Hybridized Course on
Condensed Matter Physics

Tao Xiang

txiang@itp.ac.cn

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Course Time Table

1. Panorama and basic models of Condensed Matter Theory

   Sept 4 to Sept 9 (2 weeks) Tao Xiang

2. Green's Function theory

   Sept 18 to Oct. 16 (4 weeks) Shao-Jing Qin

3. Theory of quantum phase transition

   Oct. 23 to Oct. 30 (2 weeks) Hong-Gang Luo

4. Path integral and mean-field theory

   Nov. 6 to Nov. 20 (3 weeks) Yue Yu

5. Theory of mesoscopic phenomena

   Nov. 27 to Dec. 18 (4 weeks) Zhong-Yi Lu

6. Selected topics: Quantum Hall effect, High-Tc superconductivity, Kondo problem, DFT, DMRG, etc

   Dec 25 to Jan 22 2007 (4 weeks)

What is Condensed Matter Physics?

Old believe:

Solid state physics is the physics of dirt.

Wolfgang Pauli

What is Condensed Matter Physics?

Modern Policy Maker's definition:

- >1/3 of physics
- solid + liquid
- hard + soft matter: de Gennes
- structure + transport: the PRL division
- basis of materials science and engineering

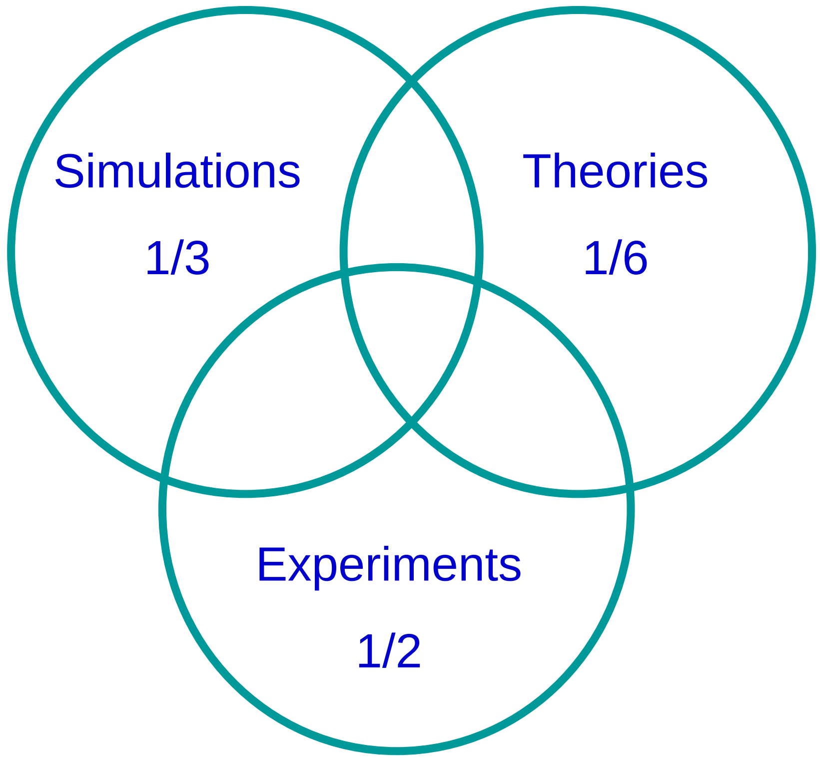
P W Anderson

1977诺贝尔物理奖

Father of "Condensed Matter"

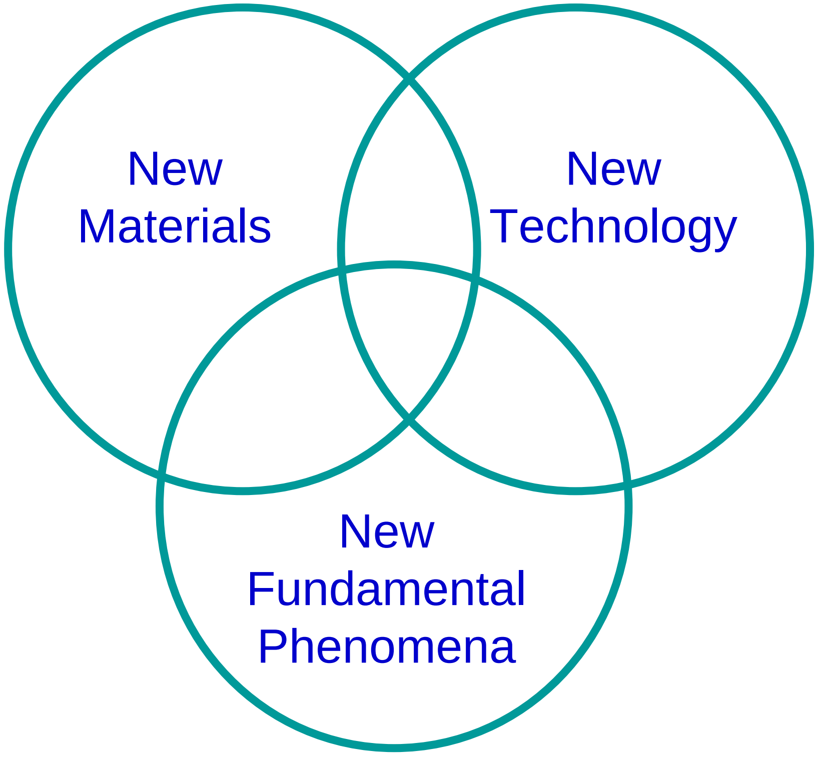
What is Condensed Matter Physics?

Technicians' definition: Methodology



What is Condensed Matter Physics?

