Strong Correlations and High Temperature Superconductivity

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Superconductivity : a typical example of a condensed matter physics problem

- 100 aniversary of its disvovery.
- Has impacted fields ranging from nuclear physics , astrophysics (pulsars, neutron stars), particle physics (Higgs mechanism)
- Emergent Phenomena

- Advances thru interplay of theory and experiment.
- Many applications resulting from basic research.
- progress in materials needed now more than ever.
- Illustrates relations technical advances, scientific discovery and understanding.
- Importance of “model Hamiltonian “ studies and first principles calculations.

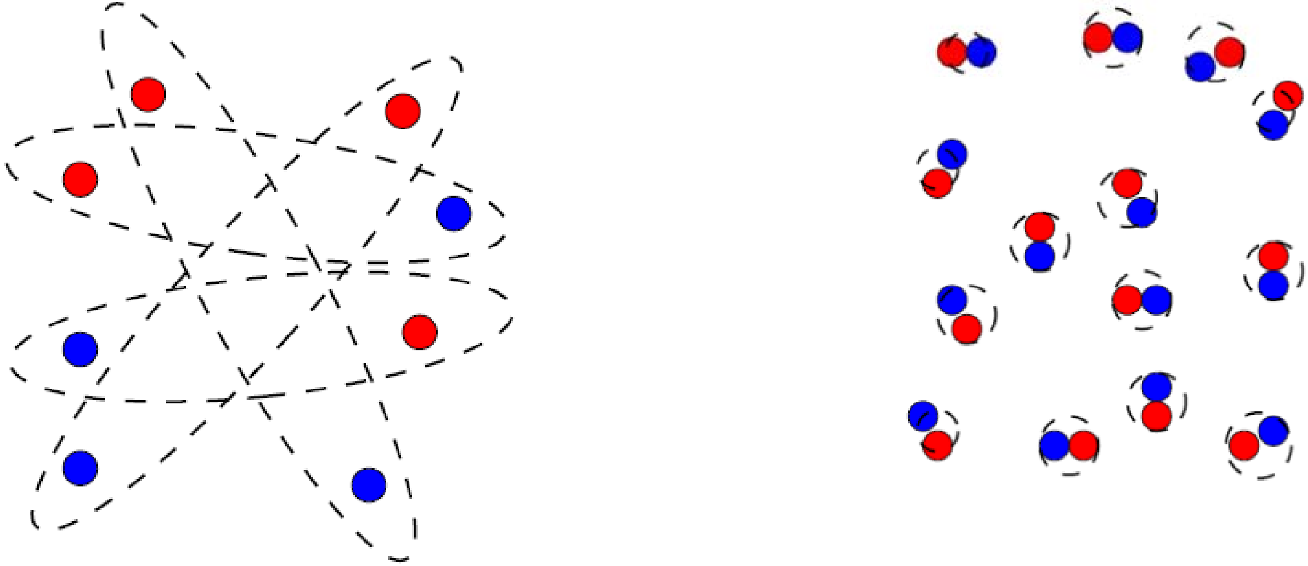
Plan of the lectures

- Give a guided tour of the landsapce of interesting superconducting materials (many strongly correlated!)
- Stress open issues as well as the current theoretical understanding of the problem. What to look for ?
- Incomplete understanding, limited experimental info, primitive theoretical tools. [lecture will combine info from theory, phenomenologies and experimental]

  - De hoc, multi nosciunt multa, omnes aliquid, nemo satis.
    (Of this many have said many things, all something, no one enough)

Bon Voyage!

It is accepted following BCS that superconductivity is due to pairing a phase coherence



Pairing and phase coherence. ODLRO in two particle quantities in the sense of C.N.Yang RMP 34 695 (1962)

SC results from BCS pairing, but very basic”big picture” questions remain

- What is the character of the wave function of the pair, in particular its symmetry
- Does superconductivity emerge from a Fermi liquid (i.e. electrons behave like a Fermi gas with effective parameters just above the transition) ? Or not, in which case what are we pairing ?
- What is the “mechanism “ for superconductivity. To be defined more rigorously later.

- Migdal Eliashberg theory was the first attempt to describe pairing when quasiparticles are ill defined due to strong scattering. Derive the equations . Discuss its applicability. Earliest theoretical attempt to address what controls Tc.

