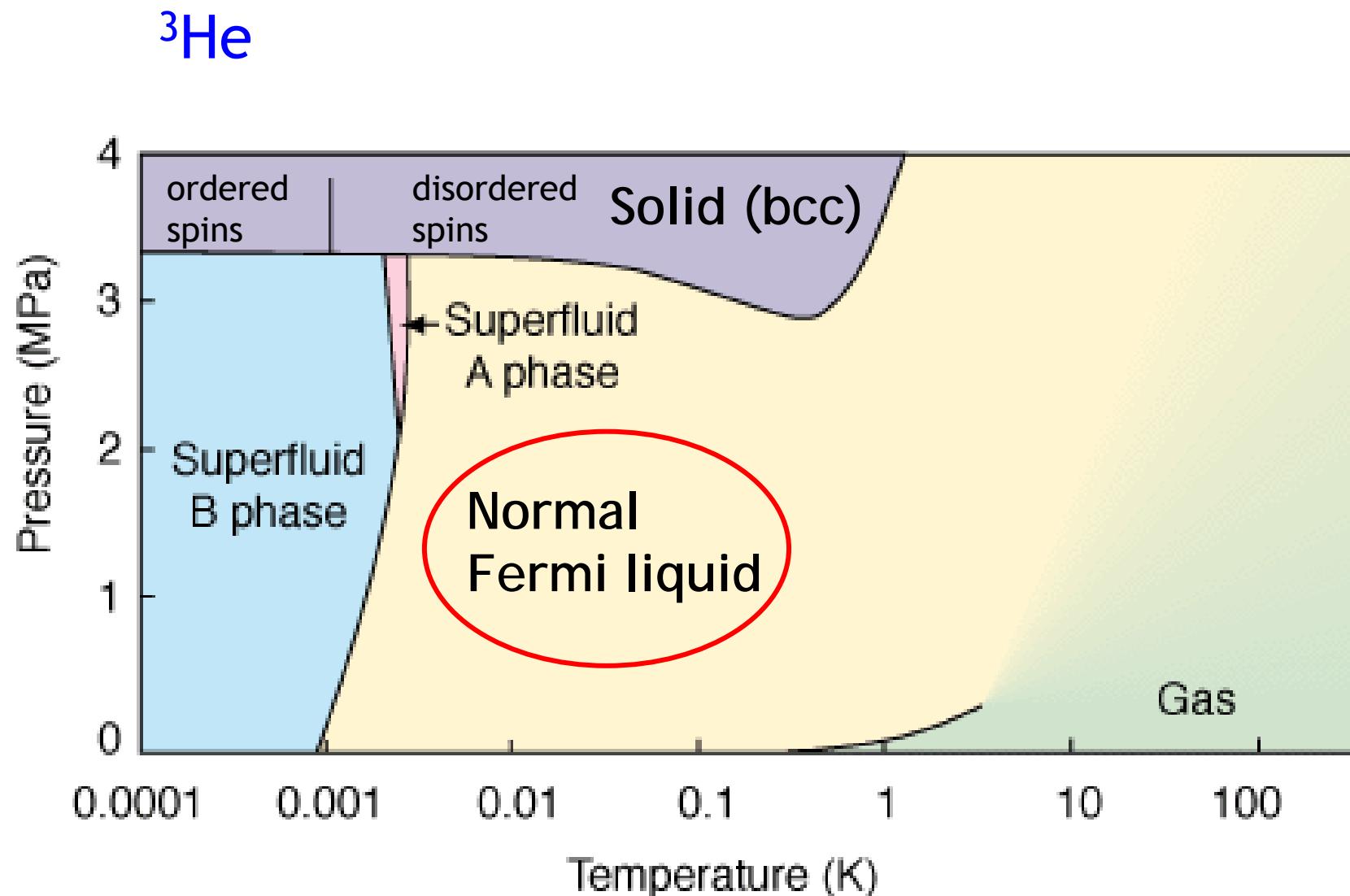
- Common properties of correlated electrons and ${}^3\text{He}$
- Emergence in many-particle systems

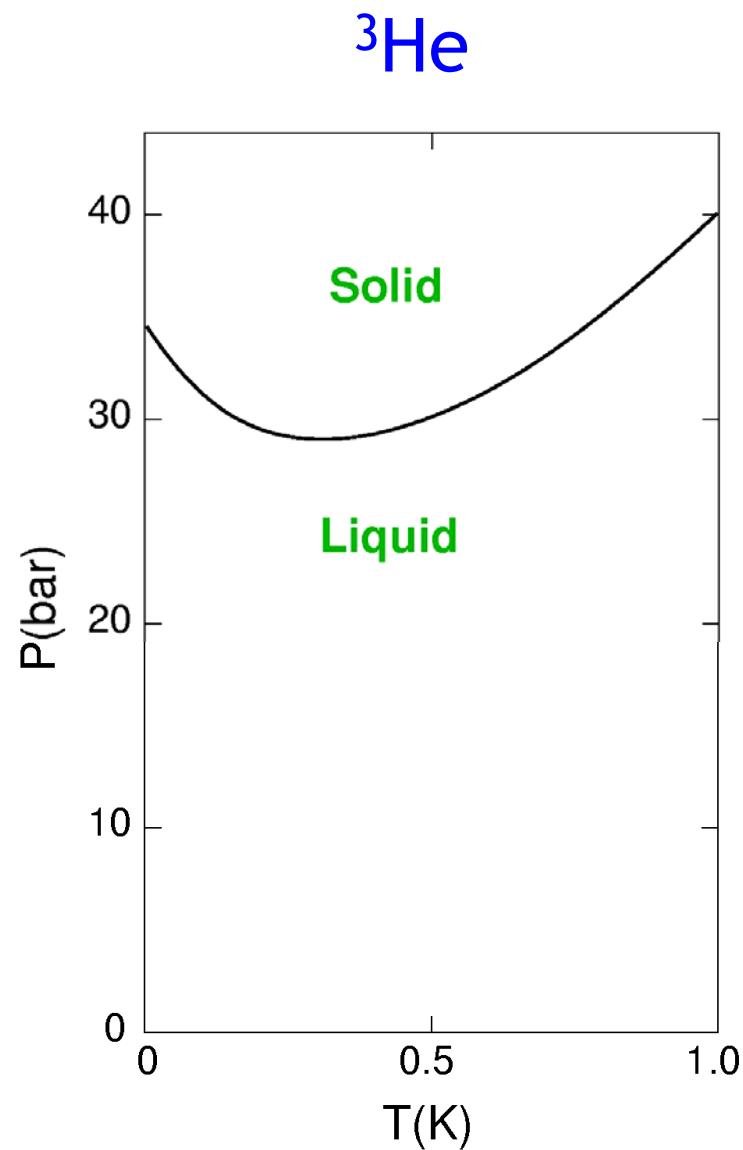
Paradigm: Helium-3

1. Normal state
2. Pair-correlated state
3. localization-delocalization transition



1. Normal state properties





Nuclear spin

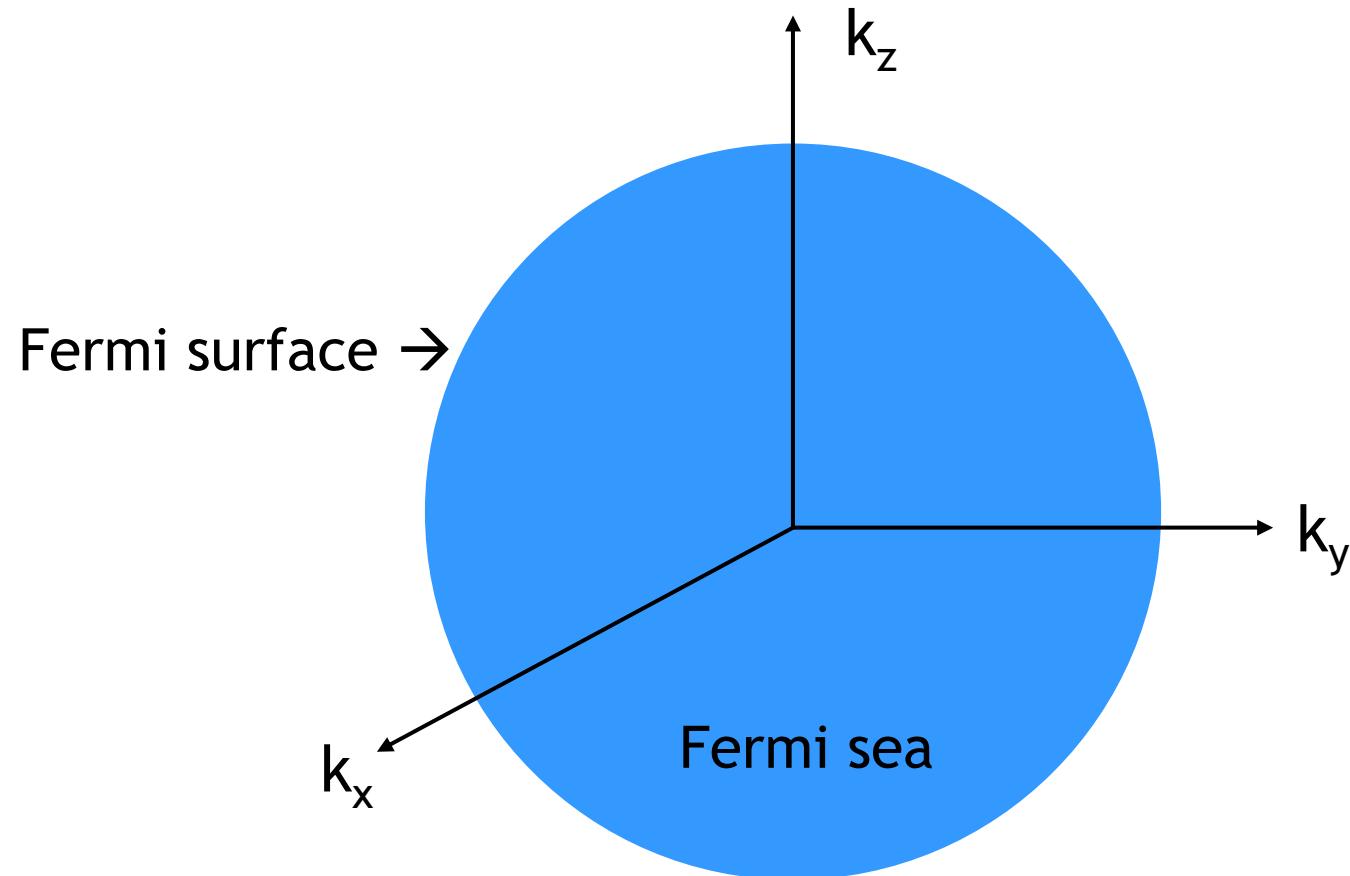
$$I = \frac{1}{2} \hbar$$

Fermion

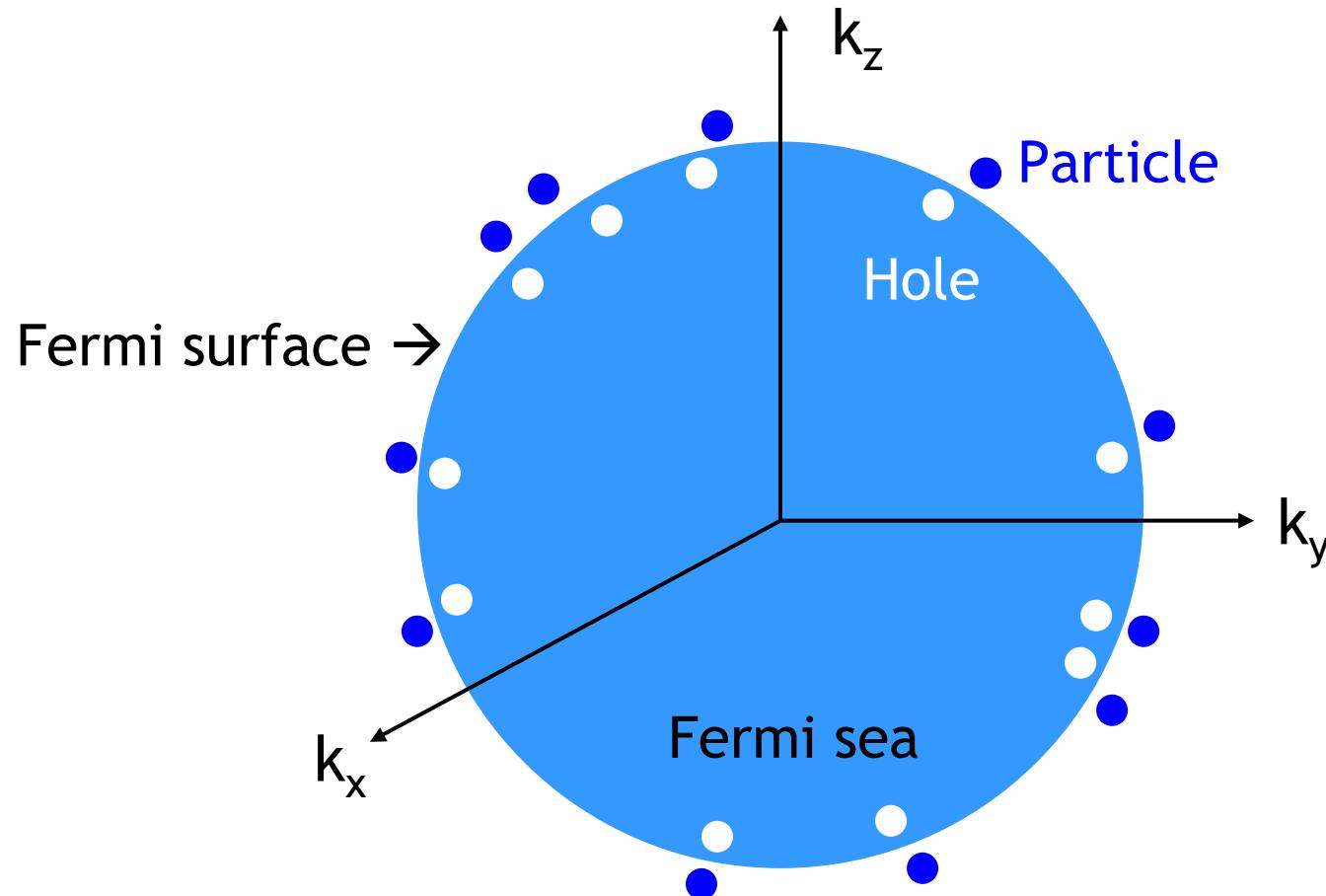
Fermi-Dirac statistics

Fermi body/surface

Fermi gas: Ground state



Fermi gas: Excited states ($T>0$)



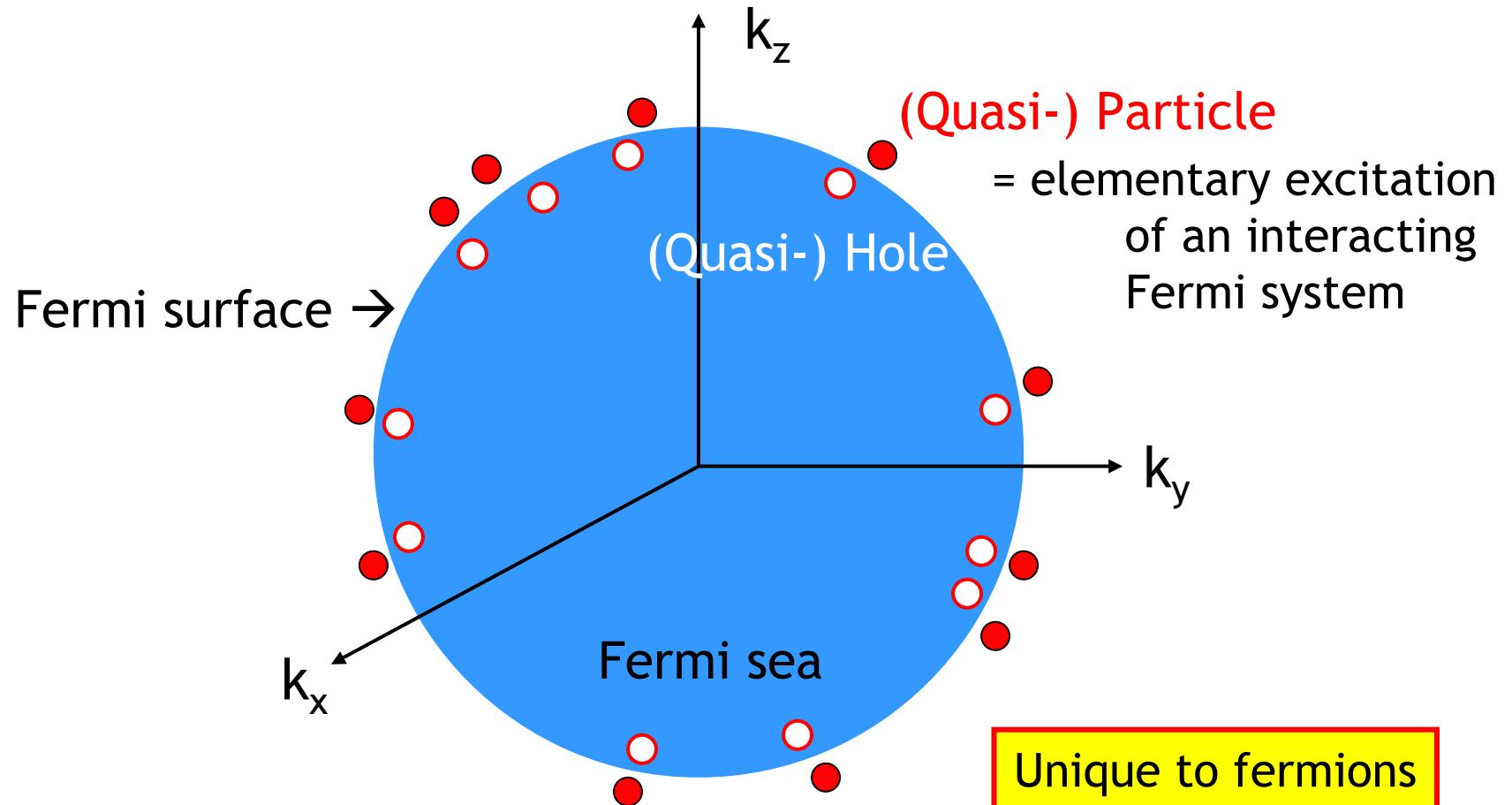
Exact k -states ('particles'): **infinite** life time