Functional definition: Applications

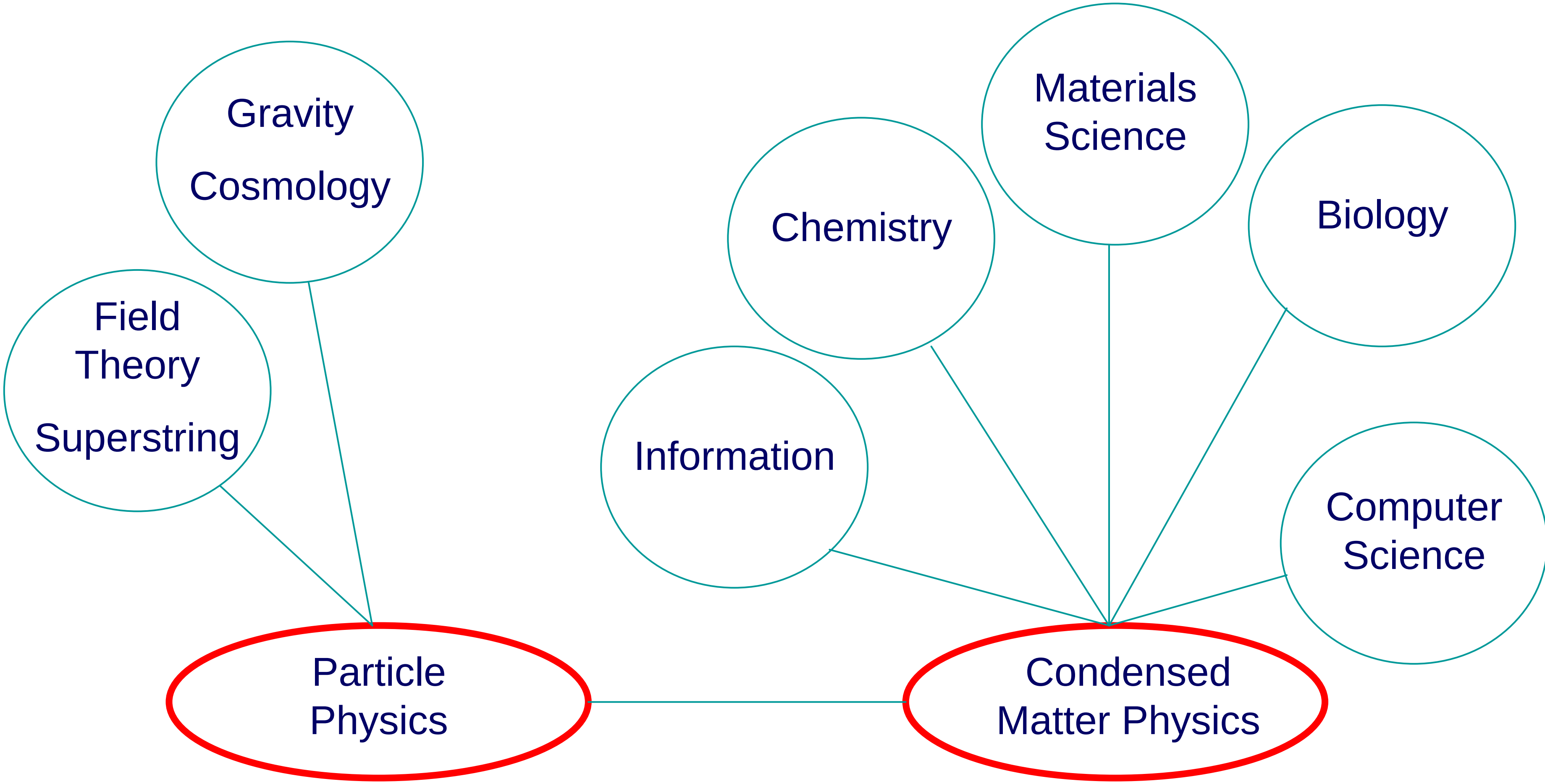


What is Condensed Matter Physics?

Specialists' definition: Universe of Complexities

- Elementary excitations:
  - quasiparticles, phonon, spin waves, plasmons, excitons, spinons and holons, …
- Elementary interactions:
  - el-el, el-ph, el-mag, …
- Elementary structures and phases:
  - charge, spin, orbitals, ions: crystal, glass, liquid …
- Endless emergent quantum phenomena
  - macroscopic quantum interference, mesoscopic size effects …