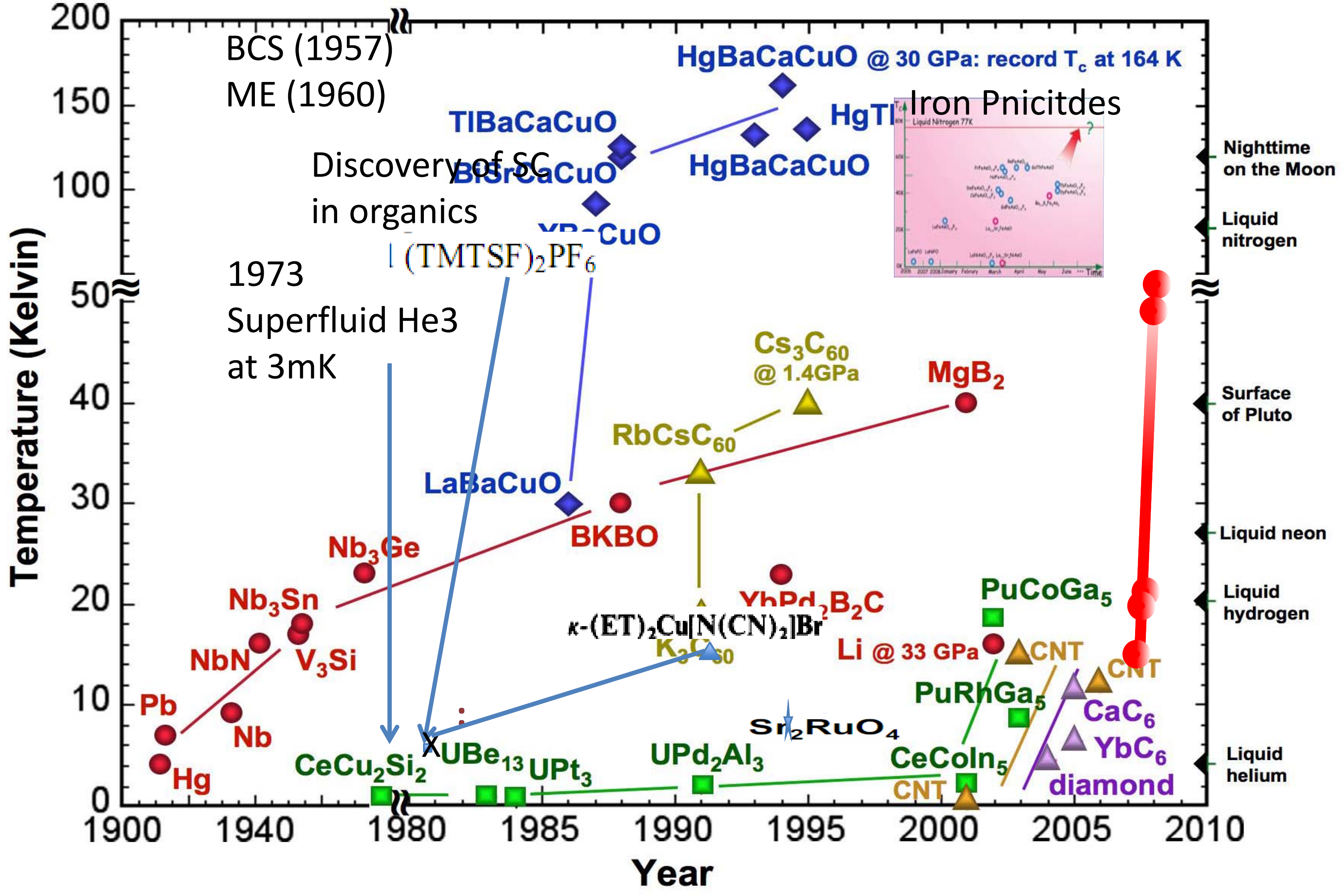
  Very much in vogue in connection with spin fluctuation theories.
- DMFT and its extensions describes well the incoherent high temperature state of many oxides. Formulate the issue of mechanism precisely in this framework.

Adress these issues thru and overview of many families of compounds discovered over many years

- Look for similarities and differences between high Tc materials with the "big picture" questions in mind.
- Search for trends within a family of materials and within families of materials. Domes. Competing orders (SDW , CDW) . Fermi Surface Nesting. Quantum Criticality]
- Existing phenomenologies correlating normal state or superconducting state properties to Tc. : [Homes law, $1/T_1T$ correlations, kinetic energy plots, Uemura plot, specific heat plots]
- Do they serve new set of "Matthias Rules" for the XXI century? [beyond expect the unexpected]
- Look at the constant interplay of theory and experiment , and the interplay of technical advances and discovery. [even if serendipity is still the driving force behind the discovery of high Tc materials]
- Show some illustrative example of the power of realistic electronic structure calculations of correlated materials in various systems.

“T_c vs. Time”

http://science.energy.gov/~/media/bes/pdf/reports/files/sc_rpt.pdf



BCS (1957)
ME (1960)

Discovery of SC
in organics

(TMTSF)$_2$PF$_6$

1973
Superfluid He3
at 3mK

Iron Pnicitdes

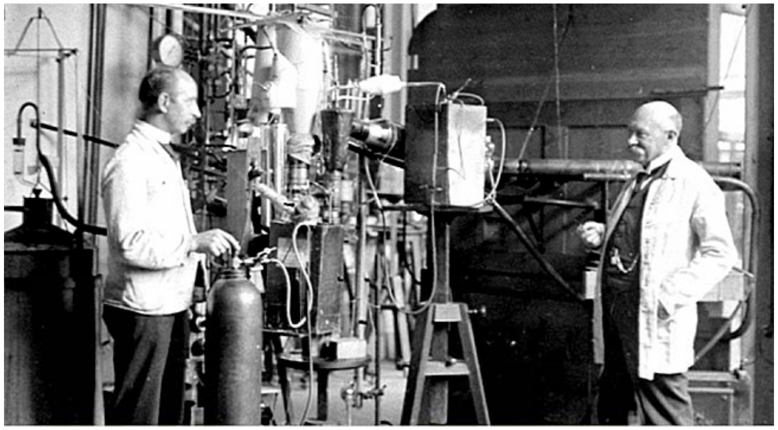
κ-(ET)$_2$Cu[N(CN)$_2$]Br

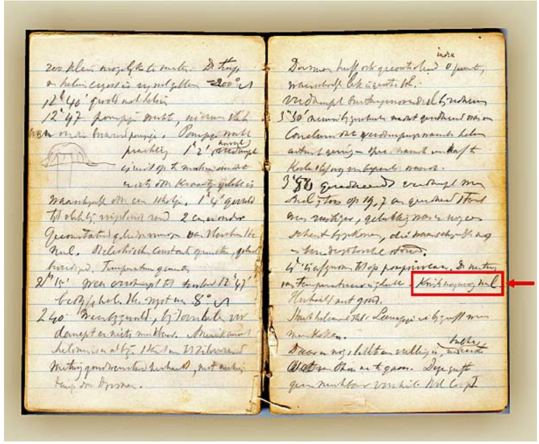
X

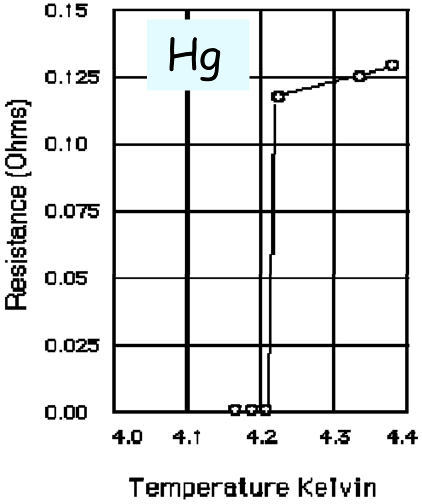
http://www.sc.doe.gov/bes/reports.lists.html

100 years ago: “mercury practically zero”