Switch on interaction adiabatically ($d=3$)

Landau Fermi liquid

Landau (1956/58)

1-1 correspondence between k-states



Well-defined k-states ("quasiparticles") with

- finite life time
- effective mass
- effective interaction

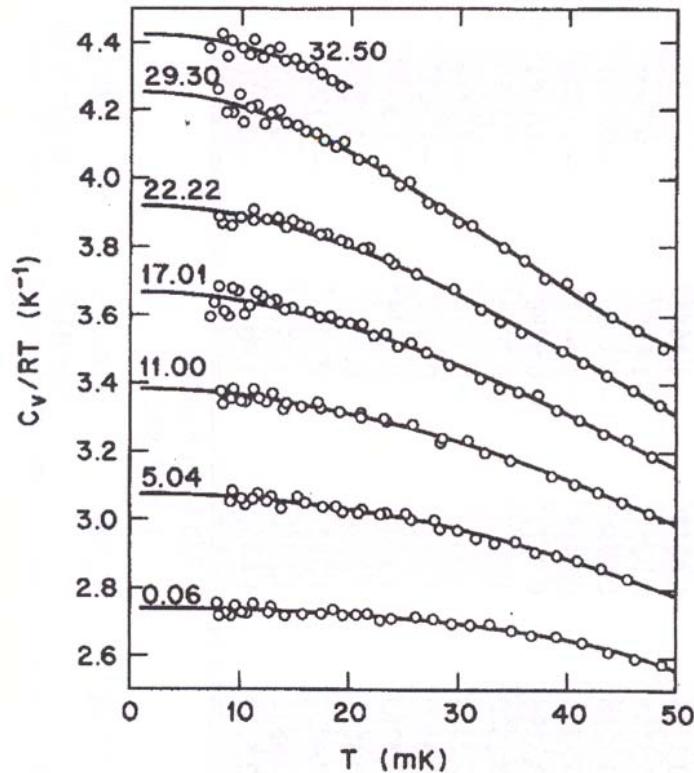
Universal Fermi liquid properties:

specific heat $c_V = \frac{m^*}{m} c_V^0$

spin susceptibility $\chi_s = \frac{m^*/m}{1 + F_0^a} \chi_s^0$

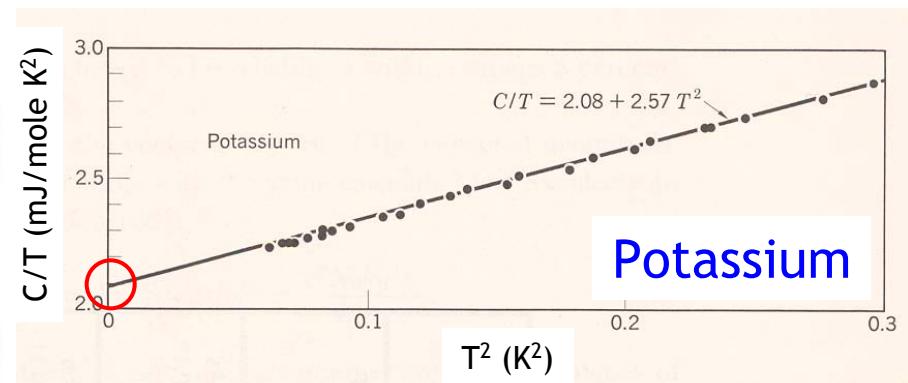
compressibility $\kappa = \frac{m^*/m}{1 + F_0^s} \kappa^0$

$$\lim_{T \rightarrow 0} \frac{c_v}{T} = \gamma \propto \frac{m^*}{m} \quad \text{quasiparticle mass}$$

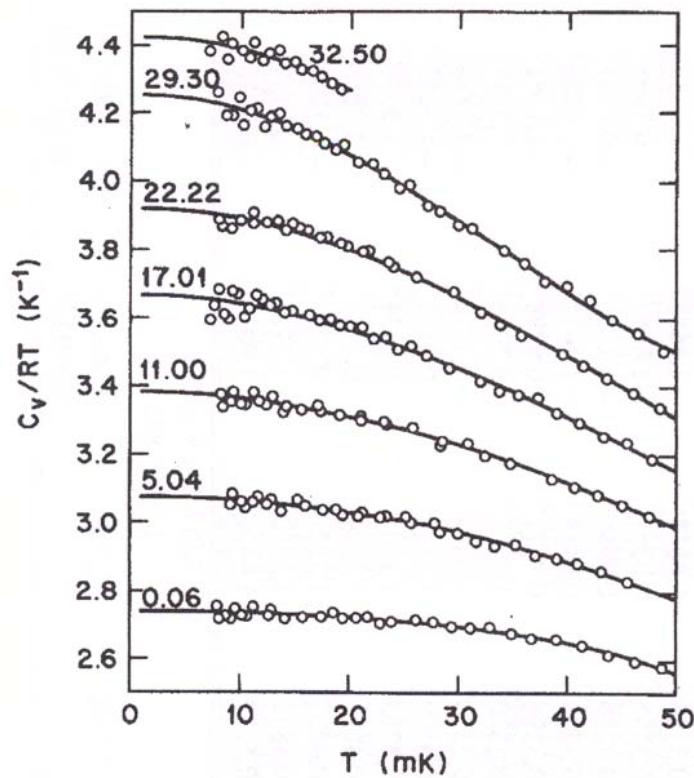


${}^3\text{He}$
Greywall (1983)

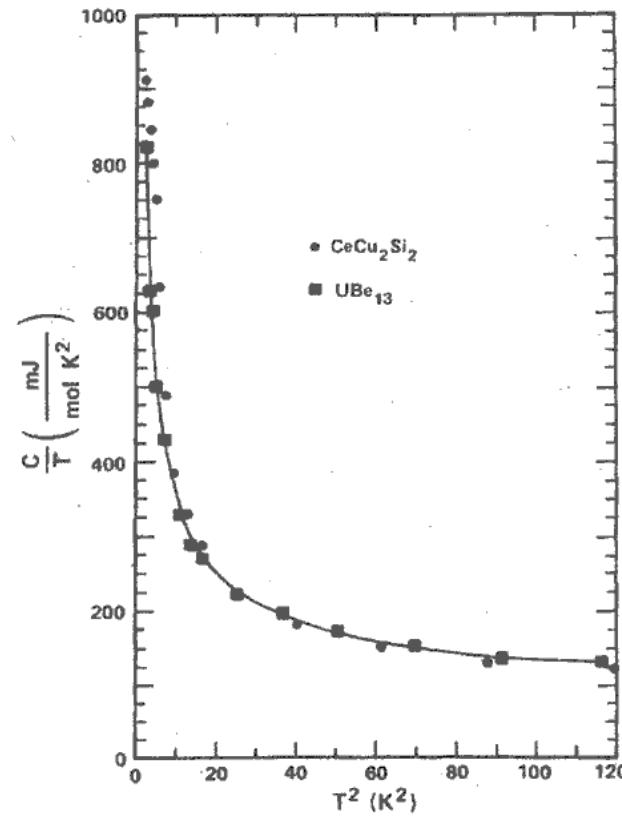
Simple metals



$$\lim_{T \rightarrow 0} \frac{c_v}{T} = \gamma \propto \frac{m^*}{m} \quad \text{quasiparticle mass}$$



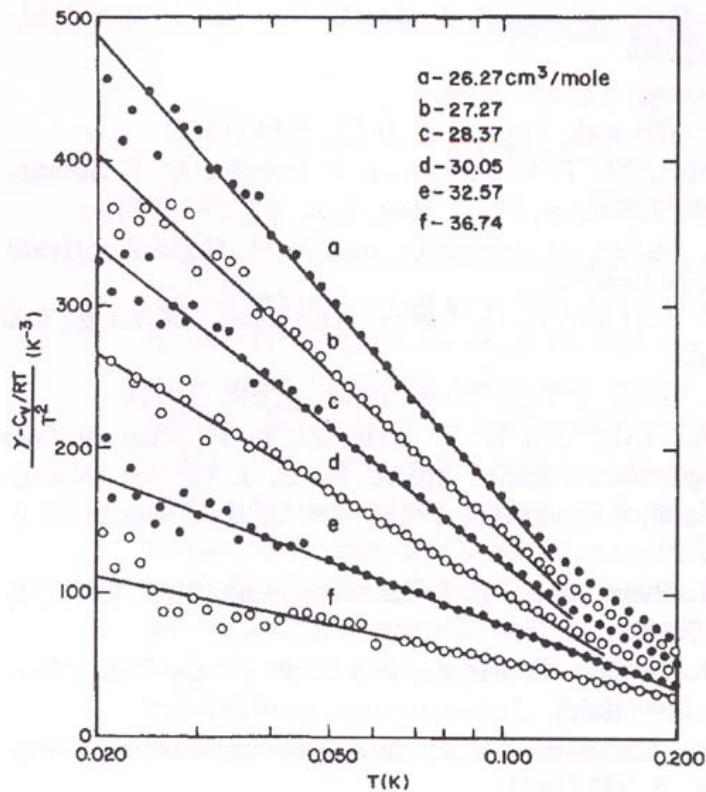
^3He
Greywall (1983)



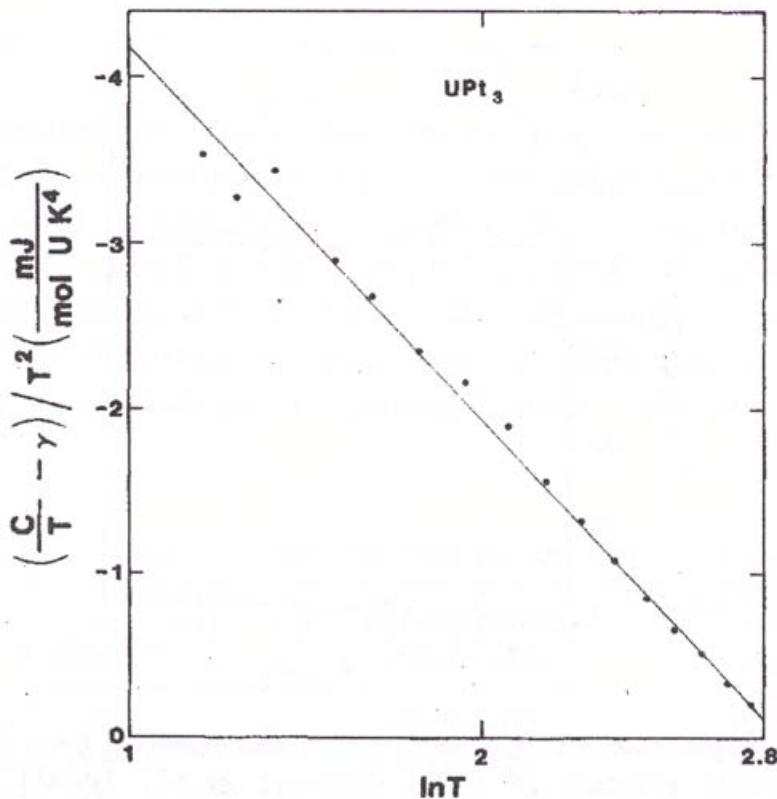
Heavy fermions: $\text{UBe}_{13}, \text{CeCu}_2\text{Si}_2$
Stewart *et al.* (1983, 1984)

$$c_V = \gamma T + \Gamma T^3 \ln T$$

Eliashberg (1960)
 Doniach, Engelsberg (1966)
 Pethick, Carneiro (1973)
 Chubukov *et al.* (2005)
 Aleiner, Efetov (2006)

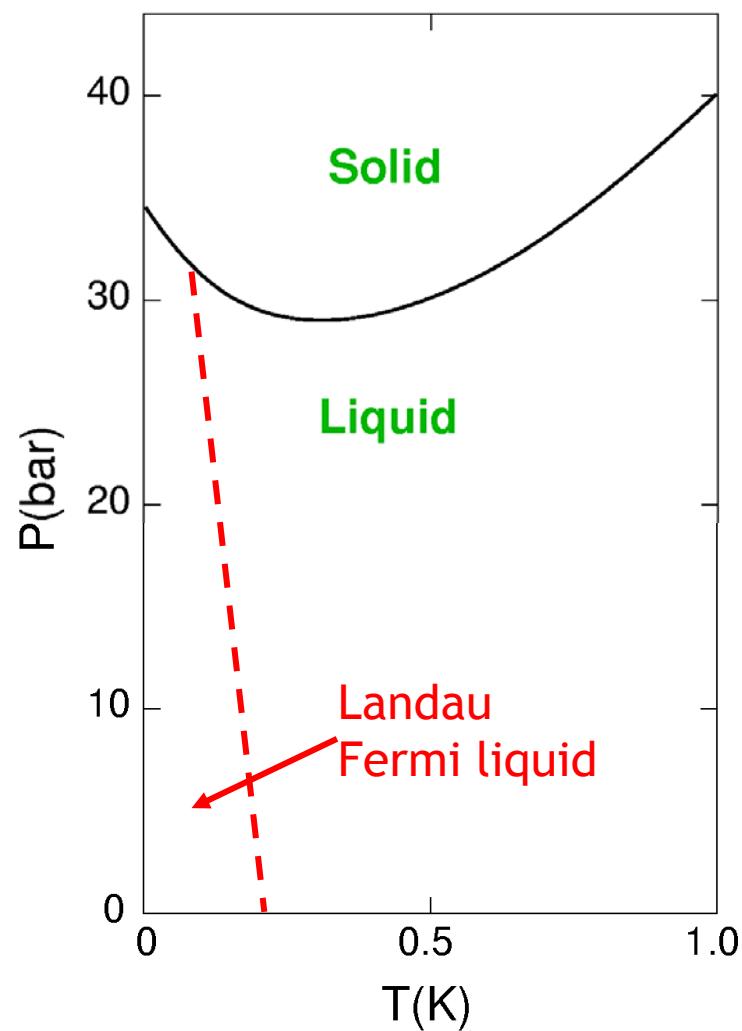


${}^3\text{He}$
 Greywall (1983)



Heavy fermions: UPt_3
 Stewart *et al.* (1983, 1984)

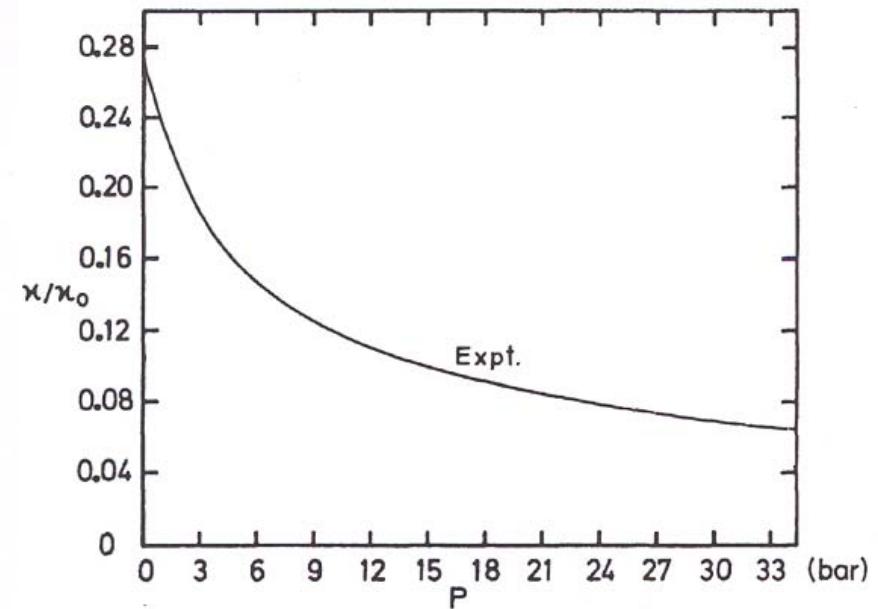
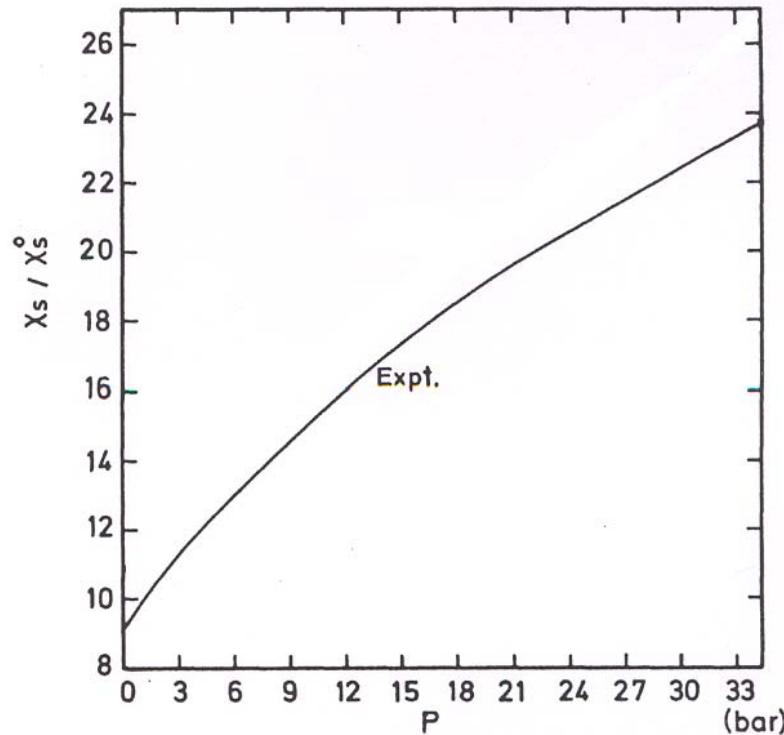
^3He



$$T_F^* = \frac{1}{k_B} \frac{\hbar^2 k_F^2}{2m^*}$$
$$= \frac{m}{m^*} T_F \approx 1.5K$$