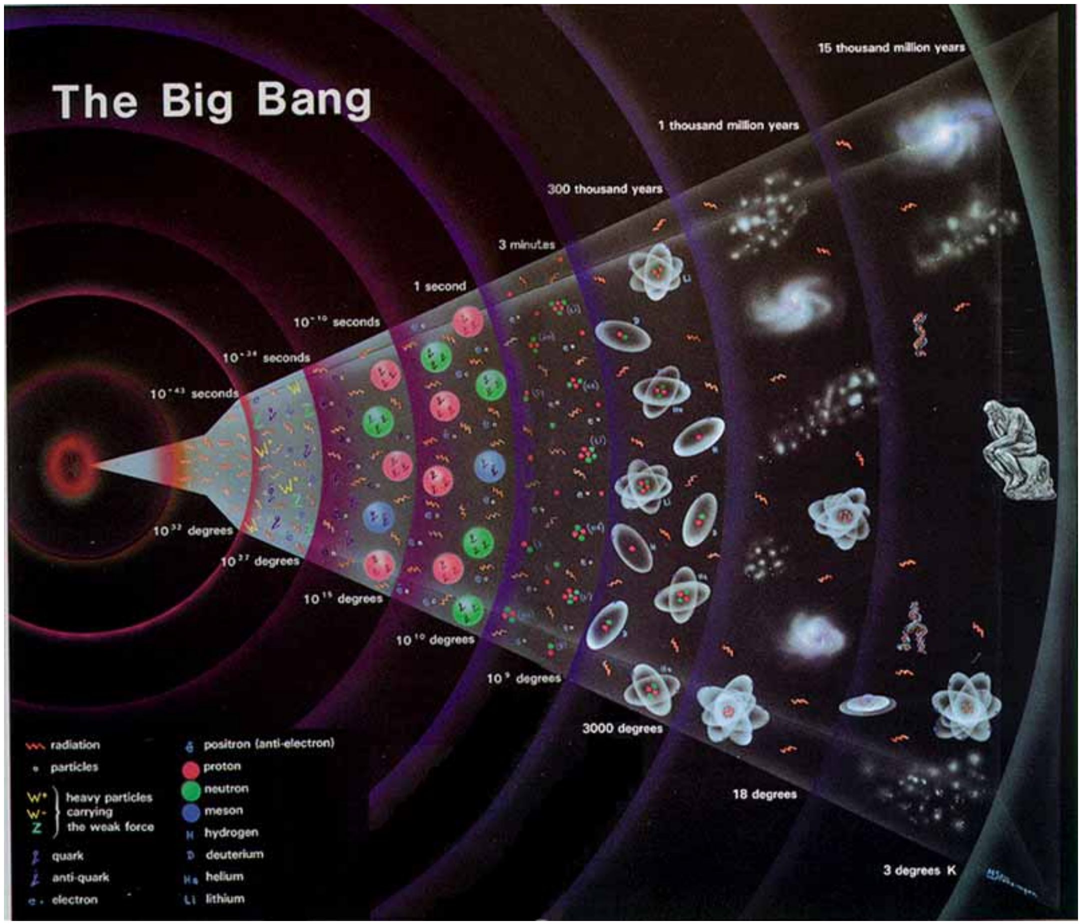
Relationship with other subjects

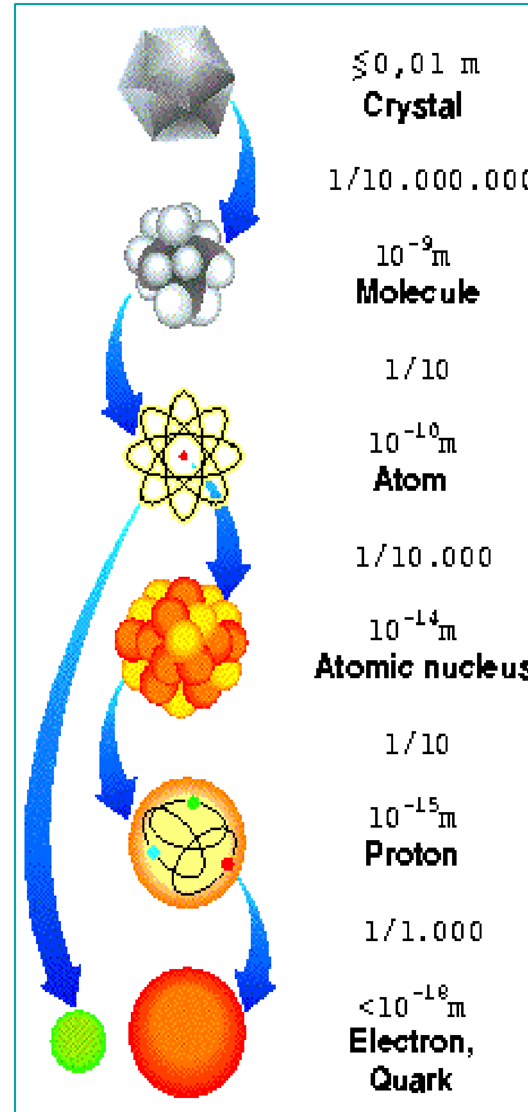


还原论 (Reductionism)：自然界的一切都由其最基本的组成单元和规律所决定

呈展论 (Emergence): 客观世界是分层次的，每个层次都有自己的基本规律

Reductionism：逐本求源

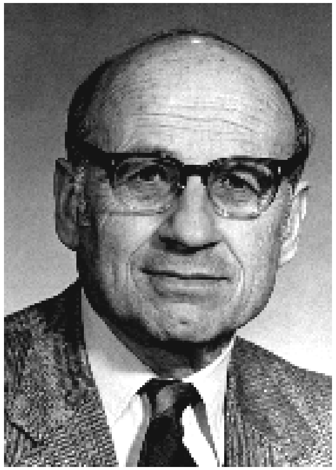




指数墙带来的困惑

由基本的相互作用力就能推出自然界的所有规律吗？

这是“大统一理论”的追求目标，但答案是否定的。



Walter Kohn
Nobel化学奖

指数墙问题

实际材料中原子数 $N \sim 10^{23}$