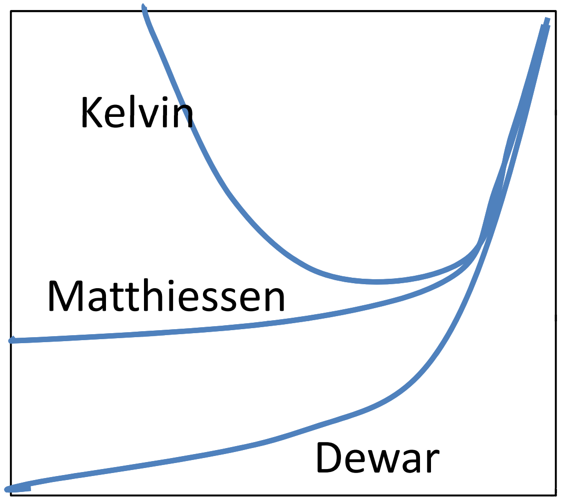
1911 Heike Kamerlingh Onnes discovery







Dirk van Delft and Peter Kes,
Physics Today 63(8), 38 (2010)



Result of a focused effort of many years to liqueify Helium to reach low temperatures. Desire to understand the behavior of metals at low T. Still serendipity at play.

Only a few structures are conduc tive to superconductivity in elements under zero pressure . FCC, HEX , BCC. Type one Superconductors

Strong coupling SC

Lead (Pb)	7.196 K	FCC
Lanthanum (La)	4.88 K	HEX
Tantalum (Ta)	4.47 K	BCC
Mercury (Hg)	4.15 K	RHL
Tin (Sn)	3.72 K	TET
Indium (In)	3.41 K	
Palladium (Pd)*	3.3 K	
Chromium (Cr)*	3 K	
Thallium (Tl)	2.38 K	
Rhenium (Re)	1.697 K	HEX
Protactinium (Pa)	1.40 K	TET
Thorium (Th)	1.38 K	FCC
Aluminum (Al)	1.175 K	FCC
Gallium (Ga)	1.083 K	ORC
Molybdenum (Mo)	0.915 K	BCC
Zinc (Zn)	0.85 K	HEX
Osmium (Os)	0.66 K	HEX
Zirconium (Zr)	0.61 K	HEX
Americium (Am)	0.60 K	HEX
Cadmium (Cd)	0.517 K	HEX
Ruthenium (Ru)	0.49 K	HEX
Titanium (Ti)	0.40 K	HEX
Uranium (U)	0.20 K	ORC
Hafnium (Hf)	0.128 K	HEX
Iridium (Ir)	0.1125 K	FCC
Beryllium (Be)	0.023 K (SRM 768)	HEX
Tungsten (W)	0.0154 K	BCC
Platinum (Pt)*	0.0019 K	
Lithium (Li)	0.0004 K	
Rhodium (Rh)	0.000325 K	FCC

Under irradiation
Thin film form

powder

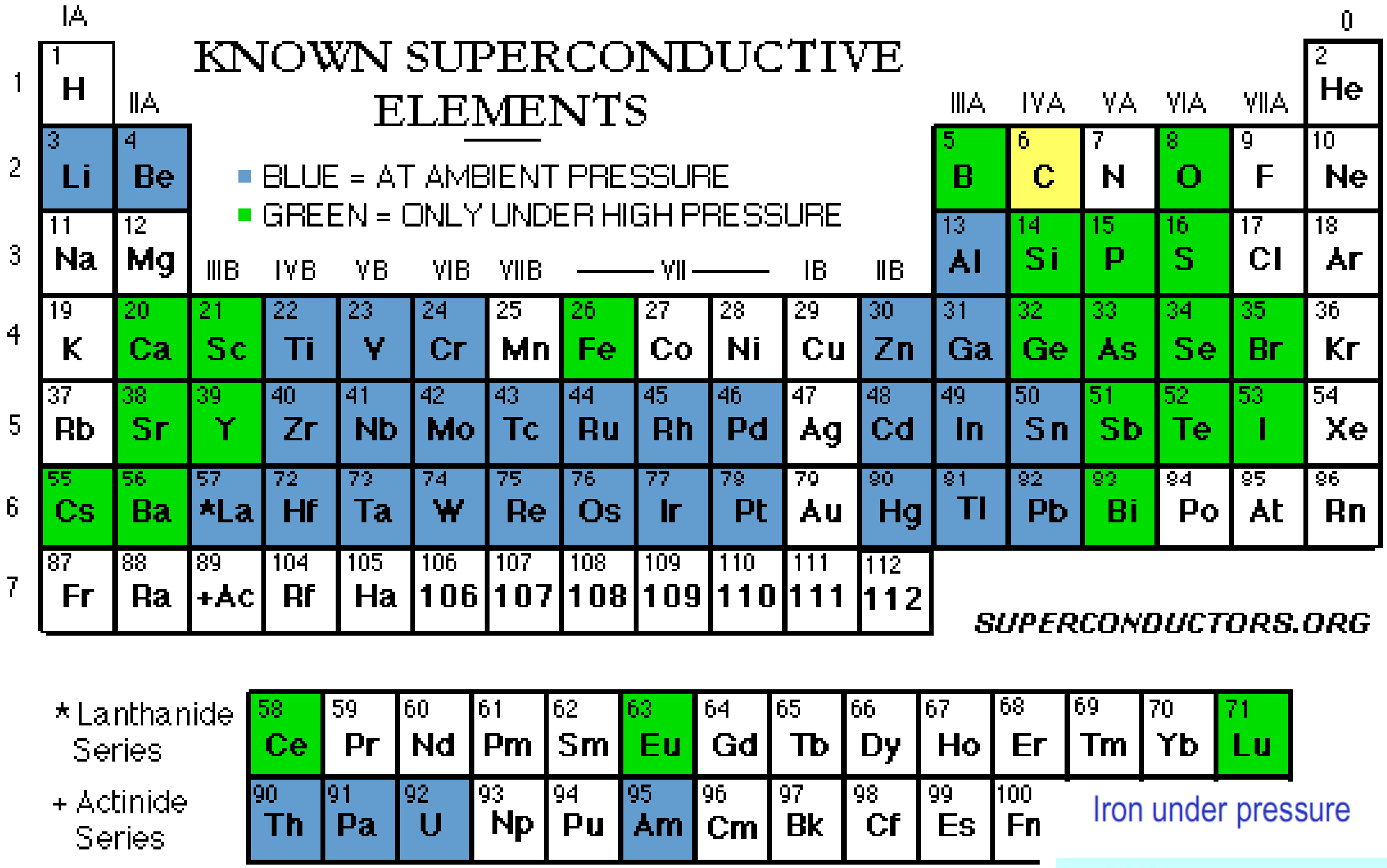
CUB	cubic	**MCL**	monoclinic
FCC	face centered cubic	**DIA**	diamond
BCC	body centered cubic	**ORC**	orthorhombic
HEX	hexagonal	**RHL**	rhombohedral
TET	tetragonal	**SCB**	simple cubic