^3He : Pressure dependence

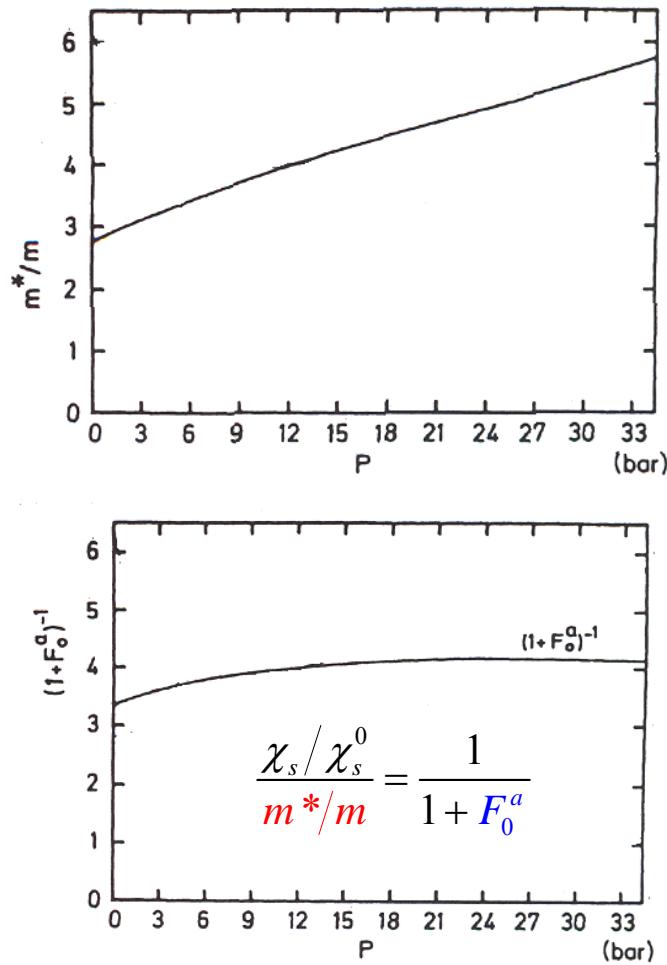
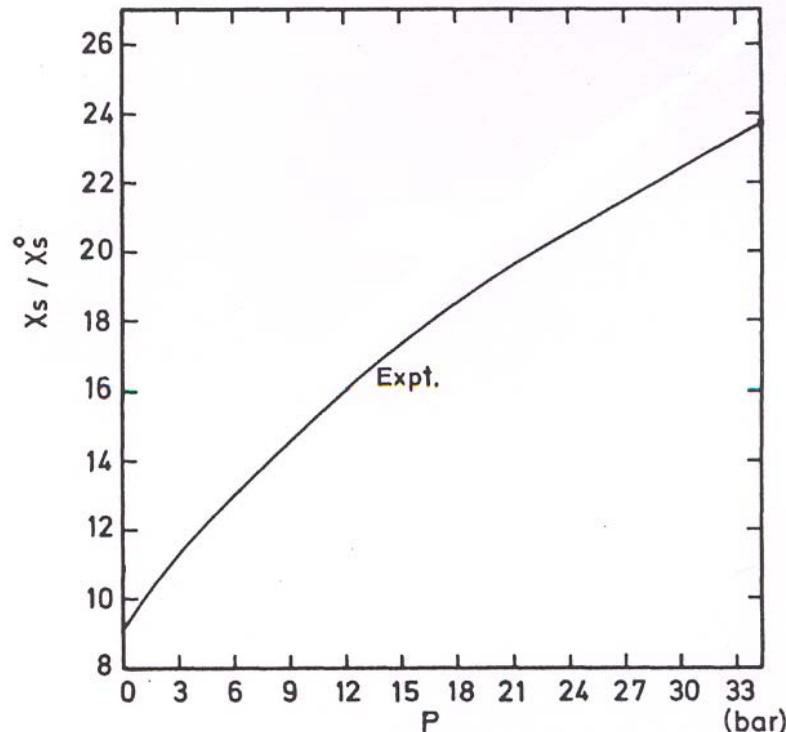
Greywall (1983)



Strong short-range, repulsive interactions →
• spin fluctuations strongly enhanced
• density fluctuations strongly suppressed

High susceptibility: “almost ferromagnetic liquid“?

^3He : Pressure dependence



$$\chi_s / \chi_s^0 = \frac{m^*/m}{1 + F_0^a}$$

Anderson, Brinkman (1975):

“Almost localized Fermi liquid”; vicinity of Mott transition

Gutzwiller-Brinkman-Rice theory

$$H = \sum_{i,j,\sigma} \color{red} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \color{red} U \underbrace{\sum_i n_{i\uparrow} n_{i\downarrow}}_{\hat{D}}$$

Gutzwiller (1963)
Hubbard (1963)
Kanamori (1963)

Gutzwiller wave function $|\psi_G\rangle = e^{-\lambda\hat{D}} |\psi_0\rangle$

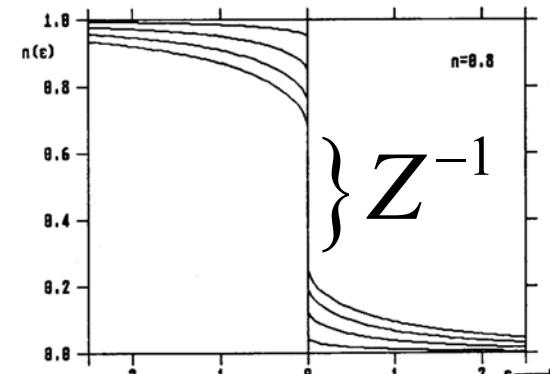
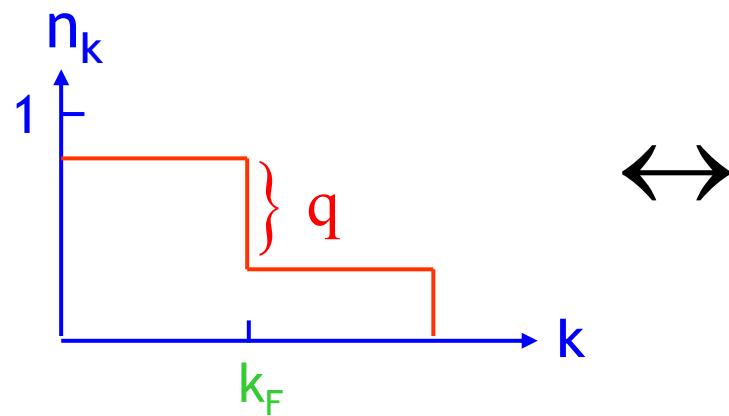
$$E_G = \frac{1}{L} \frac{\langle \psi_G | H | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}$$

One-particle wave function
(Hartree-Fock, BCS, etc.)

d=1,∞: exact analytic evaluation possible Metzner, DV (1988/89)

Gutzwiller approximation (1963/65)

$$\frac{E_G}{L} \stackrel{GA}{=} q(d) \bar{\varepsilon}_0 + U d, \quad \frac{\partial E}{\partial d} = 0$$



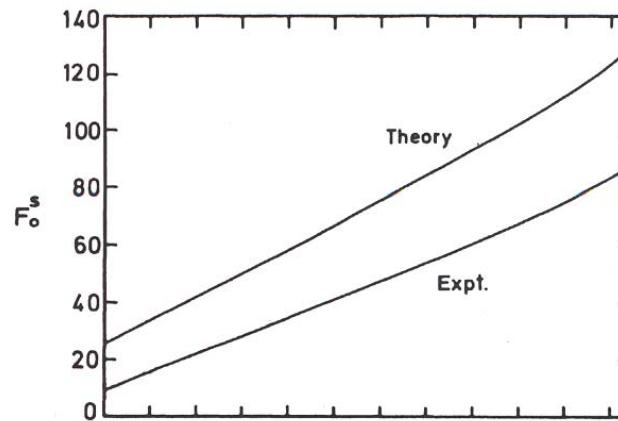
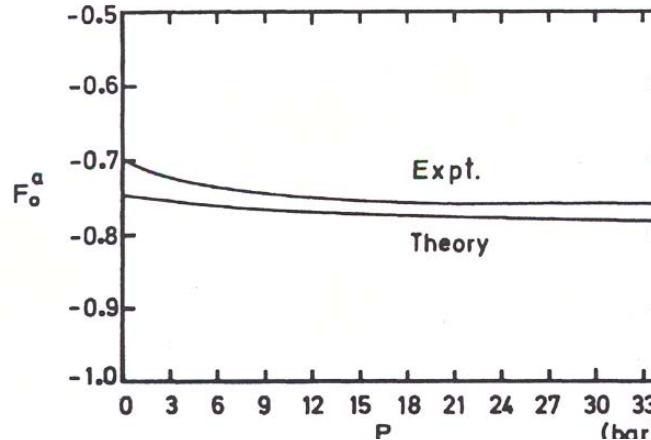
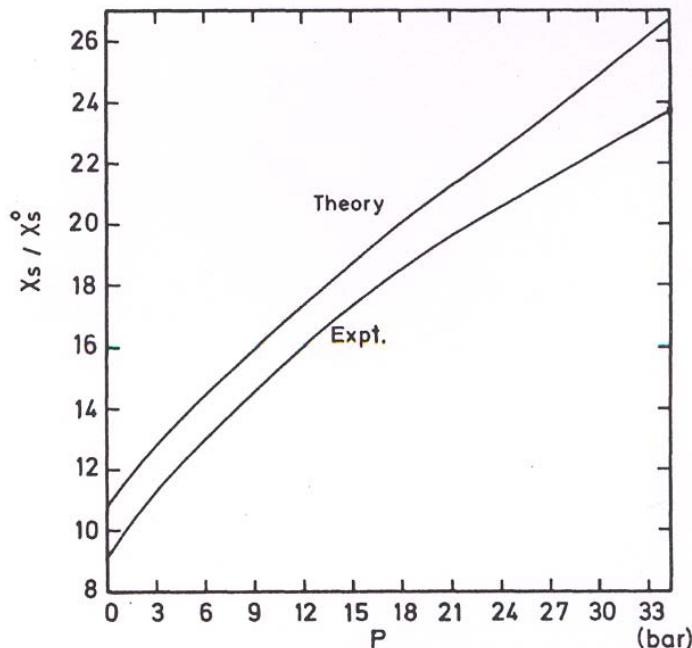
Brinkman, Rice (1970): $\frac{m^*}{m} = q^{-1} \xrightarrow{U \rightarrow U_c} \infty$

Describes metal-insulator ("Mott") transition,
→ application to V_2O_3

Gutzwiller-Brinkman-Rice theory: Application to normal liquid ^3He

DV (1984)

Gutzwiller approximation \leftrightarrow
Landau Fermi liquid theory



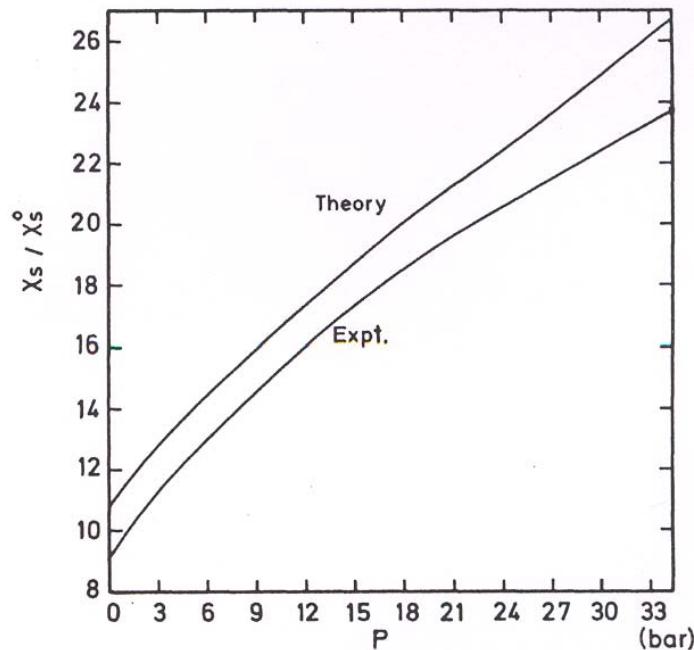
liquid ^3He :

"almost localized Fermi liquid" (vicinity of Mott transition),
not „almost ferromagnetic”

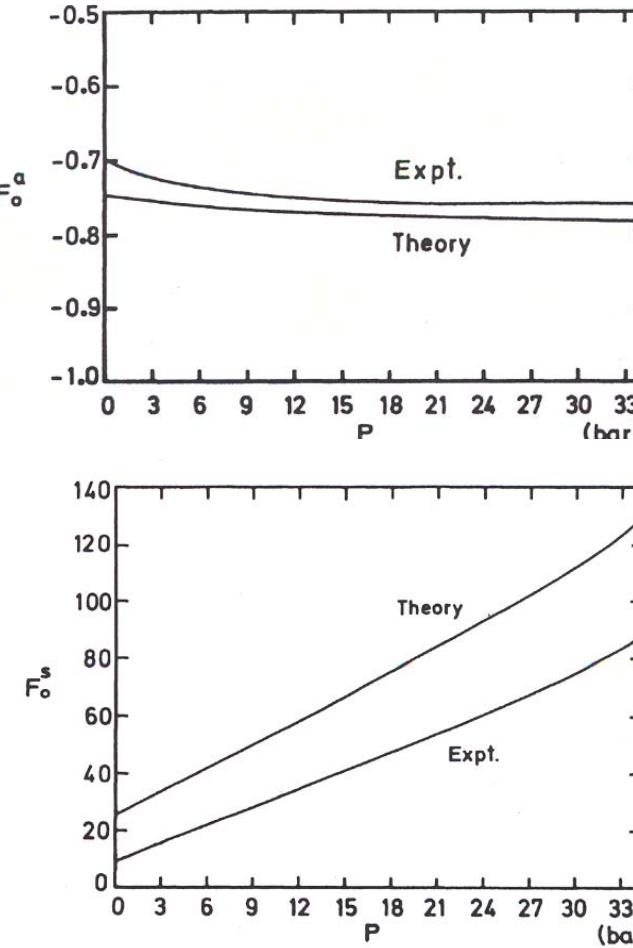
Gutzwiller-Brinkman-Rice theory: Application to normal liquid ^3He

DV (1984)

Gutzwiller approximation \leftrightarrow
Landau Fermi liquid theory



Generalization:
Gutzwiller-Hubbard
lattice gas model for ^3He



DV, Wölfle, Anderson (1987)

Gutzwiller wave function in $d \rightarrow \infty$

$$|\psi_G\rangle = e^{-\lambda \hat{H}_U} |\psi_0\rangle$$
$$E_G = \frac{\langle \psi_G | H | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}$$

Gutzwiller approximation exact in $d \rightarrow \infty$

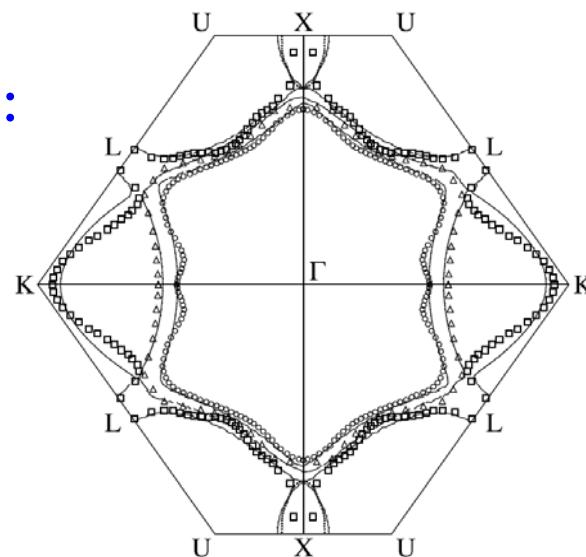
Metzner, DV (1989)