系统总的自由度数不是每个粒子自由度数相加，而是相乘！

↓

自由度随粒子数指数增加

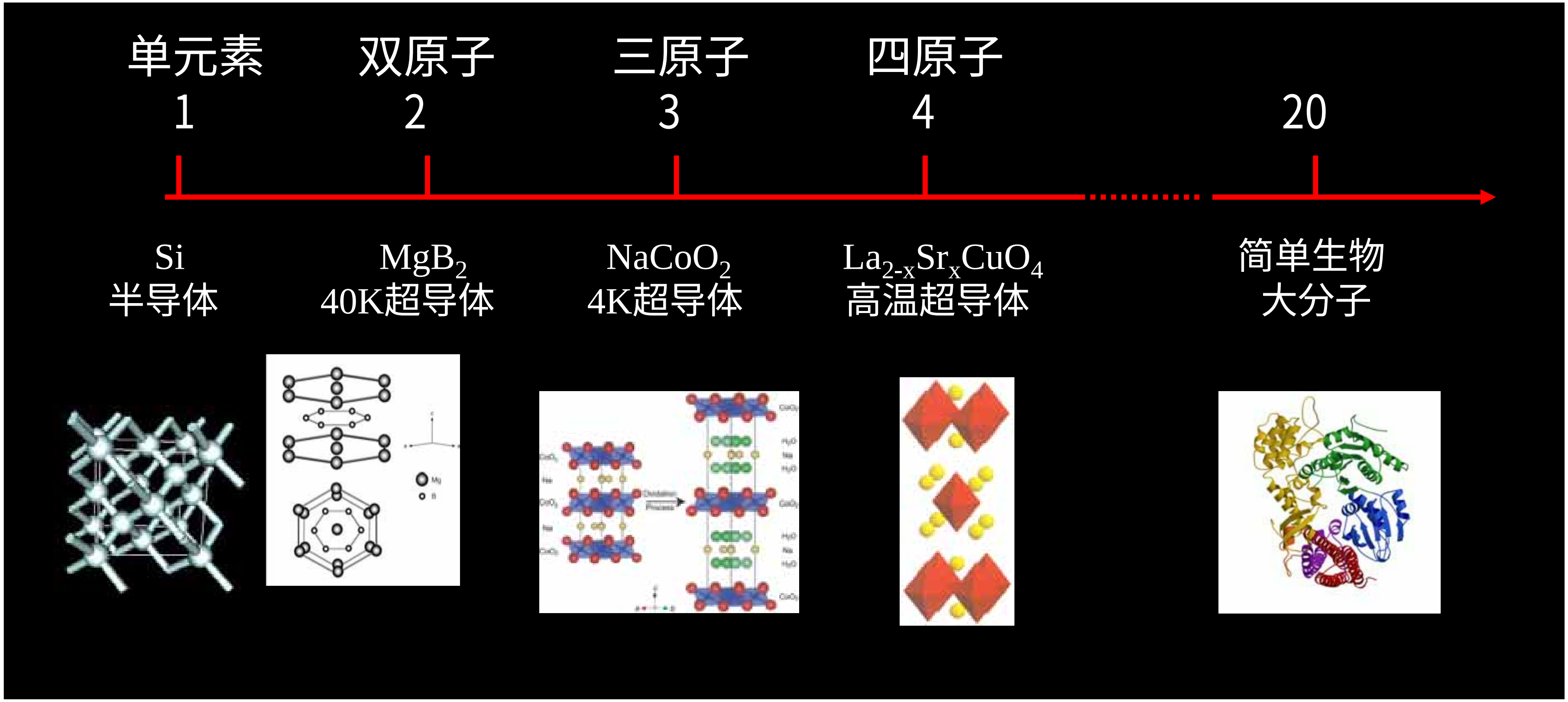
Emergence：集体行为不是个体行为的简单相加

More Is Different

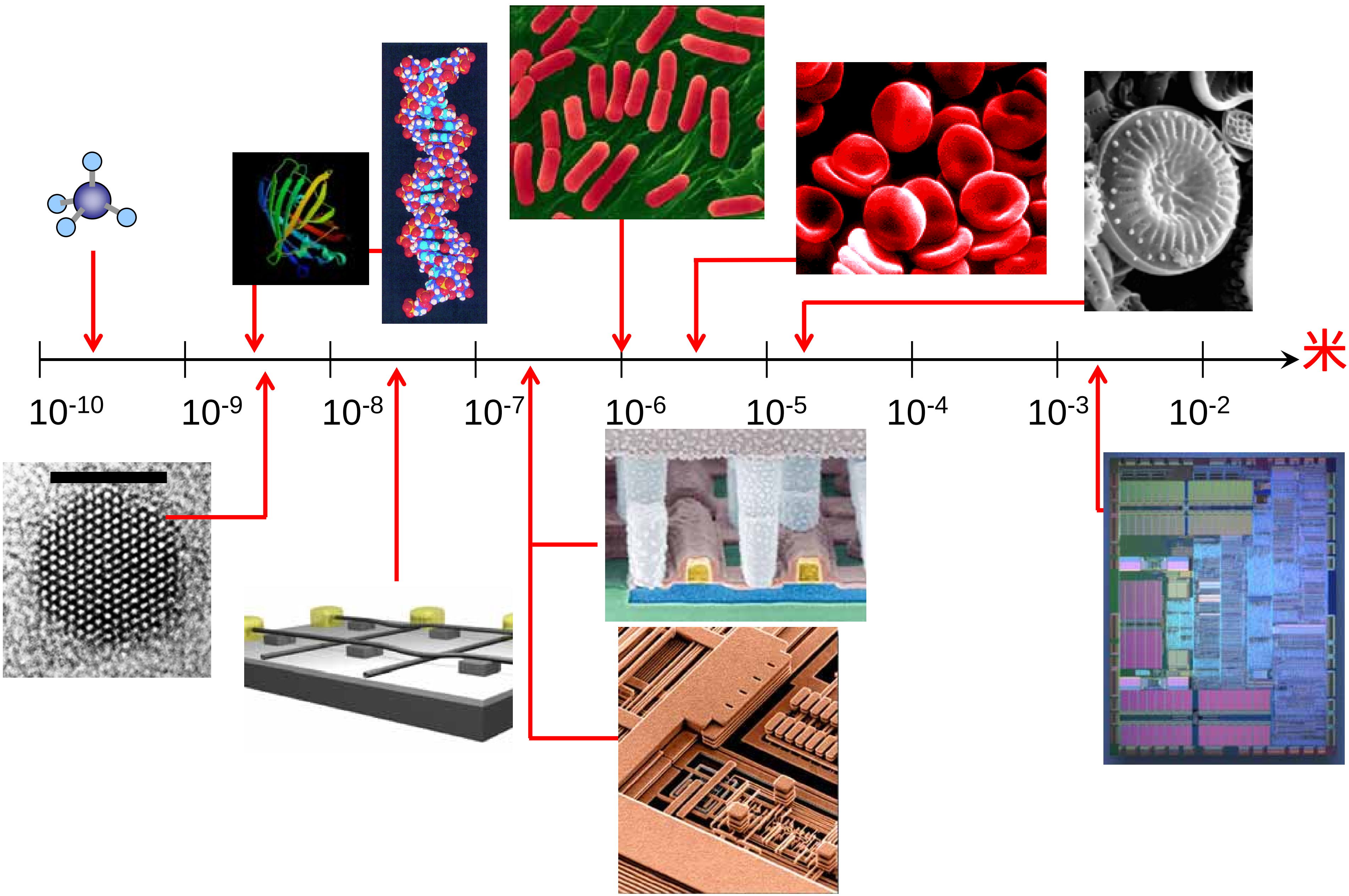
由基本粒子构成的巨大的和复杂的的集聚体的行为并不能依据少数粒子的性质作简单外推就能理解。正好相反，在复杂性的每一个层次之中会呈现全新的性质，而要理解这些新行为所需要作的研究，就其基础性而言，与其他研究相比毫不逊色。

Philip W. Anderson 1972

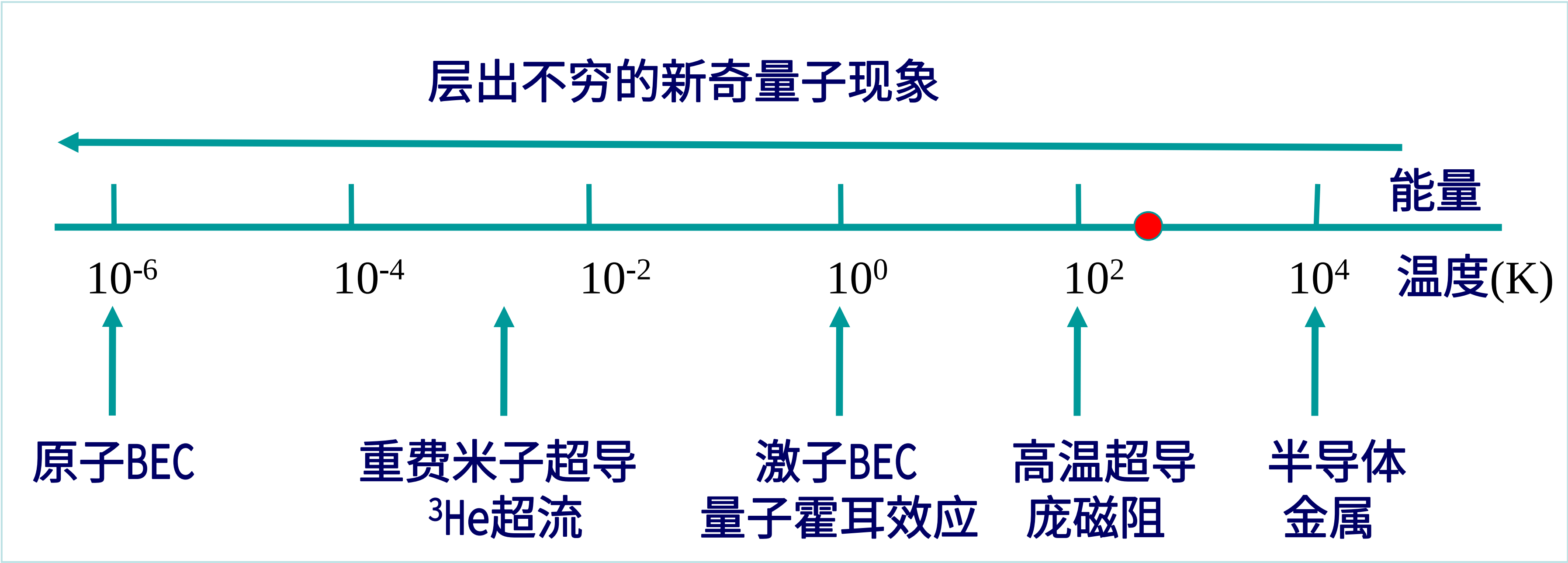
More Is Different！



More Is Different！



More is different!