Type2

C	15 K
Nb	9.25 K
Tc	7.80 K
V	5.40 K

Lattice: C=Fullerene, Nb=BCC, Tc=HEX, V=BCC

http://www.superconductors.org/TYPe1.htm



KNOWN SUPERCONDUCTIVE ELEMENTS

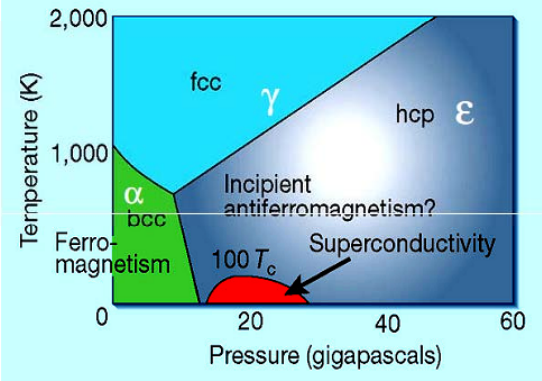
🟦 BLUE = AT AMBIENT PRESSURE
🟩 GREEN = ONLY UNDER HIGH PRESSURE

	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1	1 H																	2 He
2	🟦 3 Li	🟦 4 Be											🟩 5 B	🟨 6 C	7 N	🟩 8 O	9 F	10 Ne
3	11 Na	12 Mg											🟦 13 Al	🟩 14 Si	🟩 15 P	🟩 16 S	17 Cl	18 Ar
4	19 K	🟩 20 Ca	🟩 21 Sc	🟦 22 Ti	🟦 23 V	🟦 24 Cr	25 Mn	🟩 26 Fe	27 Co	28 Ni	29 Cu	🟦 30 Zn	🟦 31 Ga	🟩 32 Ge	🟩 33 As	🟩 34 Se	🟩 35 Br	36 Kr
5	37 Rb	🟩 38 Sr	🟩 39 Y	🟦 40 Zr	🟦 41 Nb	🟦 42 Mo	🟦 43 Tc	🟦 44 Ru	🟦 45 Rh	🟩 46 Pd	47 Ag	🟦 48 Cd	🟦 49 In	🟦 50 Sn	🟩 51 Sb	🟩 52 Te	🟩 53 I	54 Xe
6	🟩 55 Cs	🟩 56 Ba	🟦 57 *La	🟦 72 Hf	🟦 73 Ta	🟦 74 W	🟦 75 Re	🟦 76 Os	🟦 77 Ir	🟦 78 Pt	79 Au	🟦 80 Hg	🟦 81 Tl	🟦 82 Pb	🟩 83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 +Ac	104 Rf	105 Ha	106 106	107 107	108 108	109 109	110 110	111 111	112 112						

SUPERCONDUCTORS.ORG

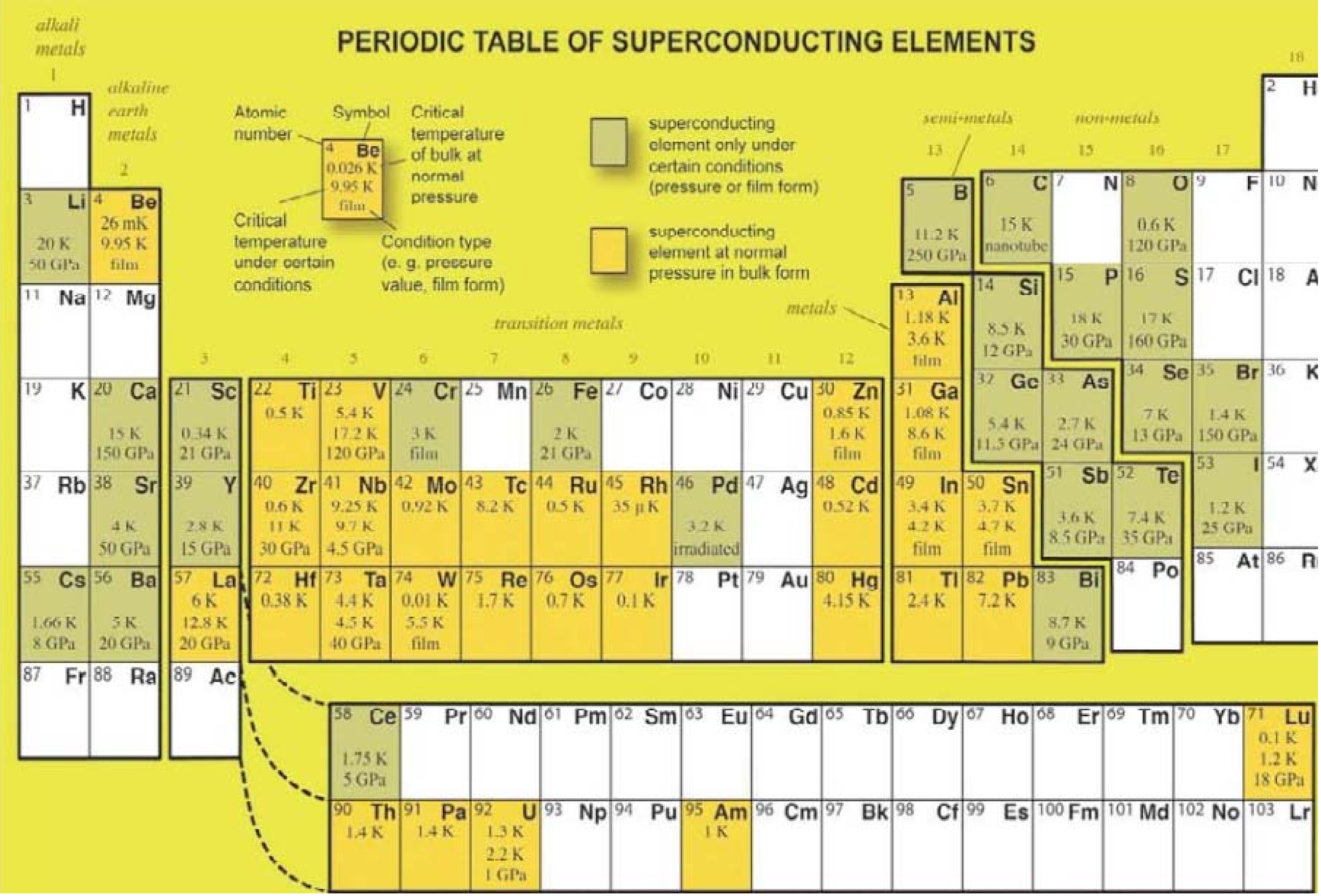
* Lanthanide Series	🟩 58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	🟩 63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	🟩 71 Lu
+ Actinide Series	🟦 90 Th	🟦 91 Pa	🟦 92 U	93 Np	94 Pu	🟦 95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fn			