$d \rightarrow \infty$: Evaluation of E_G for arbitrary $|\psi_0\rangle$

Gebhard (1990)

Multi-band generalization:

„Gutzwiller DFT“



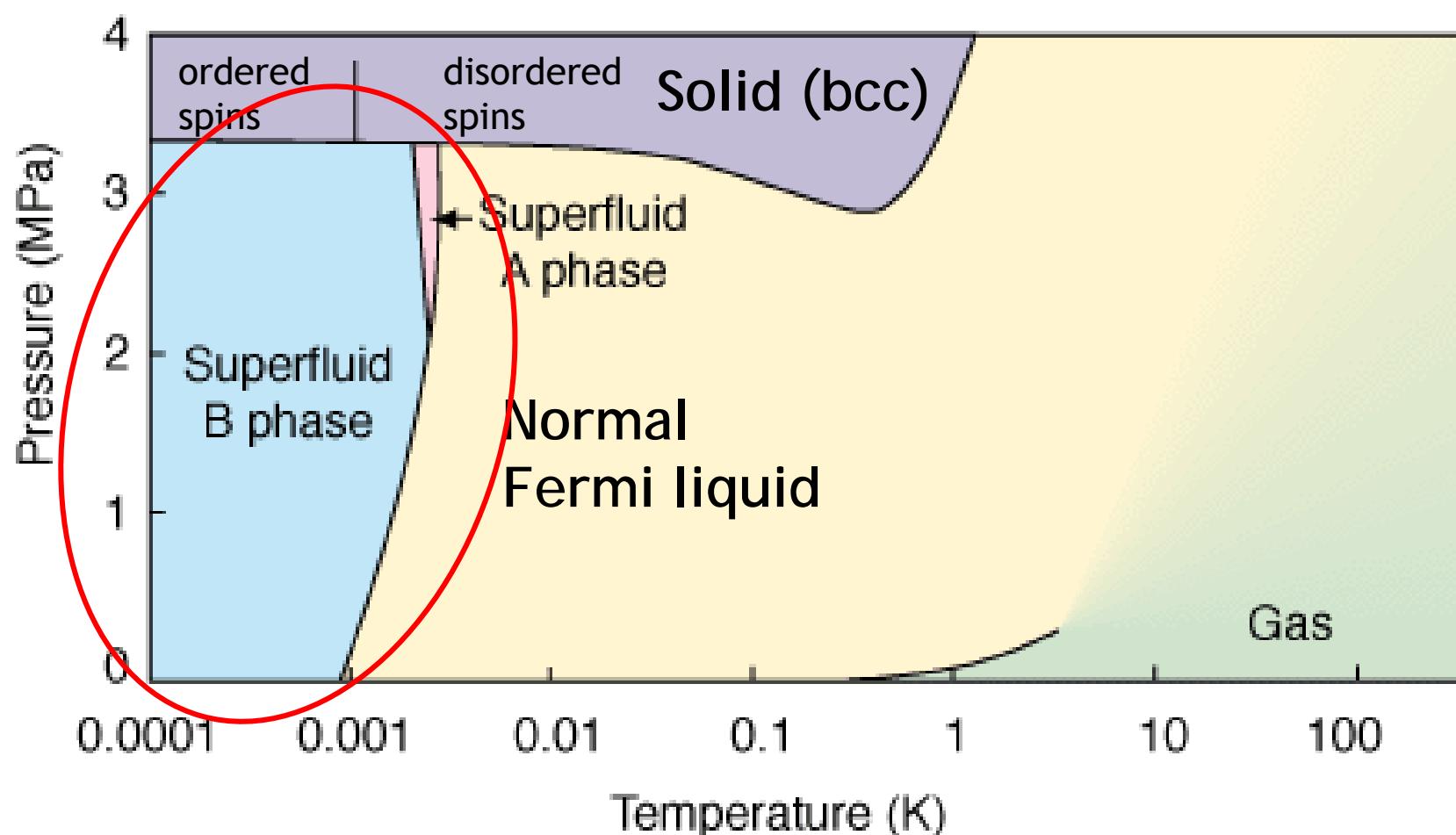
Ferromagnetic Ni:
Cut of Fermi surface

Bünemann, Gebhard, Ohm, Weiser, Weber (2005)

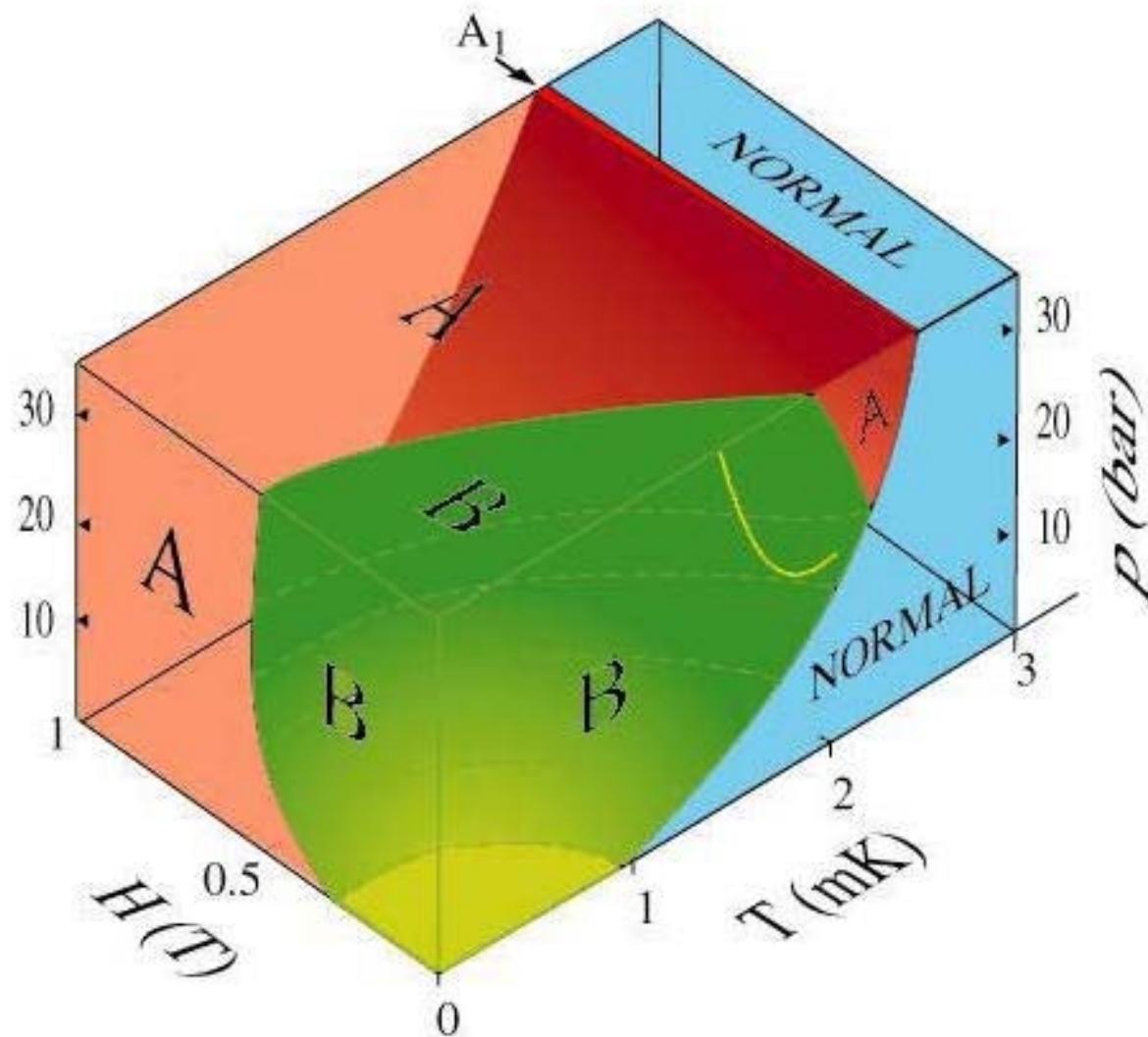
2. Pair-correlated state

Osheroff, Richardson, Lee (1972)

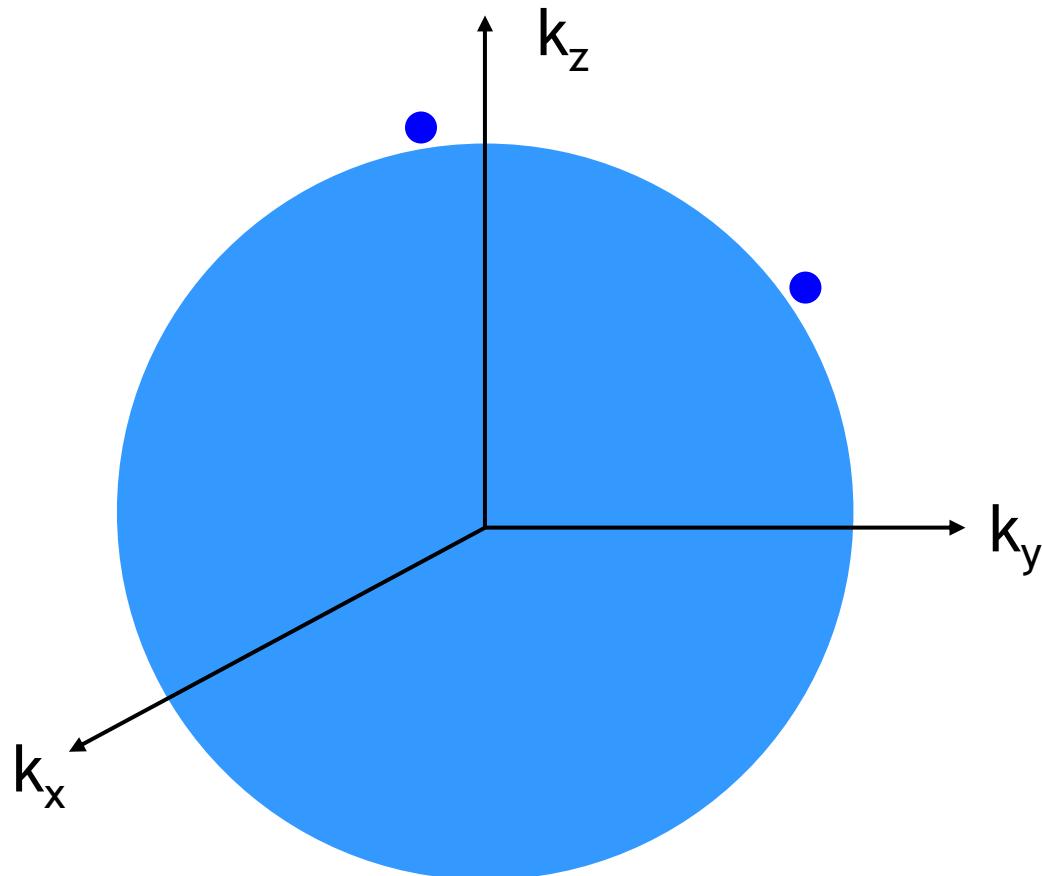
^3He : P-T phase diagram



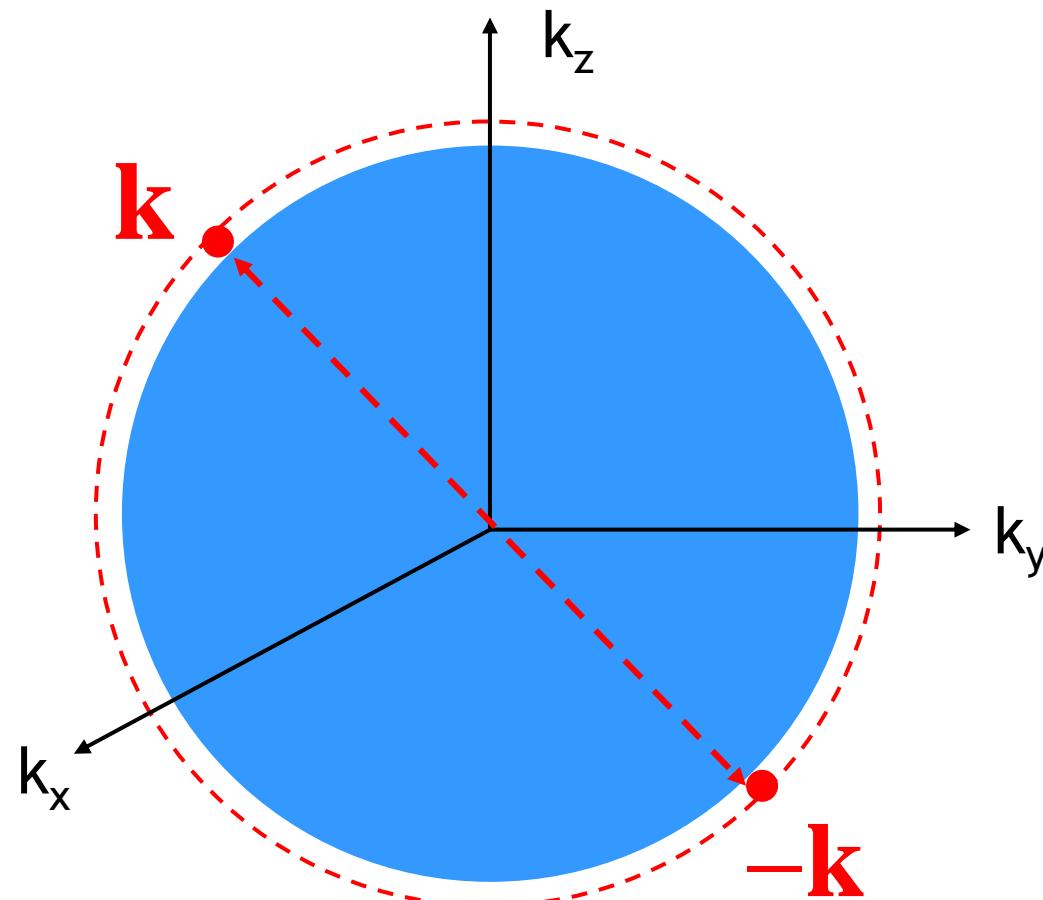
${}^3\text{He}$: H-P-T phase diagram



Landau Fermi liquid



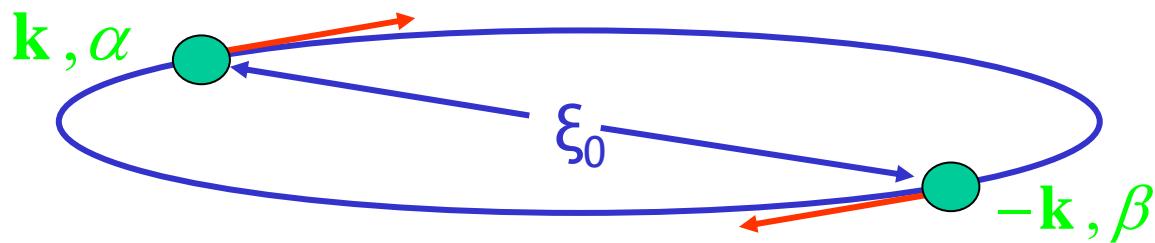
Arbitrarily weak attraction \Rightarrow Cooper instability



Universal fermionic property

Arbitrarily weak attraction:

Cooper pair $(\mathbf{k}, \alpha; -\mathbf{k}, \beta)$



$$\Psi_{L=0,2,4,\dots} = \psi(\mathbf{r}) |\uparrow\downarrow - \downarrow\uparrow\rangle$$

S=0
(singlet)

$$\begin{aligned} \Psi_{L=1,3,5,\dots} = & \psi_+(\mathbf{r}) |\uparrow\uparrow\rangle \\ & + \psi_0(\mathbf{r}) |\uparrow\downarrow + \downarrow\uparrow\rangle \\ & + \psi_-(\mathbf{r}) |\downarrow\downarrow\rangle \end{aligned}$$

S=1
(triplet)

Cooper pairing of Fermions vs. Bose-Einstein condensation

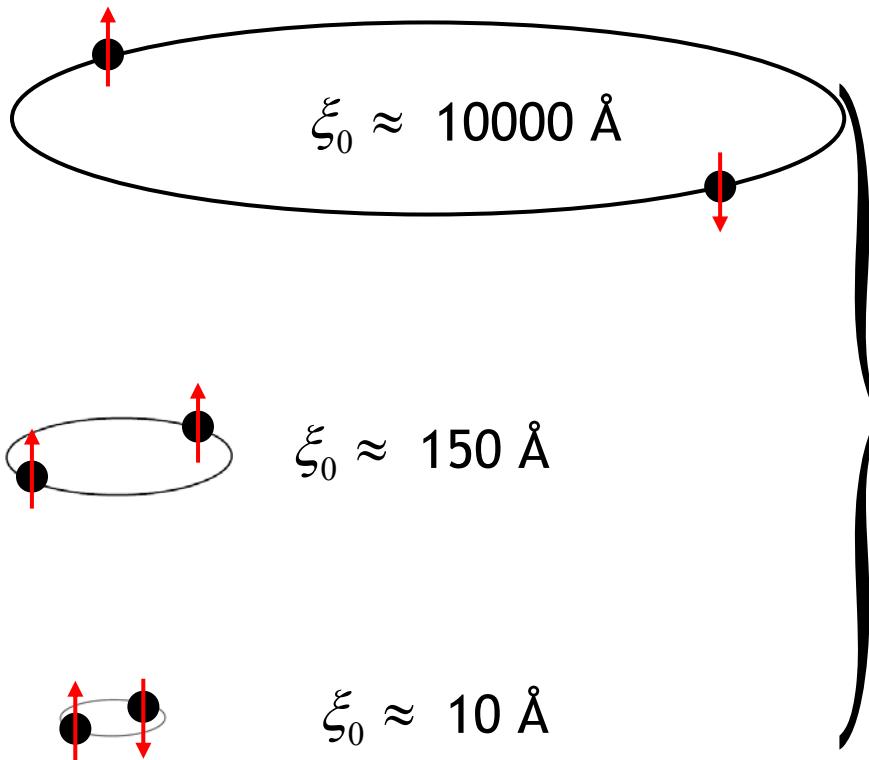
Cooper pair: “Quasi-boson”

Conventional superconductors

Superfluid ^3He

High T_c superconductors

Tightly packed bosons



BCS

Continuous crossover?