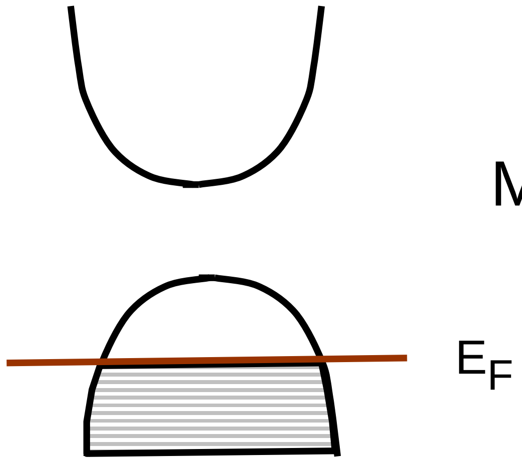
Role of theory in this field

- To develop useful models for experimental systems
- To reveal mechanisms for observed phenomena
- To develop accurate methods to predict properties
- To establish a systematic world view of condensed matter (and the universe)

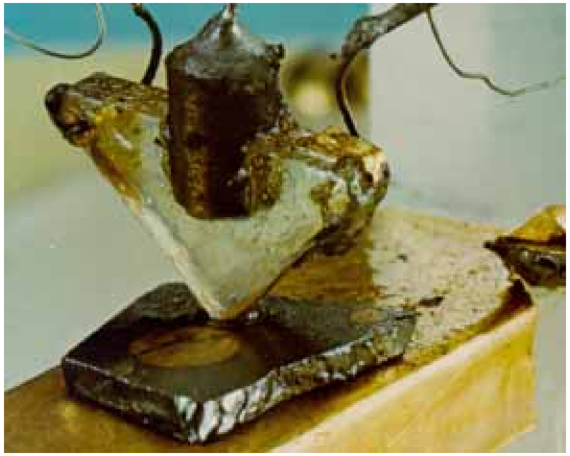
Two Milestones of the 1st Half 20th Century

1. Crystal Dynamics
   - 1848: 空间点阵学说(Bravais)
   - 1889: 空间群理论(Federov 和 Schvenflies)
   - 1907: 独立振子的量子理论(Einstein)
   - 1912: 连续介质中的弹性波的量子理论(Debye)
2. Band Theory
   - 1900: 金属电导和热传导的经典自由电子理论(Drude)
   - 1924: 基于Fermi统计的自由电子理论(Pauli 和 Sommerfield)
   - 1907: 铁磁性相变的分子场理论(Weiss)
   - 金属导电的能带理论(Bloch)

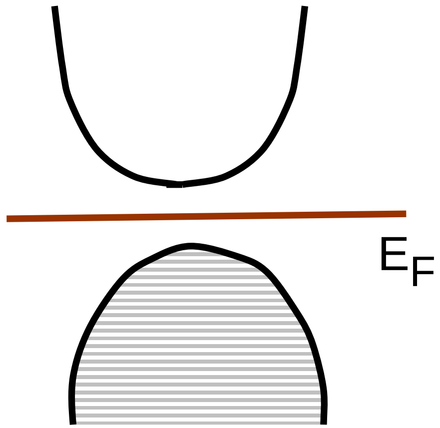
Standard Picture of Metel and Insulator



Metals



First semiconductor transistor



Insulators
and
Semiconductors

Main Stream of Modern Condensed Matter Theory

Understanding of collective motions of electrons

- Main Actors: electrons (charge + spin)
- Key Concept: Symmetry breaking
- Achievements
  - Landau Fermi Liquid Theory
  - Landau Theory of Continuous Phase Transition
  - BCS Theory of Superconductivity
  - Anderson Theory of Localization
  - Theory of Quantum Hall Effects
  - ……

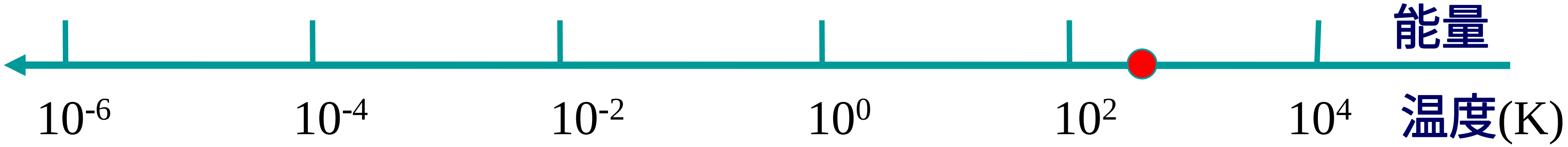
Main Stream of Modern Condensed Matter Theory

- Driving force:
  - Challenging problems raised in emergent quantum phenomena

- Theoretical frameworks
  - Single-electron approximation: Band theory, Landau Fermi Liquid
  - Correlated electrons: Unified theory is still absent

- Development of theoretical methods
  - Analytical: path integral, Green's function, mean-field theory …
  - Numerical: density functional, Monte Carlo, DMRG, DMFT …