Iron under pressure



Only a few fermi liquids survive low T and high P.
New physics even in simple elements!

http://www.superconductors.org/Type1.htm



PERIODIC TABLE OF SUPERCONDUCTING ELEMENTS

Atomic number — Symbol — Critical temperature of bulk at normal pressure

4 Be
0.026 K
9.95 K
film

Critical temperature under certain conditions — Condition type (e. g. pressure value, film form)

🟩 superconducting element only under certain conditions (pressure or film form)

🟨 superconducting element at normal pressure in bulk form

alkali metals · *alkaline earth metals* · *transition metals* · *metals* · *semi-metals* · *non-metals*

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H																	2 H
3 Li 20 K 50 GPa	4 Be 26 mK 9.95 K film											5 B 11.2 K 250 GPa	6 C 15 K nanotube	7 N	8 O 0.6 K 120 GPa	9 F	10 N
11 Na	12 Mg											13 Al 1.18 K 3.6 K film	14 Si 8.5 K 12 GPa	15 P 18 K 30 GPa	16 S 17 K 160 GPa	17 Cl	18 A
19 K	20 Ca 15 K 150 GPa	21 Sc 0.34 K 21 GPa	22 Ti 0.5 K	23 V 5.4 K 17.2 K 120 GPa	24 Cr 3 K film	25 Mn	26 Fe 2 K 21 GPa	27 Co	28 Ni	29 Cu	30 Zn 0.85 K 1.6 K film	31 Ga 1.08 K 8.6 K film	32 Ge 5.4 K 11.5 GPa	33 As 2.7 K 24 GPa	34 Se 7 K 13 GPa	35 Br 1.4 K 150 GPa	36 K
37 Rb	38 Sr 4 K 50 GPa	39 Y 2.8 K 15 GPa	40 Zr 0.6 K 11 K 30 GPa	41 Nb 9.25 K 9.7 K 4.5 GPa	42 Mo 0.92 K	43 Tc 8.2 K	44 Ru 0.5 K	45 Rh 35 µK	46 Pd 3.2 K irradiated	47 Ag	48 Cd 0.52 K	49 In 3.4 K 4.2 K film	50 Sn 3.7 K 4.7 K film	51 Sb 3.6 K 8.5 GPa	52 Te 7.4 K 35 GPa	53 I 1.2 K 25 GPa	54 X
55 Cs 1.66 K 8 GPa	56 Ba 5 K 20 GPa	57 La 6 K 12.8 K 20 GPa	72 Hf 0.38 K	73 Ta 4.4 K 4.5 K 40 GPa	74 W 0.01 K 5.5 K film	75 Re 1.7 K	76 Os 0.7 K	77 Ir 0.1 K	78 Pt	79 Au	80 Hg 4.15 K	81 Tl 2.4 K	82 Pb 7.2 K	83 Bi 8.7 K 9 GPa	84 Po	85 At	86 R
87 Fr	88 Ra	89 Ac															

58 Ce 1.75 K 5 GPa	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu 0.1 K 1.2 K 18 GPa
90 Th 1.4 K	91 Pa 1.4 K	92 U 1.3 K 2.2 K 1 GPa	93 Np	94 Pu	95 Am 1 K	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

PRL **94,** 097002 (2005) PHYSICAL REVIEW LETTERS week ending 11 MARCH 2005

Superconductivity in the Americium Metal as a Function of Pressure: Probing the Mott Transition

J.-C. Griveau, J. Rebizant, and G. H. Lander
European Commission, Joint Research Centre, Institute for Transuranium, Elements Postfach 2340, 76125 Karlsruhe, Germany