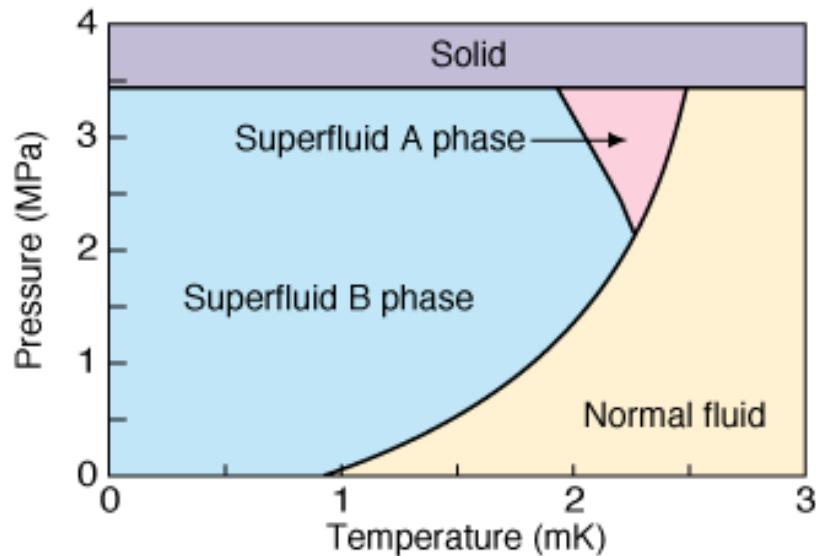
BEC

New insights from BEC of cold atoms

Leggett (1980)

Superfluid ^3He

$L=1, S=1$

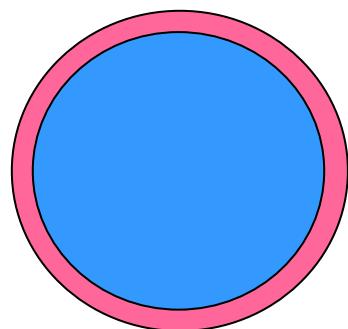


Order parameter matrix

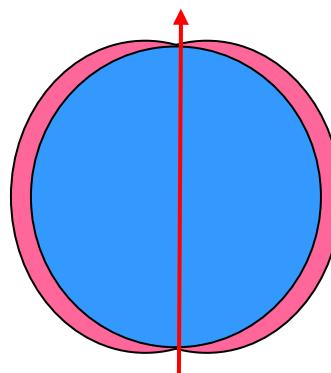
$$A_{i\mu}$$

$3 \times 3 \times 2 = 18$ real numbers

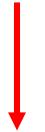
B phase



A phase



$\text{SO}(3)_S \times \text{SO}(3)_L \times \text{U}(1)_\varphi$ symmetry broken

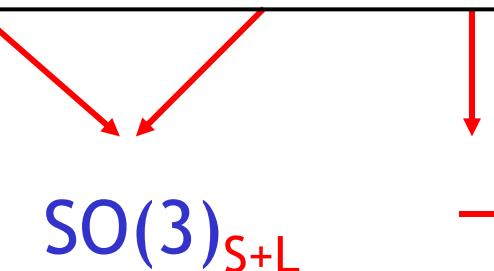


Leggett (1975)
Mineev (1980)
Bruder, DV (1986)

s-wave pairing

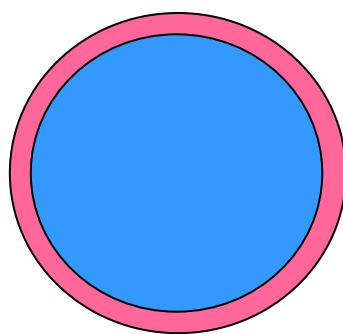
"conventional" superfluidity/superconductivity

$\text{SO}(3)_S \times \text{SO}(3)_L \times \text{U}(1)_\varphi$ symmetry broken



Leggett (1975)
Mineev (1980)
Bruder, DV (1986)

B phase



Spontaneously broken spin-orbit symmetry (SBSOS)

Leggett (1972)

"unconventional" superfluidity

$$c_V \propto e^{-\Delta/k_B T}$$

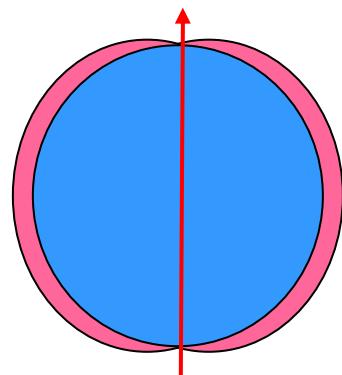
only stable phase in mean-field theory

$\text{SO}(3)_S \times \text{SO}(3)_L \times \text{U}(1)_\varphi$ symmetry broken

$$\downarrow$$
$$\text{U}(1)_{S_z} \times \text{U}(1)_{L_z - \varphi}$$

Leggett (1975)
Mineev (1980)
Bruder, DV (1986)

A phase



"unconventional" superfluidity

$$c_V \propto T^3$$

stabilization by
strong-coupling effects

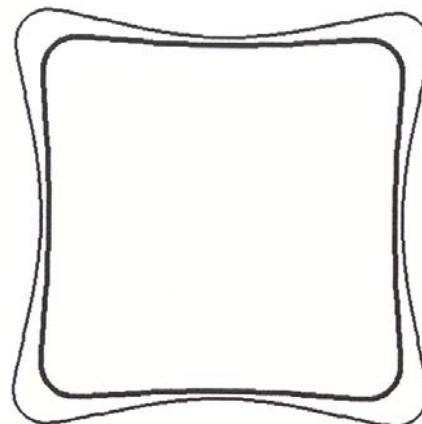
Unconventional superconductivity

$G \times SO(3)_S \times T \times U(1)_\varphi$ symmetry broken

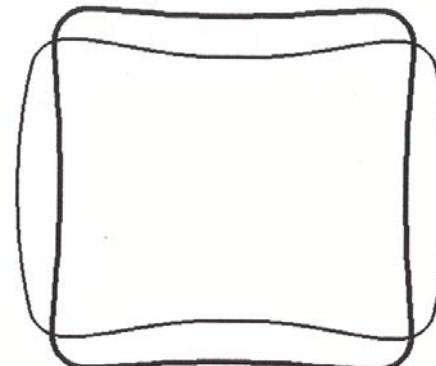
G : point symmetry group of solid

Anderson (1985)
Volovik, Gorkov (1985)
Ueda, Rice (1985)
Blount (1985)

Example: Tetragonal crystal (D_{4h})



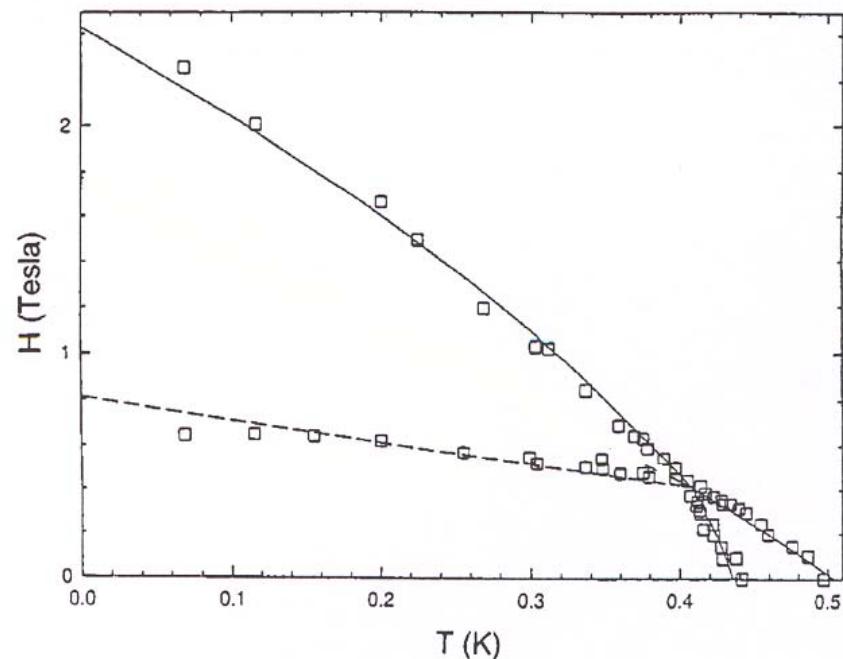
conventional



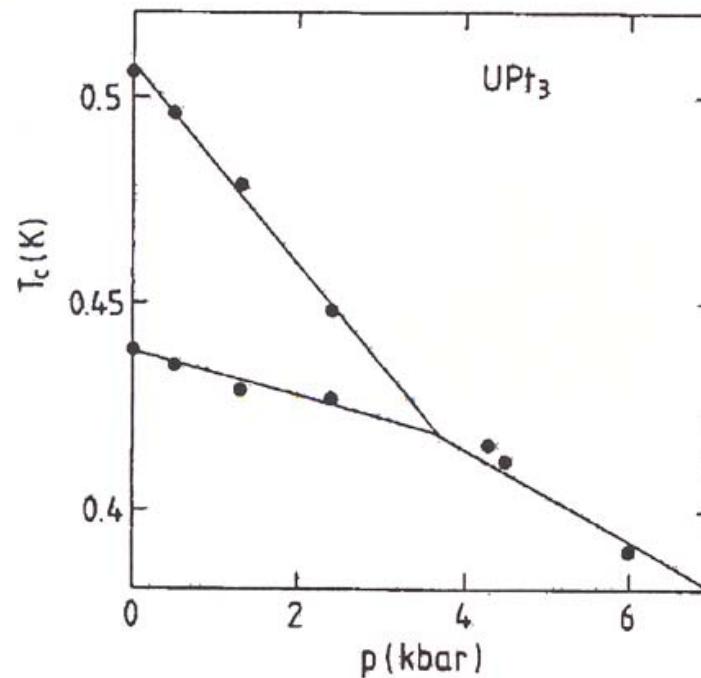
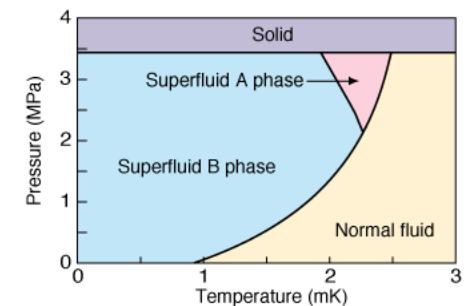
D_{2h} : unconventional

Unconventional superconductivity

UPt₃



H-T phase diagram
Adenwalla *et al.* (1990)
Park, Joynt (1995)



T-P phase diagram
v. Löhneysen, Trappmann,
Taillefer (1992)

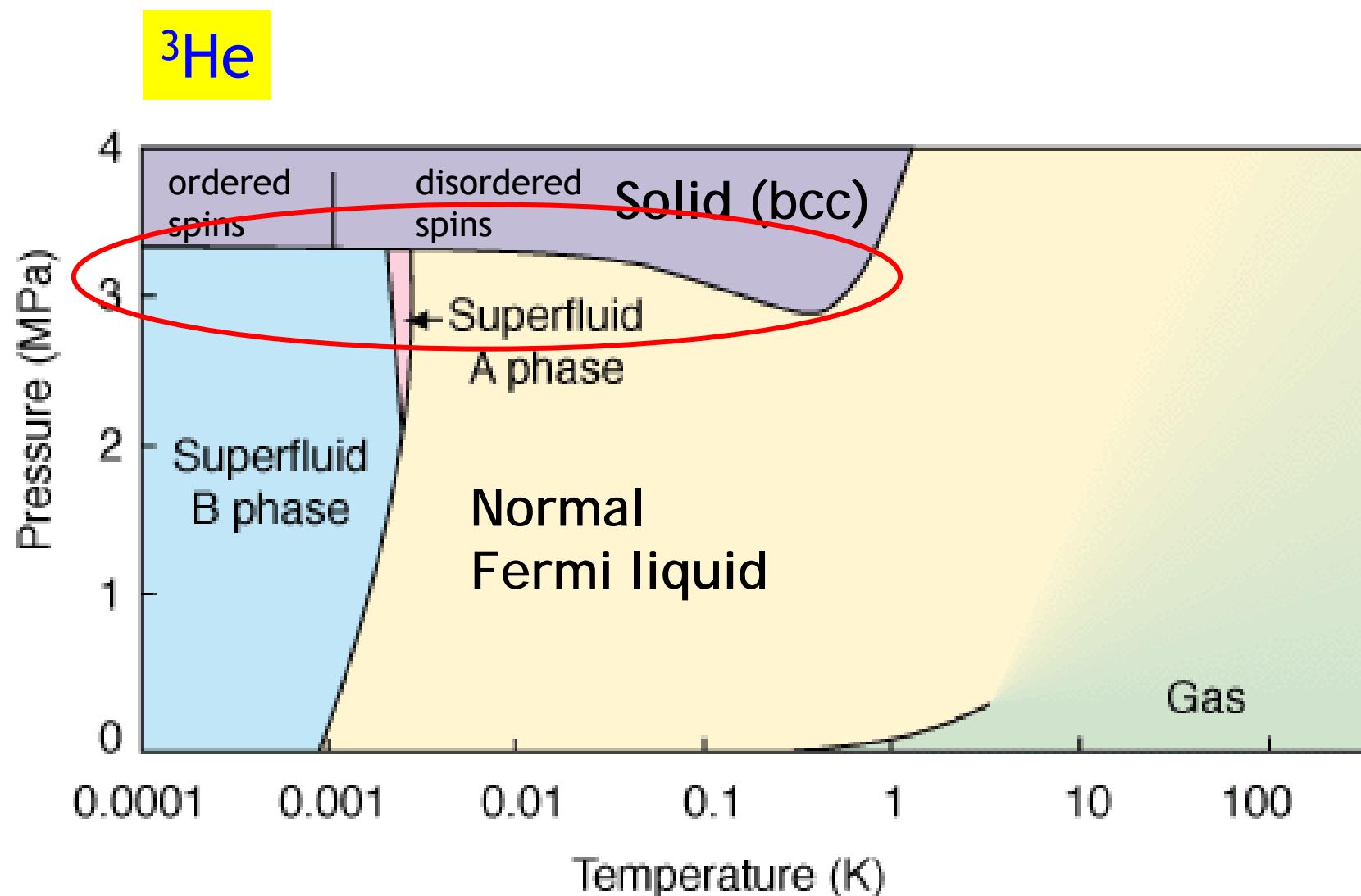
Unconventional superconductivity

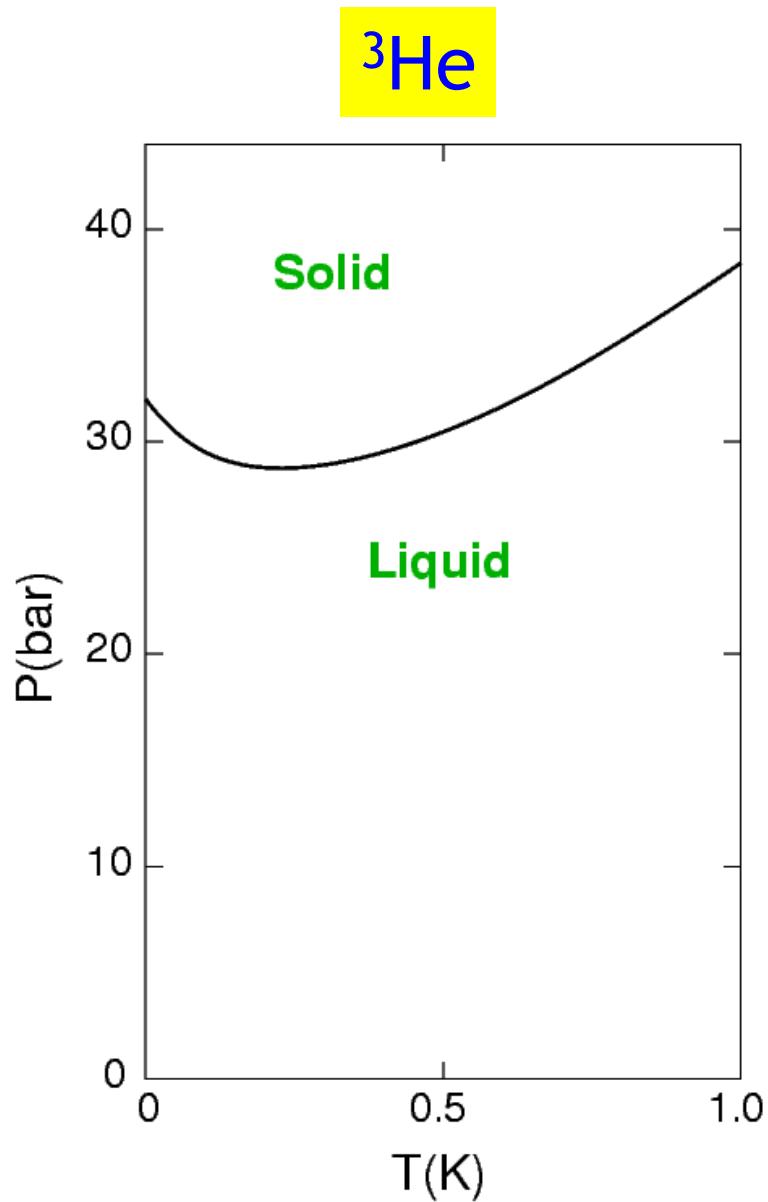
Other systems:

$\text{U}_{1-x}\text{Th}_x\text{Be}_{13}$ Ott *et al.* (1985)

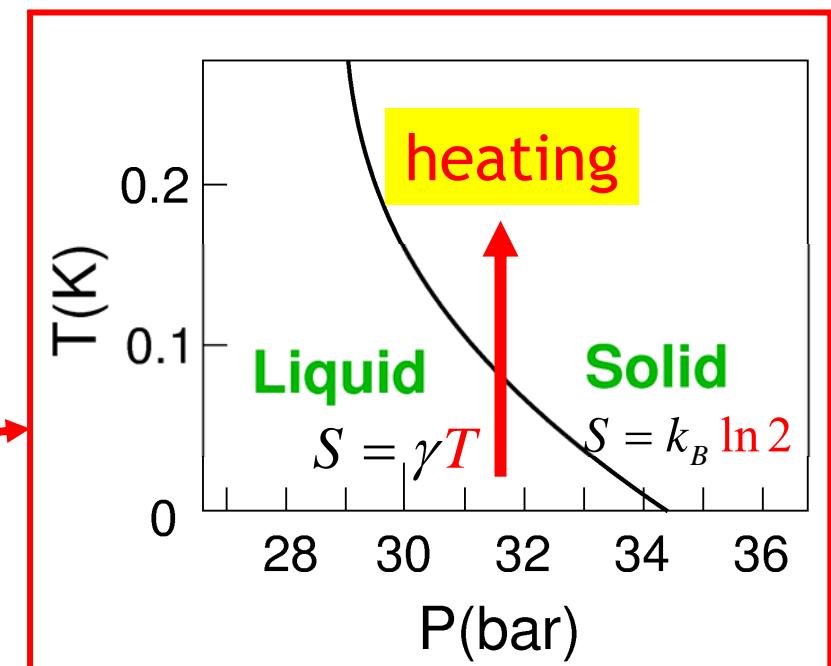
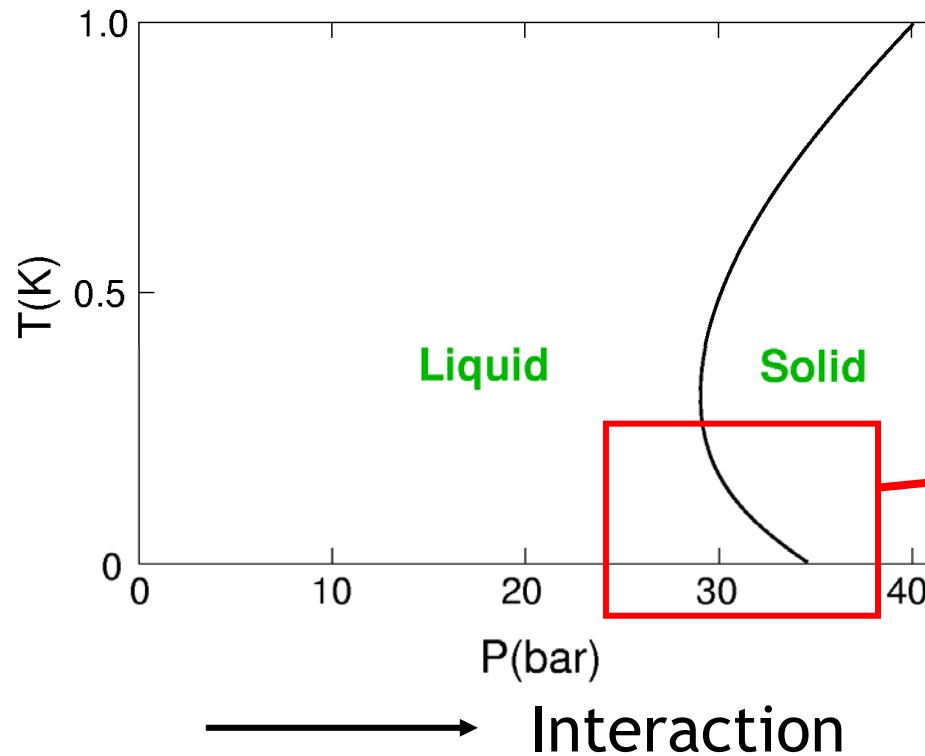
Sr_2RuO_4 Maeno *et al.* (1994) → triplet pairing

3. Localization-delocalization transition





^3He



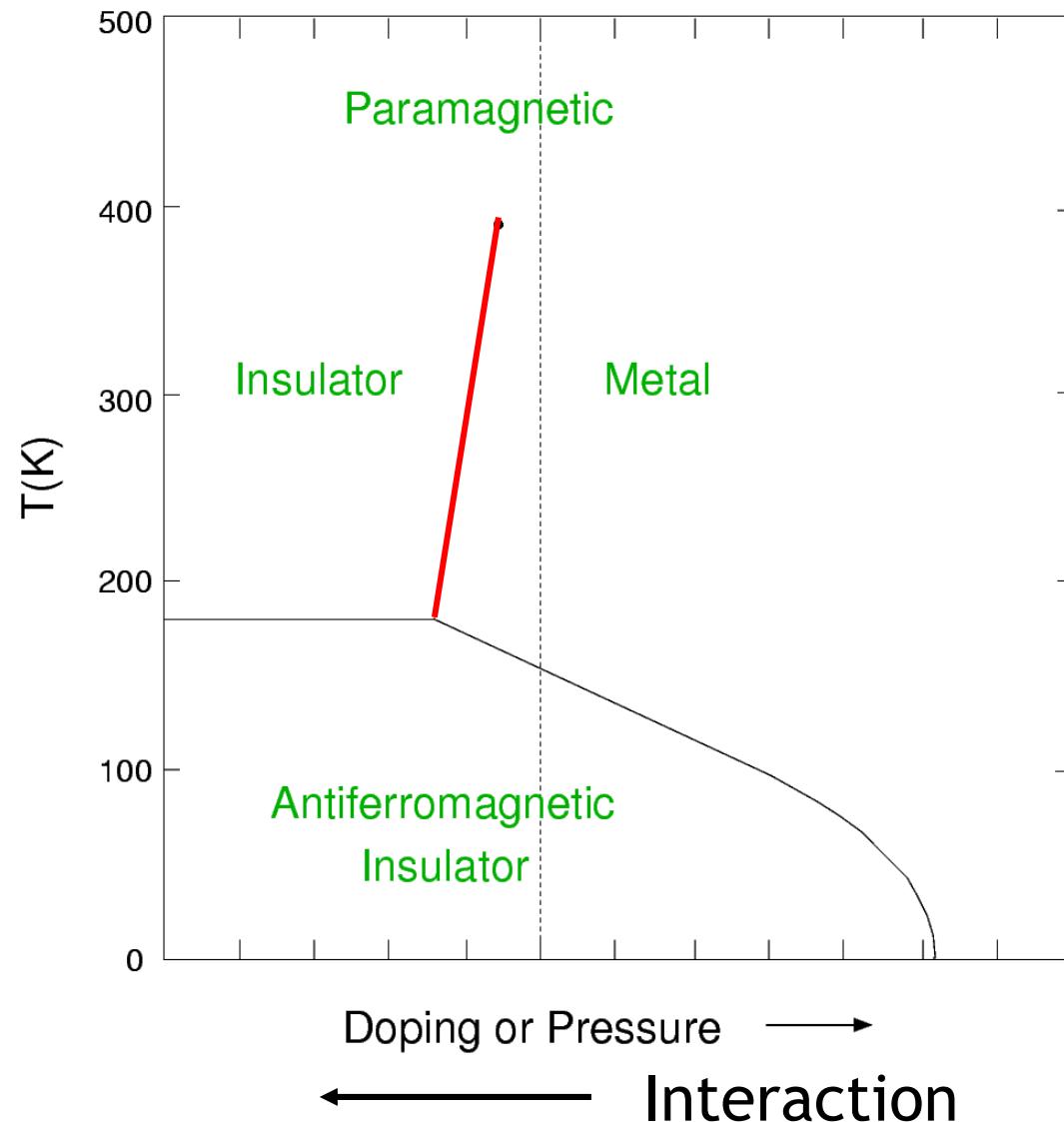
Clausius-Clapeyron eq.:

$$\frac{dP}{dT} = \frac{s_2 - s_1}{v_2 - v_1} = \frac{\Delta s}{\Delta v}.$$

anomalous
("Pomeranchuk")
effect

V_2O_3

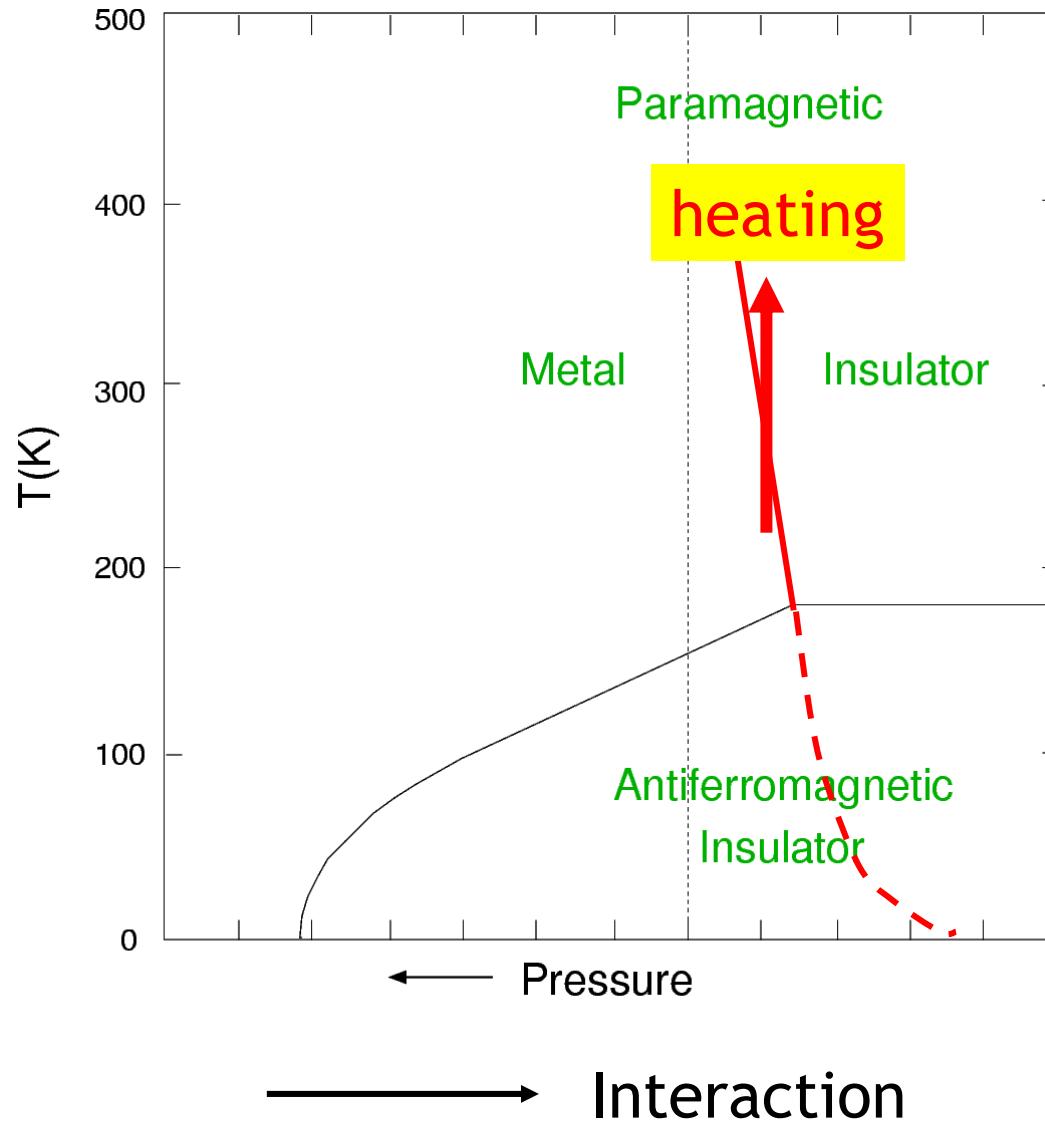
McWhan *et al.* (1971)



Correlation induced ("Mott-Hubbard") metal-insulator transition

V2O3

McWhan *et al.* (1971)



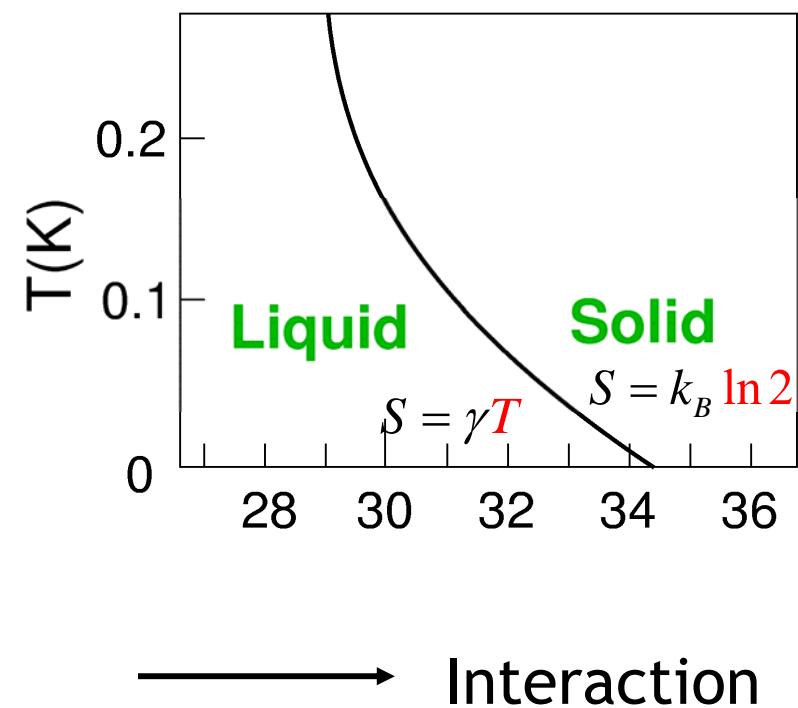
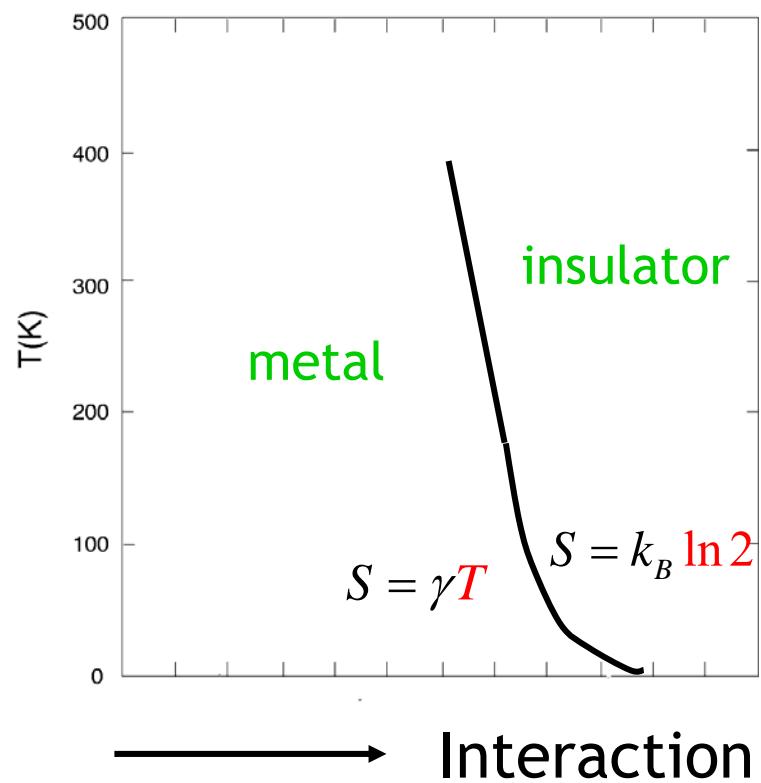
Clausius-Clapeyron eq.:

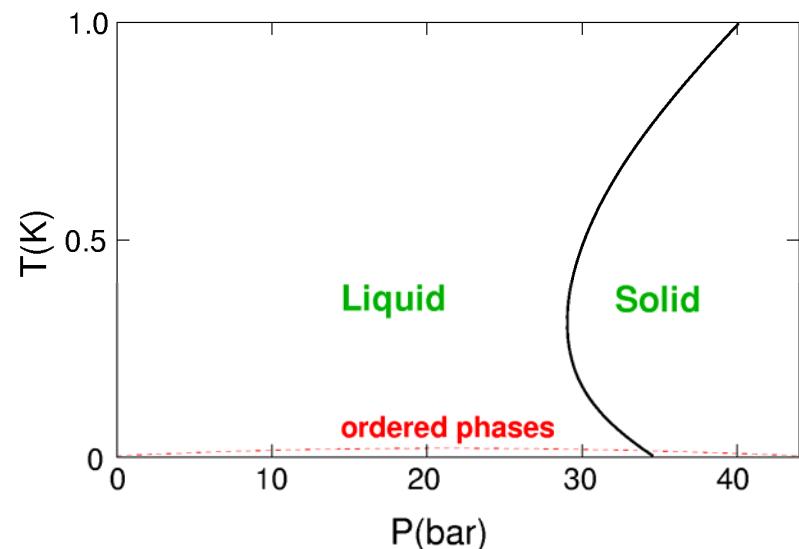
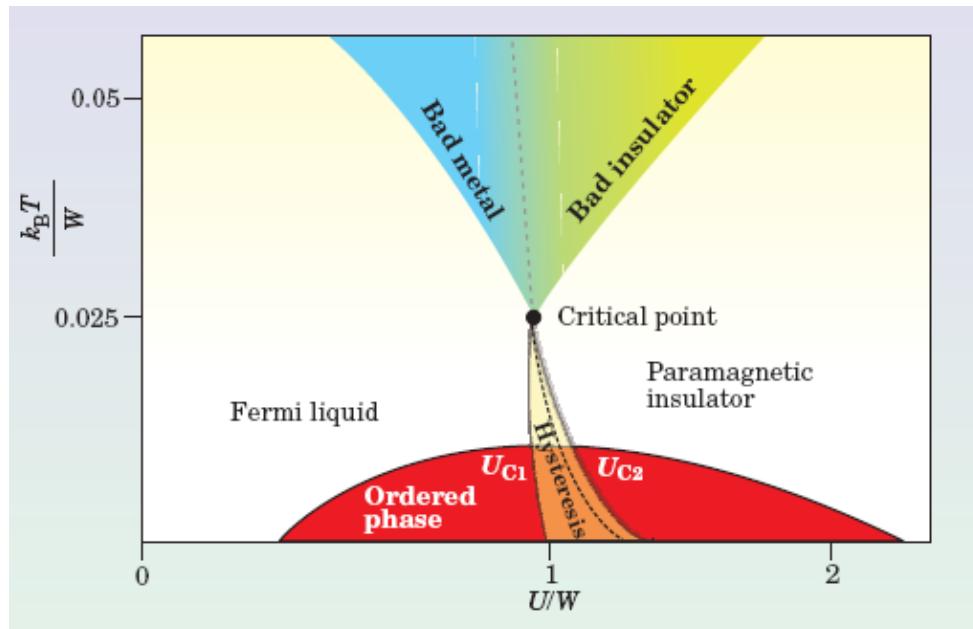
$$\frac{dP}{dT} = \frac{s_2 - s_1}{v_2 - v_1} = \frac{\Delta s}{\Delta v}.$$

Localization-delocalization transition

V_2O_3 :
Mott metal-insulator transition

3He :
liquid-solid transition





Strongly correlated
electron materials:
 V_2O_3 , $\text{NiSe}_{2-x}\text{S}_x$, κ -organics, ...

Helium-3

Universality due to
Fermi statistics + correlations

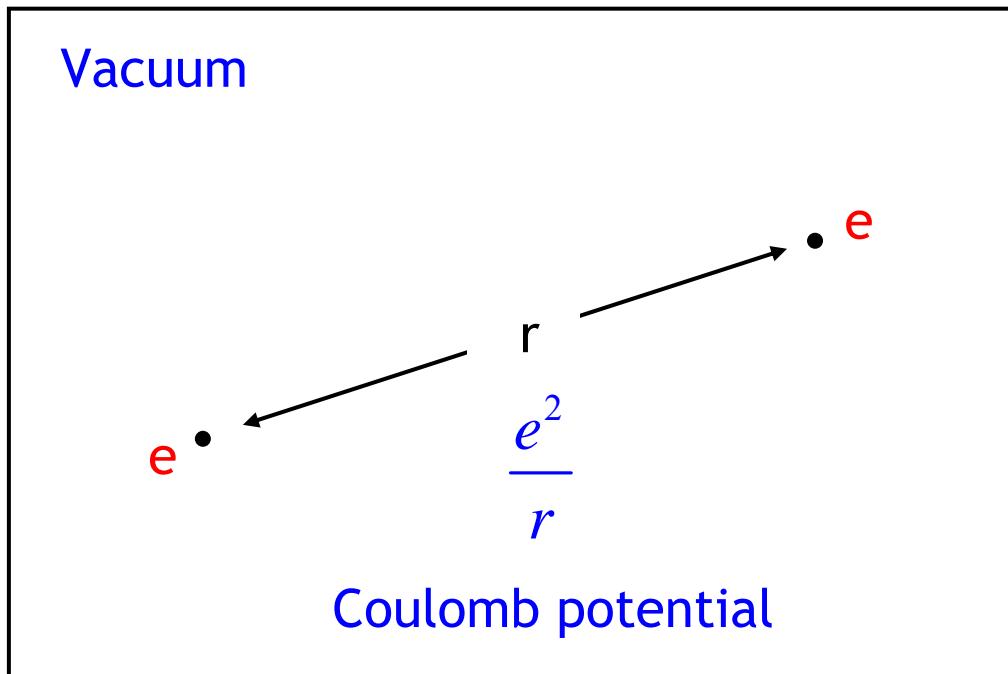
Peculiarities of Many-Particle Systems and “Emergence“

Interacting many-particle systems

Elementary (“bare”) particles + interactions

$$\downarrow \quad N \rightarrow \infty$$

effective (“quasi”) particles + effective interactions



Interacting many-particle systems

Elementary (“bare”) particles + interactions

$$\downarrow \quad N \rightarrow \infty$$

effective (“quasi”) particles + effective interactions

Electron gas: Screening

Simplest approximation: Thomas-Fermi

$$\frac{e^2}{r} e^{-r/\xi}$$

Effective Yukawa potential

Interacting many-particle systems

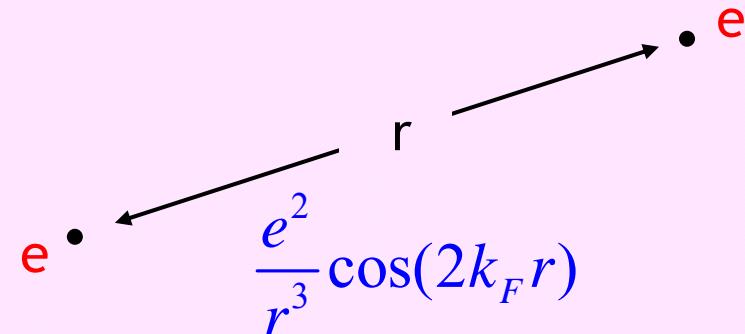
Elementary (“bare”) particles + interactions

$$\downarrow \quad N \rightarrow \infty$$

effective (“quasi”) particles + effective interactions

Electron gas: Screening

Better approximation: Lindhard



Friedel oscillations

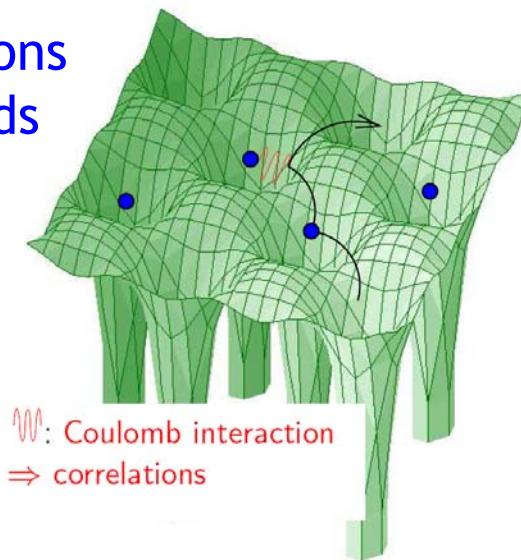
Interacting many-particle systems

Elementary (“bare”) particles + interactions

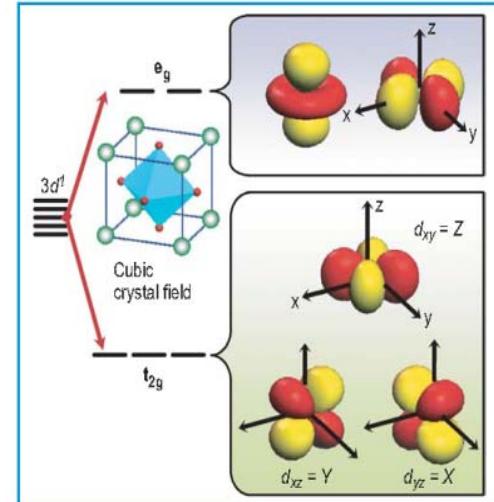
$$\downarrow \quad N \rightarrow \infty$$

effective (“quasi”) particles + effective interactions

Electrons
in solids



⌚: Coulomb interaction
⇒ correlations



“Strong interaction” of
electrons in localized orbitals

Interacting many-particle systems

Elementary (“bare”) particles + interactions

$$\downarrow \quad N \rightarrow \infty$$

effective (“quasi”) particles + effective interactions

Entirely new phenomena arise, e.g., phase transitions

Strategy of Statistical Physics to detect Phase Transitions

Hamiltonian of many-body system

$$H(V, N)$$



Energy of microstate i

$$E_i(V, N)$$



Partition function

$$Z(T, V, N) = \sum_i e^{-E_i/k_B T}$$



Free energy

$$F(T, V, N) = -k_B T \ln Z$$



Chemical potential

$$G(T, P, N) = N\mu(T, P)$$

Sum of analytic terms
→ Z analytic ?!

Thermodynamic limit:
 $N, V \rightarrow \infty, N/V = const.$

→ infinitely many terms
→ Z, μ can become
non-analytic



↓ Lee, Yang (1952)

Singularity in $\mu^{(n)}(T, P)$ ↔ Phase transition

Strategy of Statistical Physics to detect Phase Transitions

Hamiltonian of
many-body system

$$H(V, N)$$



Energy of microstate i

$$E_i(V, N)$$



Partition function

$$Z(T, V, N) = \sum_i e^{-E_i/k_B T}$$



Free energy

$$F(T, V, N) = -k_B T \ln Z$$



Chemical potential

$$G(T, P, N) = N\mu(T, P)$$

Sum of analytic terms
→ Z analytic ?!

Thermodynamic limit:
 $N, V \rightarrow \infty, N/V = const.$
→ infinitely many terms
→ Z, μ can become
non-analytic

↓ Lee, Yang (1952)

Thermodynamic limit → unpredicted new phenomena

Interacting many-particle systems

$$\downarrow \quad N \rightarrow \infty$$

Entirely new phenomena, e.g., phase transitions



Unpredicted “emergent” behavior

We used to think that if we knew one, we knew two,
because one and one are two.

We are finding out that we must learn a great deal more about 'and'.

Arthur Eddington (1882-1944)

“More is different”

Anderson (1972)

Interacting many-particle systems

↓ $N \rightarrow \infty$

Emergence

Examples:

Superconductivity
Magnetism
Galaxy formation

Traffic
Weather
Stock market

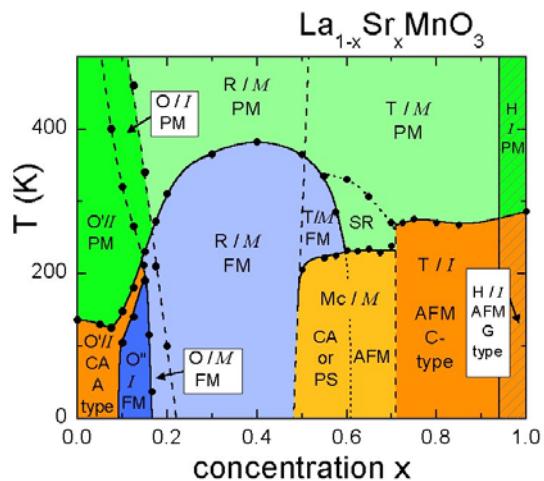
Ants
Human body
Consciousness

© The Institute for Complex Adaptive matter (ICAM)

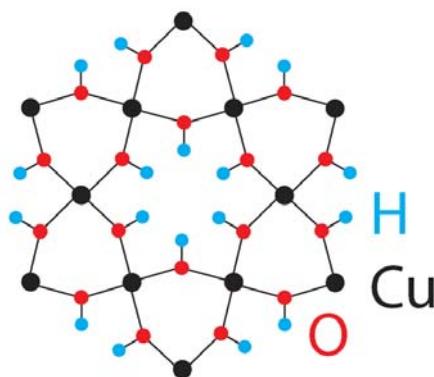
New Developments & Perspectives

(i) Complex correlated electron materials

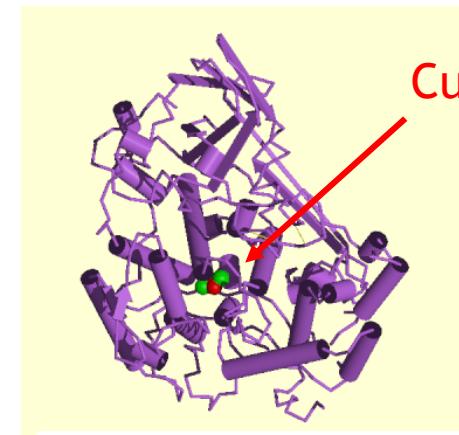
Explanation & prediction of properties of complex materials



Phase diagram of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$
Hemberger *et al.* (2002)



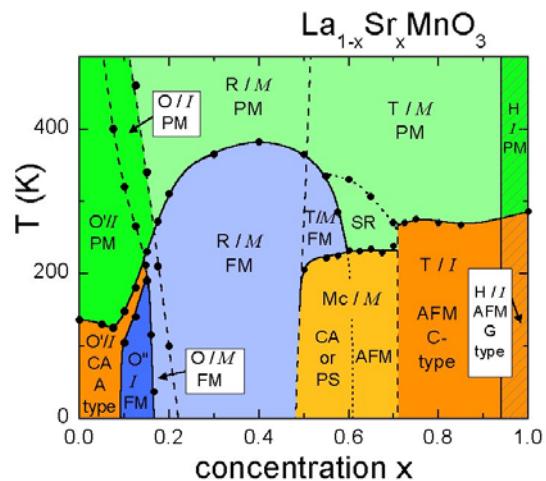
Kagome layer in
 $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$
(herbertsmithite):
Spin liquid behavior



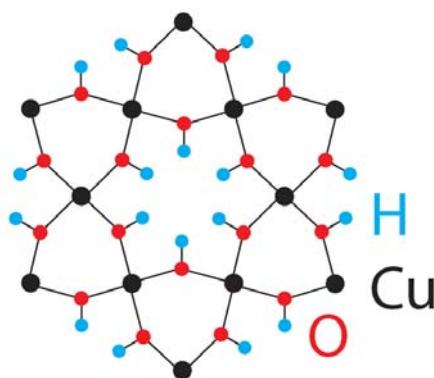
1, 2, ... multi-electron
transfer in
metalloprotein
complexes
→ Photosynthesis

(i) Complex correlated electron materials

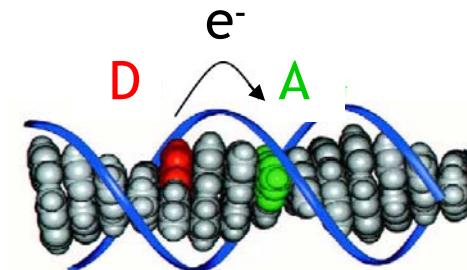
Explanation & prediction of properties of complex materials



Phase diagram of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$
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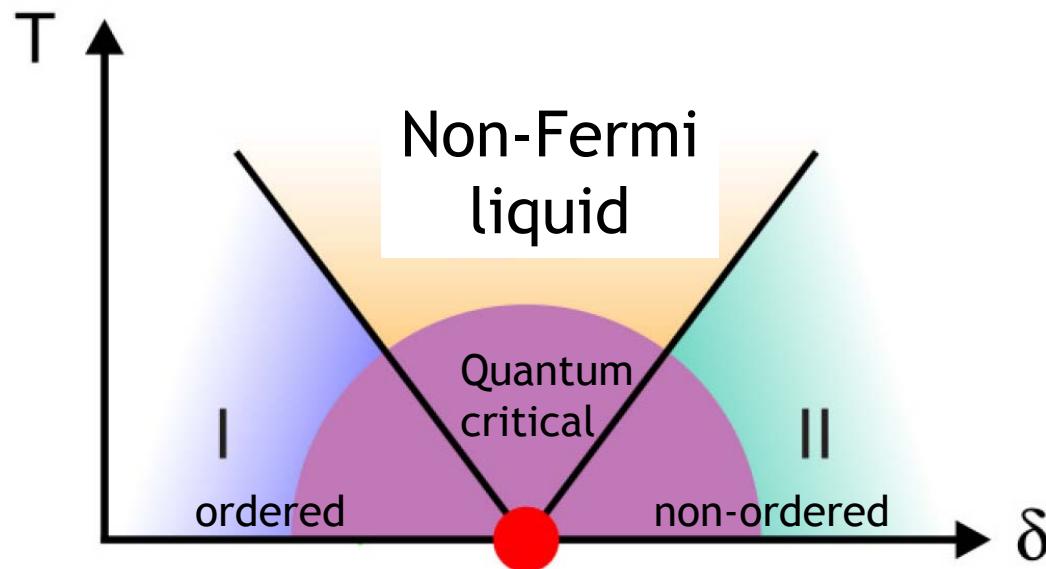