Challenging Problems

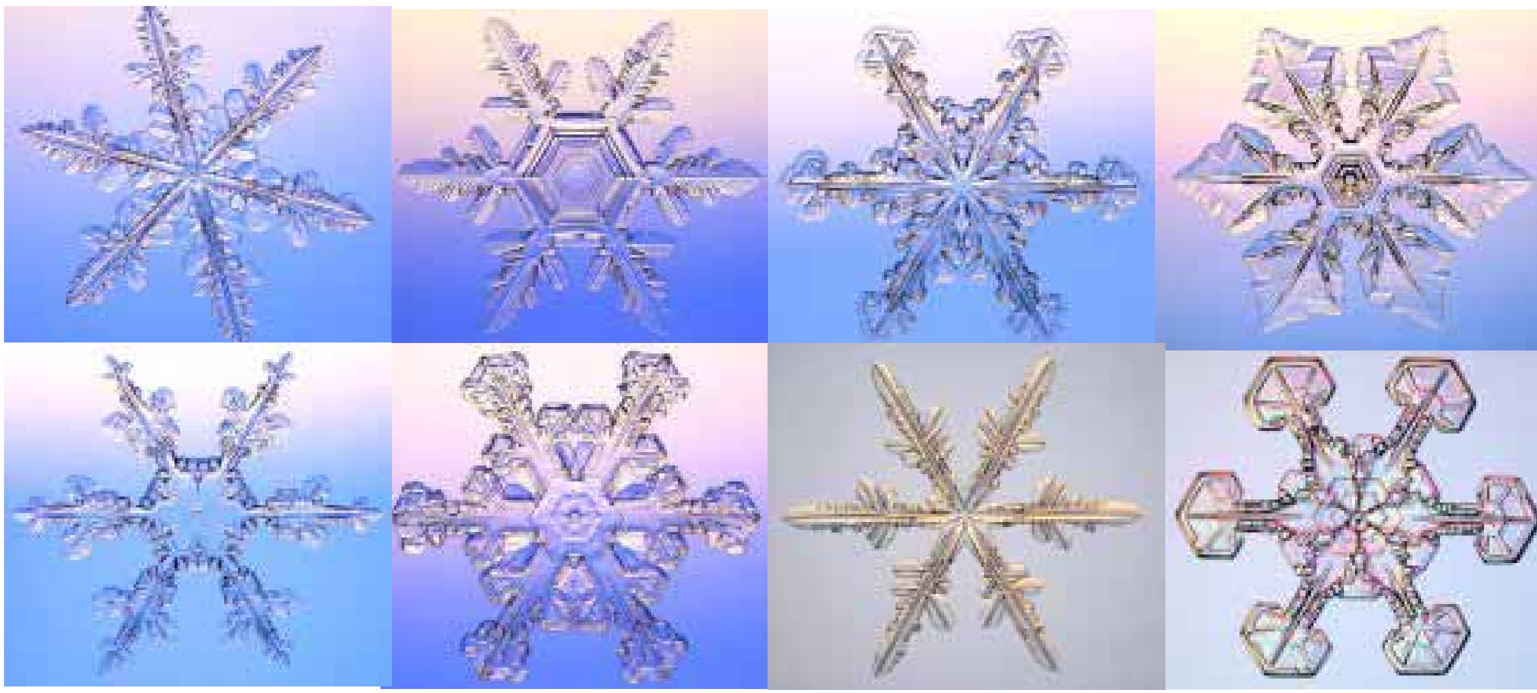


- Superconductivity: cuprates, heavy fermions, …
- Quantum Hall Effects: integer, fractional, graphene, …
- Superfluid and supersolid: ^{4}He, ^{3}He
- Bose-Einstein condensation: excitons, cold atoms
- (Anti)-ferromagnetism and Mott transition
- Kondo effects
- Anderson localization
- Quantum criticality
- ……
- More to come

$T = 273K$

100 °C 水沸腾成蒸汽

0 °C 水冻结成冰

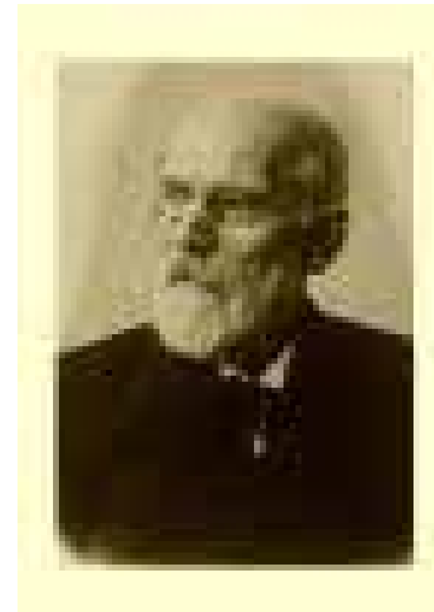


为什么10^{23}个水分子，单个水分子结构不变、相互作用不变，会“集体地”、“不约而同地”从一个相“变”到另一个相？

经典粒子的合作行为：统计力学描述

Complex assemblies of atoms and molecules require a STATISTICAL description

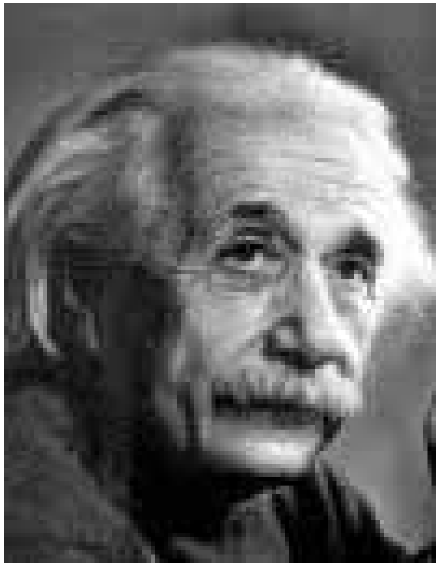
分子间的作用力为范德瓦耳斯力



1873 范德瓦耳斯

$$\left(P+\left(\frac{N}{V}\right)^2 a\right)(V-Nb)=NkT$$

全同粒子的关联现象：量子统计

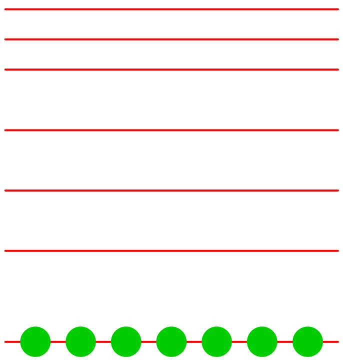


Satyan N. Bose Albert Einstein Enrico Fermi Paul A.M. Dirac

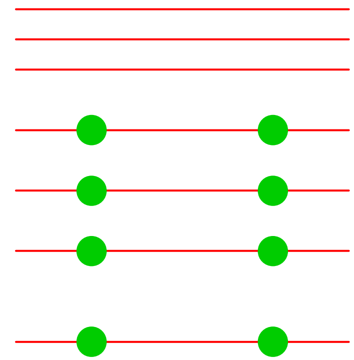
玻色统计：
每个状态可容纳任意多个粒子

费米统计：
每个状态最多可容纳一个粒子

Fermi Statistics：Foundation of Chemistry



Bosons have no Chemical Bonds



Fermions can form Chemical Bonds

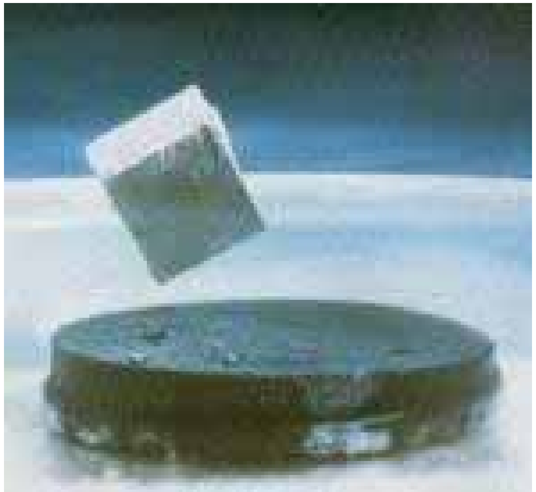
"With a heavy heart, I have been converted to the idea that Fermi-Dirac, not Einstein-Bose is the correct statistics" (for electrons)