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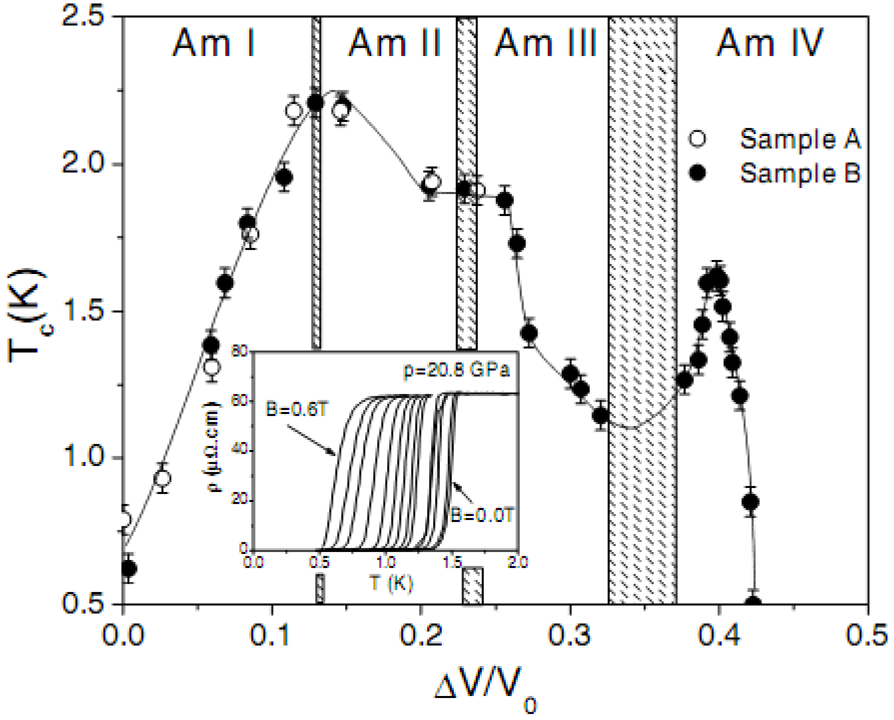
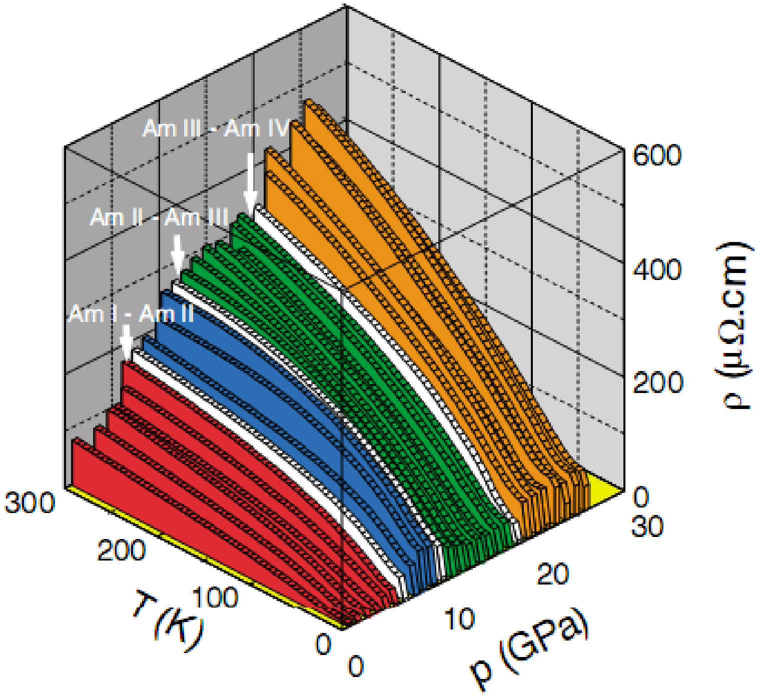
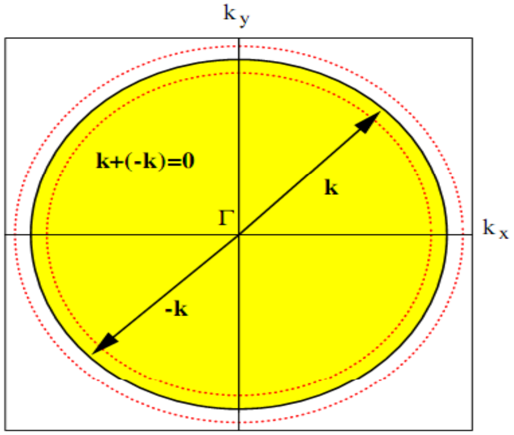




1972

$$H = H(band) + H(el.\text{-}phonon) + H(phonon) + H(el.\text{-}el.)$$

$$H_{red} = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{kk'} V_{k,k'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow} ,$$



Reduced Hamiltonian and mean field solution!

phase transition
Meissner effect
Josephson effect
ultrasonic attenuation

order parameter
zero resistance
specific heat
NMR

energy gap
flux quantization
spin susceptibility
fluctuation phenomena

Summary of BCS Mean Field Theory

$$\Delta_{\mathbf{k}} = -\frac{1}{N}\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}}\tanh\frac{\beta E_{\mathbf{k}'}}{2}$$

$$n = 1 - \frac{1}{N}\sum_{\mathbf{k}}\frac{\epsilon_{\mathbf{k}} - \mu}{E_{\mathbf{k}}}\tanh\frac{\beta E_{\mathbf{k}}}{2}.$$

where

$$E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + \Delta_{\mathbf{k}}^2}$$

$$\frac{1}{\lambda} = \int_0^{\beta\omega_D/2} dx\,\frac{\tanh x}{x}$$

$$\lambda \equiv N(\mu)V$$

$$T_c = 1.13\omega_D \exp(-1/\lambda).$$

Vkk'   = -V

At T=0 one can solve for the gap

$$\Delta = 2\omega_D\frac{\exp(-1/\lambda)}{1 - \exp(-1/\lambda)}$$

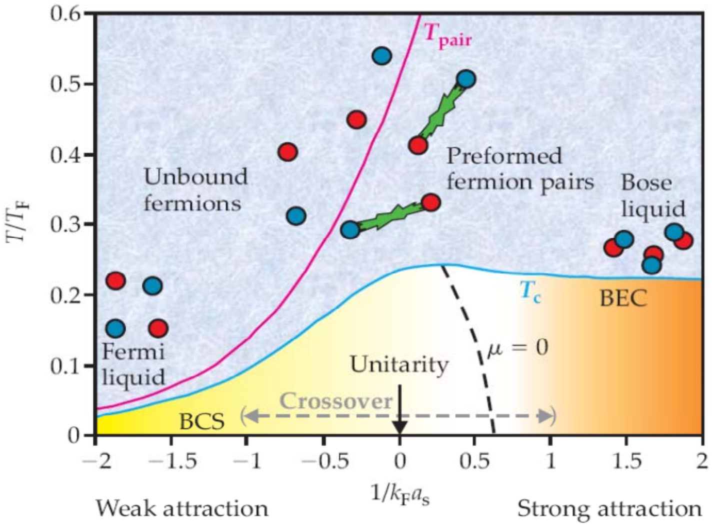
At weak coupling Δ=exp(-1/λ)