Kagome layer in
 $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$
(herbertsmithite):
Spin liquid behavior



1, 2, ... multi-electron
transfer in DNA
→ damage & repair

(ii) Quantum phase transitions



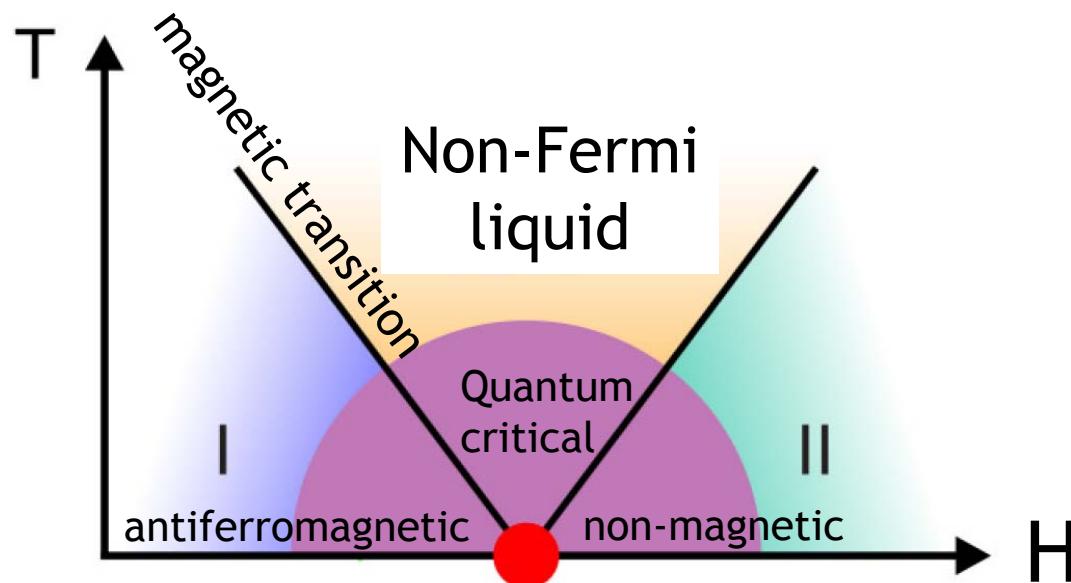
Quantum critical point

© DFG Research Unit
(Augsburg-Dresden-Göttingen-Karlsruhe-Köln-München, 2007)

Driven by quantum fluctuations

- Non-Fermi liquid behavior
- Emergence of novel degrees of freedom
- New phases of matter

(ii) Quantum phase transitions



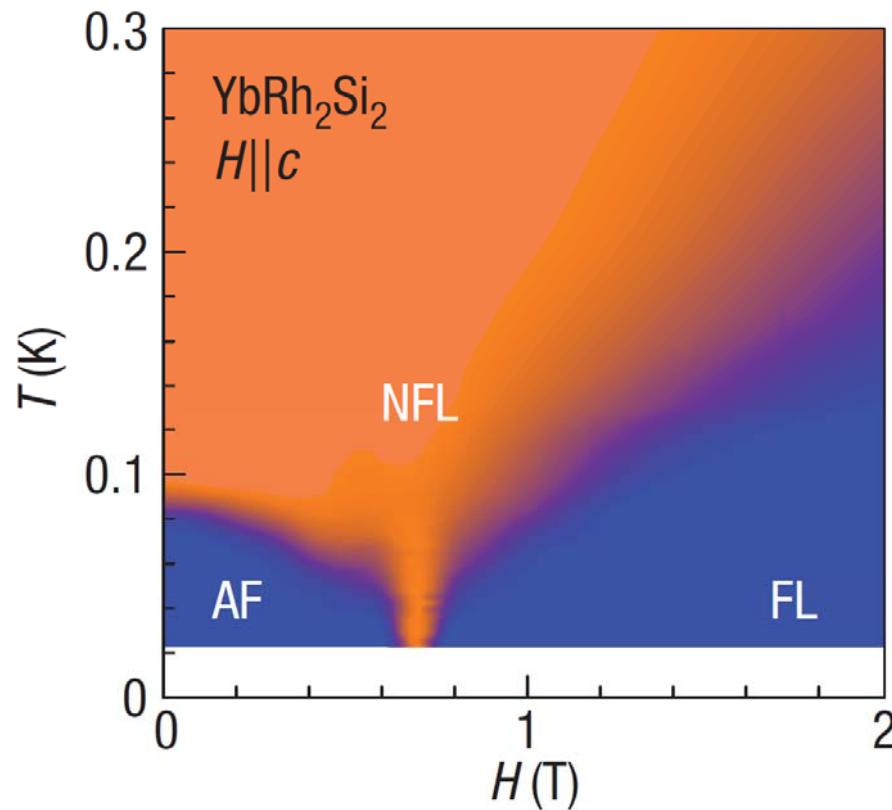
Quantum critical point

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(Augsburg-Dresden-Göttingen-Karlsruhe-Köln-München, 2007)

Driven by quantum fluctuations

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(ii) Quantum phase transitions



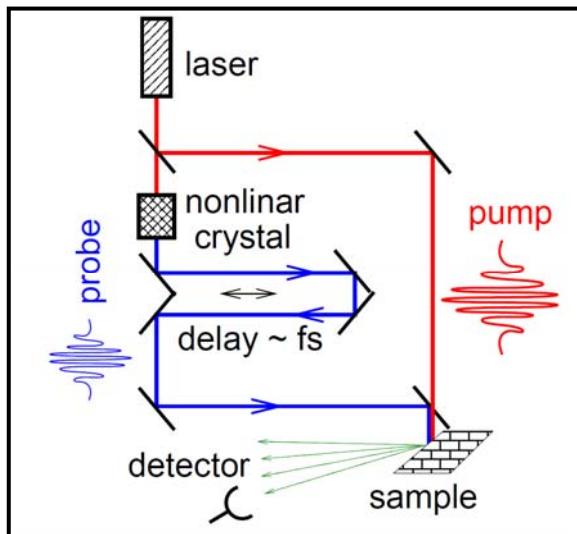
Custers *et al.* (2003)

Driven by quantum fluctuations

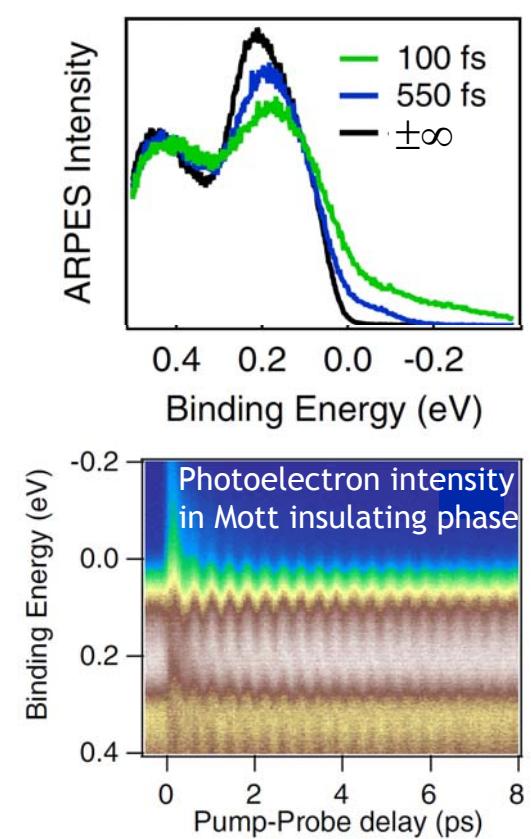
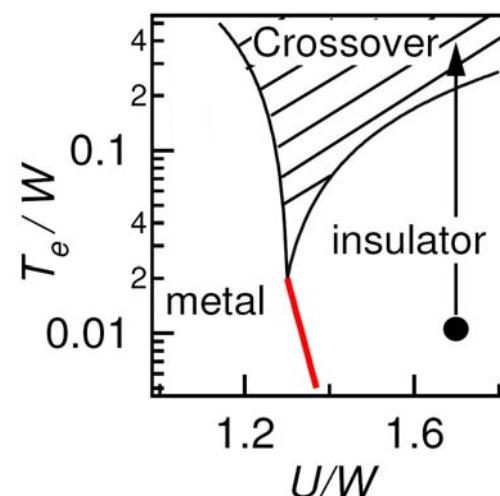
- Non-Fermi liquid behavior
- Emergence of novel degrees of freedom
- New phases of matter

(iii) Correlated electrons in non-equilibrium

Real time evolution of correlation phenomena, e.g.,
time-resolved optical photoemission



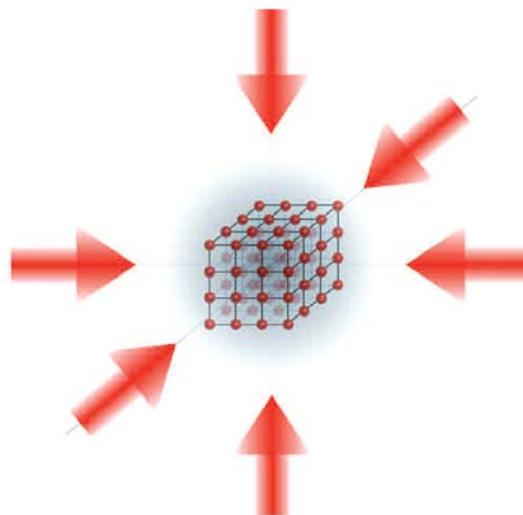
Pump-probe experiment



Perfetti *et al.* (2006)

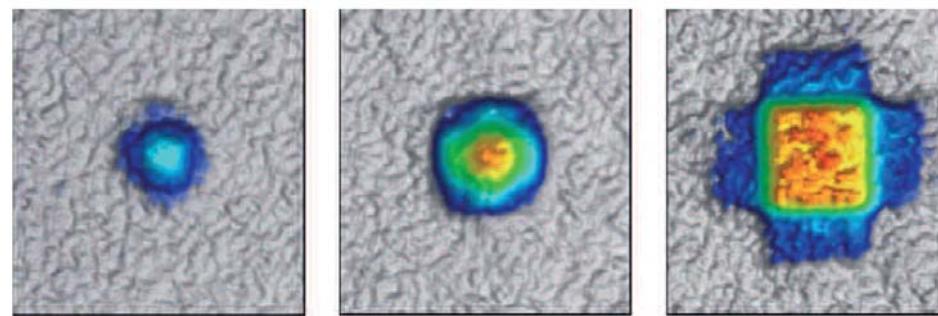
Required: Theory of non-equilibrium beyond
linear response in correlated bulk materials

(iv) Correlated fermionic/bosonic atoms in optical lattices



Modugno et al. (2003)

Bosonic/fermionic atoms in optical lattices

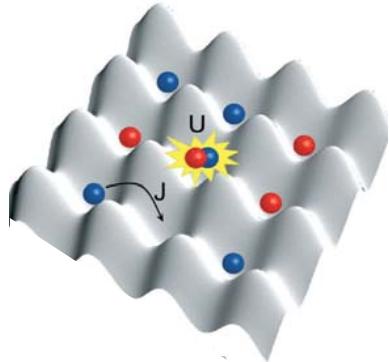


Köhl, Esslinger (2006)

Observation of Fermi surface (^{40}K atoms)

High degree of tunability: “Many-body tool box”

(iv) Correlated fermionic/bosonic atoms in optical lattices



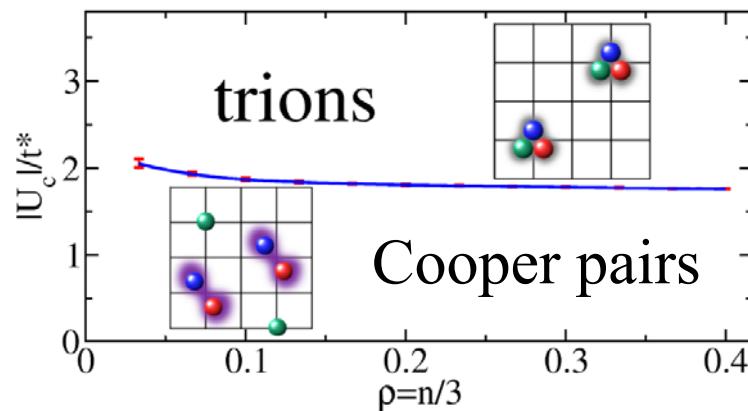
Hubbard model with ultracold atoms Jaksch *et al.* (1998)

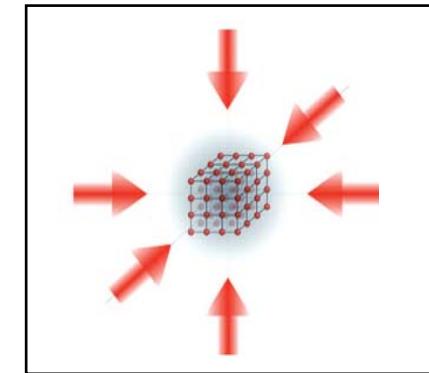
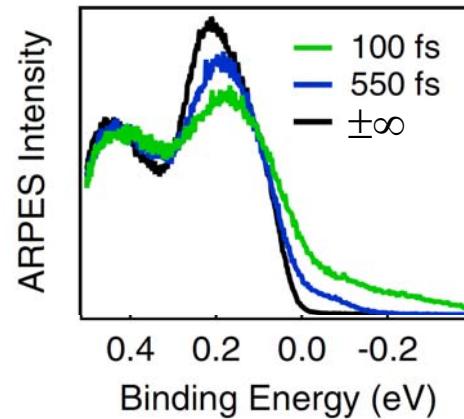
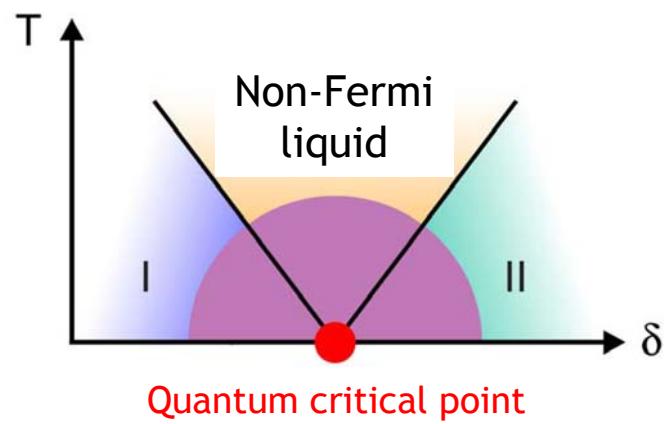
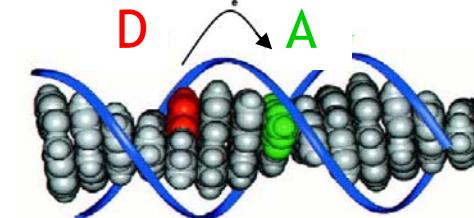
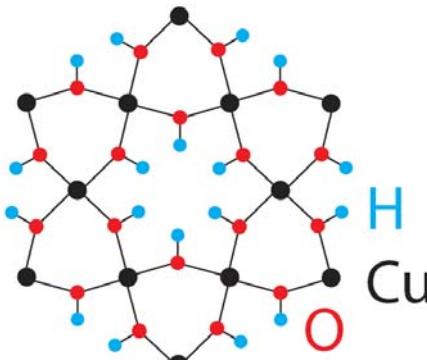
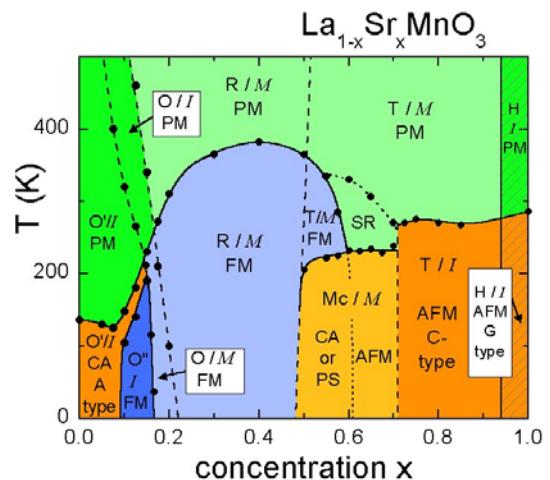
Angular momentum $L^{\text{tot}} = F \rightarrow N=2F+1$ hyperfine states

→ SU(N) Hubbard models

Honerkamp, Hofstetter (2004)

$N=3$, e.g. ${}^6\text{Li}$, $U<0$: Color superconductivity, baryon formation (QCD)
Rapp *et al.* (2006)





Correlated many-particle systems:
More manifold and fascinating than ever