Pauli, letter to Schrodinger, Dec 1926

T ~ 10^1 K Superconductivity

1911 Onnes discovered the phenomenon of superconductivity

1957 BCS established the microscopic theory of superconductivity



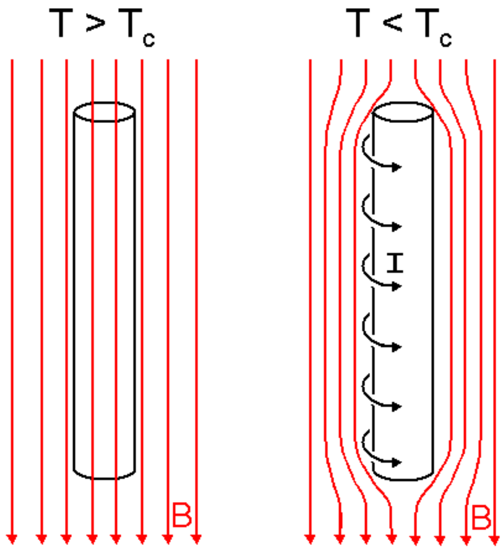
H. Kamerlingh Onnes
(1913)

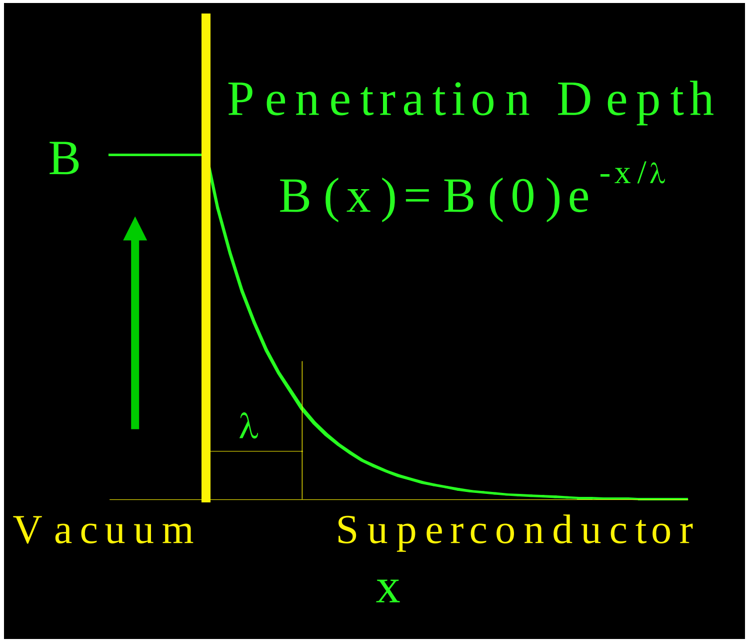
John Bardeen

Leon N. Cooper
(1972)

J. Robert Schrieffer

Meissiner Effect：Anderson-Higgs Mechanism





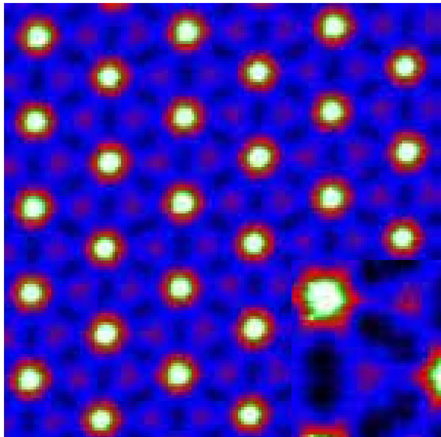
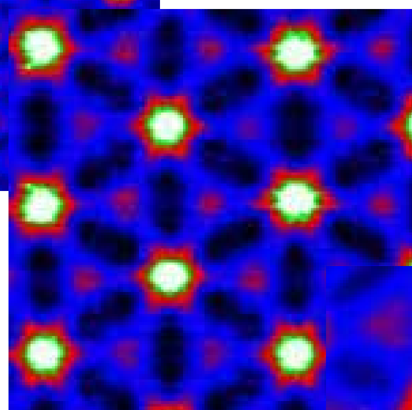
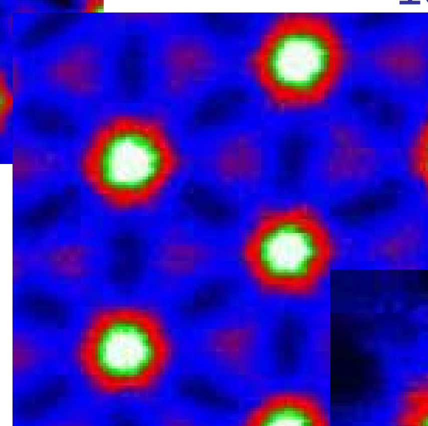
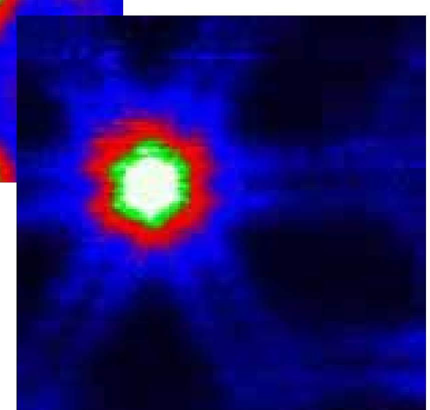
Anderson-Higgs机制：

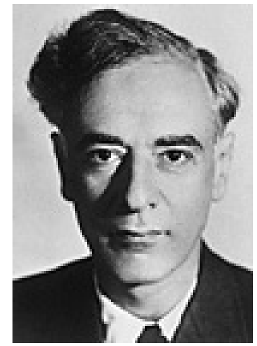
规范场（磁场）与自发破缺的Goldstone粒子耦合，可以获得质量(能隙)，导致磁场在表面的快速衰减