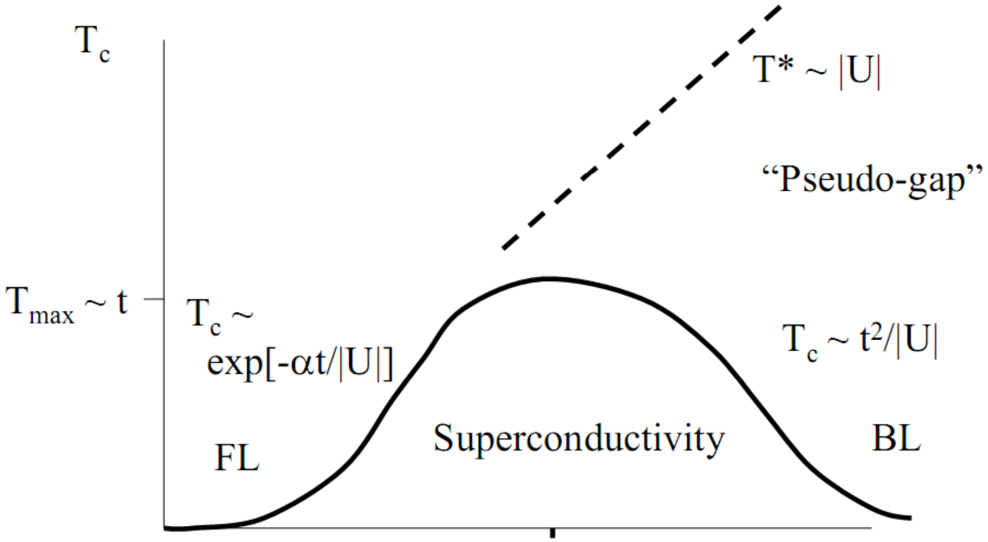
At strong coupling $\Delta = 2\omega_D\lambda.$

BCS approximations break down at strong coupling.

- Q1:   Why (and when !!!!) does MFT work.
- Q2 : When is the effective Hamiltonian a good guide to reality, and how do we estimate its parameter.

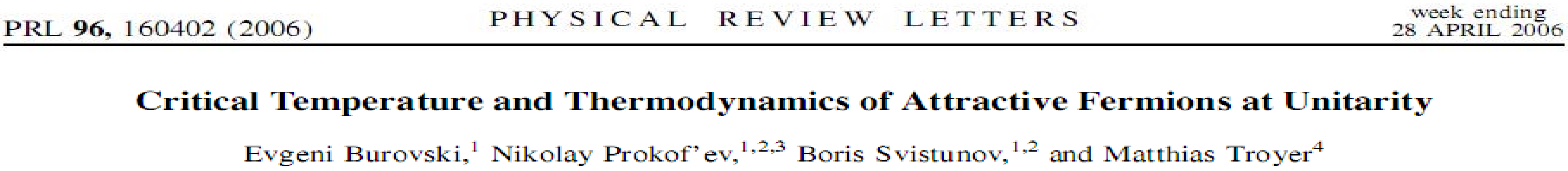
- BEC-BCS Crossover Problem
- A.J. Leggett, Karpacz Lectures (1980)
- P. Nozieres & S. Schmitt-Rink, JLTP 59, 195 (1985)





Review : Sa de Melo, Phys.Today (Oct. 2008)

Negative U Hubbard



PRL **96,** 160402 (2006) PHYSICAL REVIEW LETTERS week ending 28 APRIL 2006

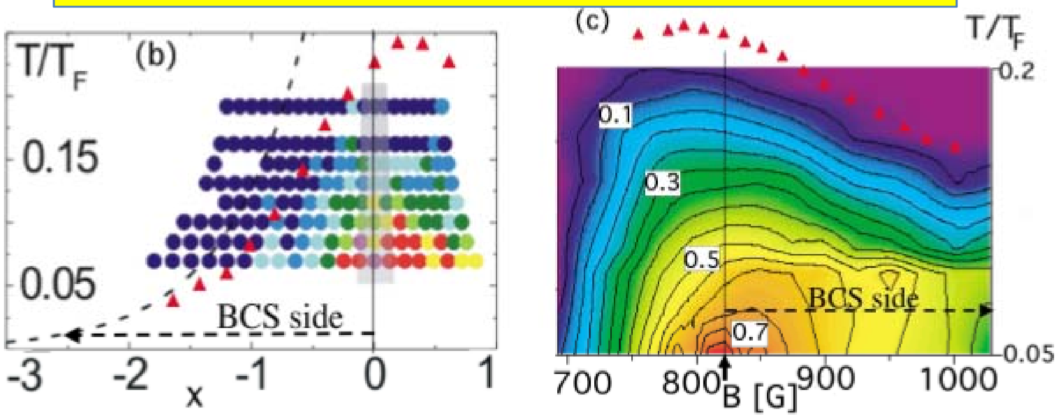
Critical Temperature and Thermodynamics of Attractive Fermions at Unitarity

Evgeni Burovski,[1] Nikolay Prokof'ev,[1,2,3] Boris Svistunov,[1,2] and Matthias Troyer[4]

PRL **96,** 160402 (2006) PHYSICAL REVIEW LETTERS week ending 28 APRIL 2006

Scaling to the continuum the attractive Hubbard model. Diagrammatic QMC

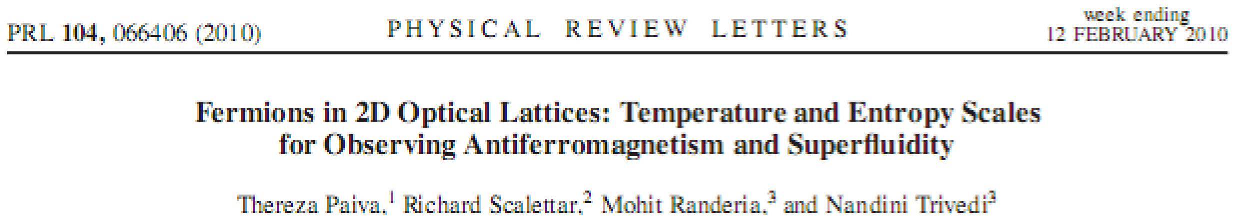
Tc/EF ~ .15



Experimental data:

K: Regal, Greiner & Jin, PRL ('04)
Li: Zwierlein, *et al.*, PRL ('04)

Tc/TF~ .2 , .25

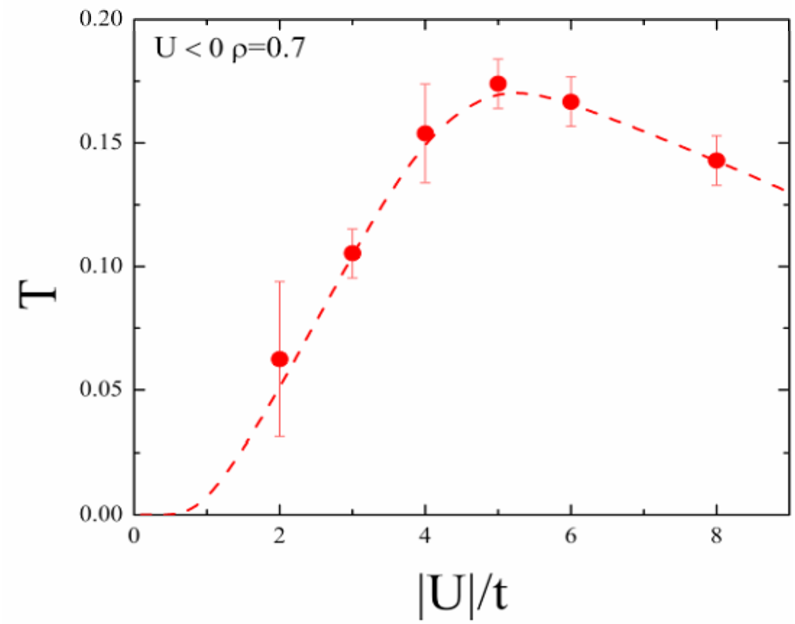


PRL 104, 066406 (2010) PHYSICAL REVIEW LETTERS week ending 12 FEBRUARY 2010

Fermions in 2D Optical Lattices: Temperature and Entropy Scales for Observing Antiferromagnetism and Superfluidity

Thereza Paiva,[1] Richard Scalettar,[2] Mohit Randeria,[3] and Nandini Trivedi[3]

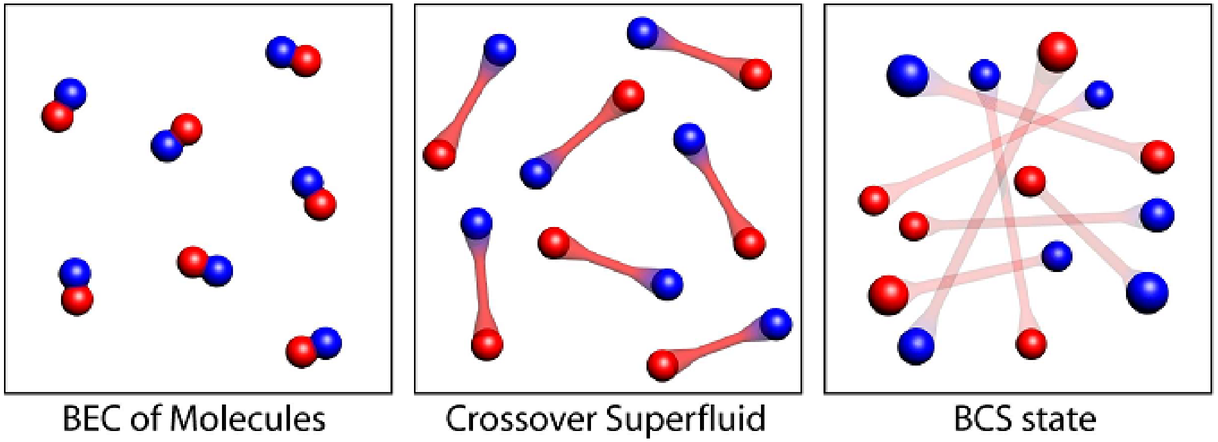
Determinantal Montecarlo on the negative U Hubbard model on a lattice at a particle density of . 7. Tc/t vs U. D=4t (half bandwidth). Tc extracted from SF den



Notice that most results are in the crossover region.
BCS regime is hard to access for simulations and experiments on cold atoms. Solid state materials have much lower Tc /TF.
Continuum models seem to have higher Tc/TF.

Making, probing and understanding ultracold Fermi gases

Wolfgang Ketterle and Martin W. Zwierlein



BEC of Molecules

Crossover Superfluid

BCS state

Fig. 1. – The BEC-BCS crossover. By tuning the interaction strength between the two fermionic spin states, one can smoothly cross over from a regime of tightly bound molecules to a regime of long-range Cooper pairs, whose characteristic size is much larger than the interparticle spacing. In between these two extremes, one encounters an intermediate regime where the pair size is comparable to the interparticle spacing.

System	T_C	T_F	T_C/T_F
Metallic lithium at ambient pressure [88]	0.4 mK	55 000 K	10^{-8}
Metallic superconductors (typical)	1–10 K	50 000 – 150 000 K	$10^{-4\cdots-5}$
^{3}He	2.6 mK	5 K	$5 \cdot 10^{-4}$
MgB_2	39 K	6 000 K	10^{-2}
High-T_C superconductors	35–140 K	2000 – 5000 K	$1 \ldots 5 \cdot 10^{-2}$
Neutron stars	10^{10} K	10^{11} K	10^{-1}
Strongly interacting atomic Fermi gases	200 nK	1 μK	0.2

Table I. – *Transition temperatures, Fermi temperatures and their ratio T_C/T_F for a variety of fermionic superfluids or superconductors.*