伦敦方程

$$\nabla^2 H = \frac{\mu_0 n_s e^2}{m} H$$

Landau-Ginzberg Theory and Quantized Magnetic Flux Vortices



Landau

1962

Ginzberg

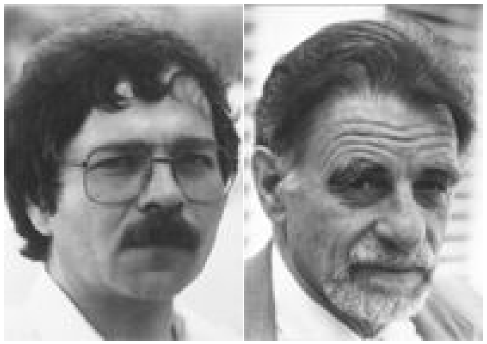
2003

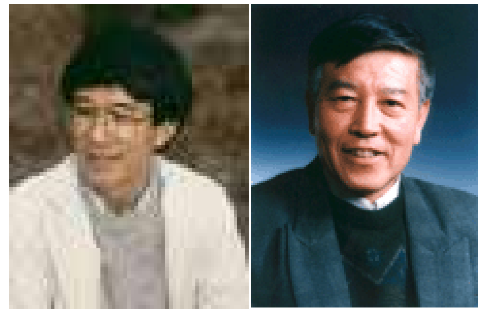
Alexei A Abrikosov

2003 Nobel Prize

Vortices of $NbSe_2$

T ~ 10^2 *K* ：High-Tc superconductors

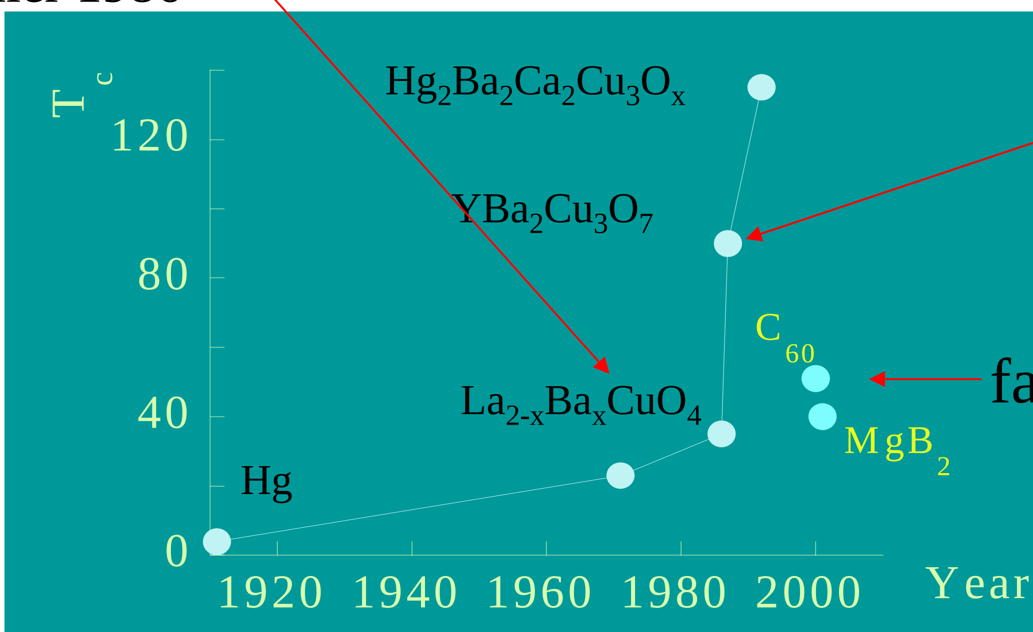




朱经武　　赵忠贤

One of the most challenging problems left last century

Bednorz & Muller 1986



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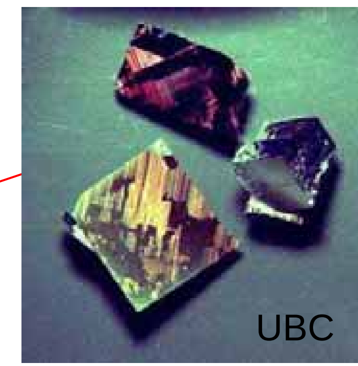
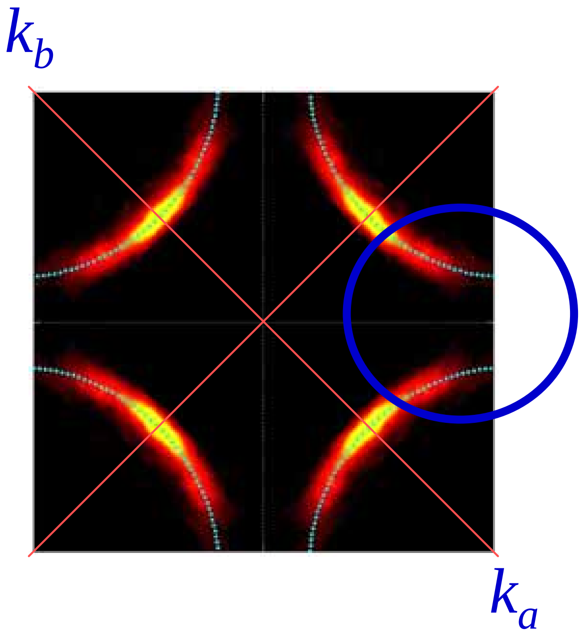
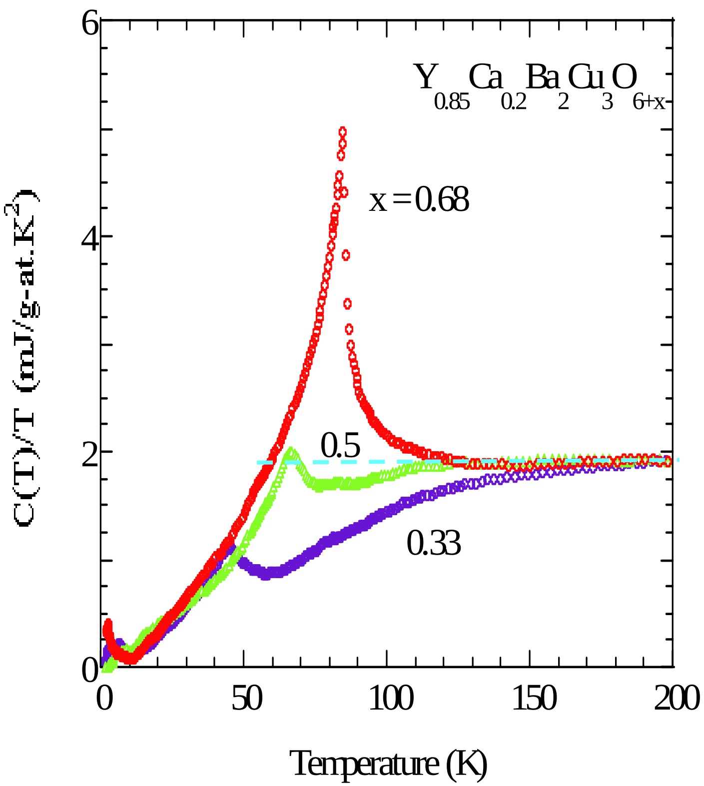


赝能隙：高温超导反常现象之根源



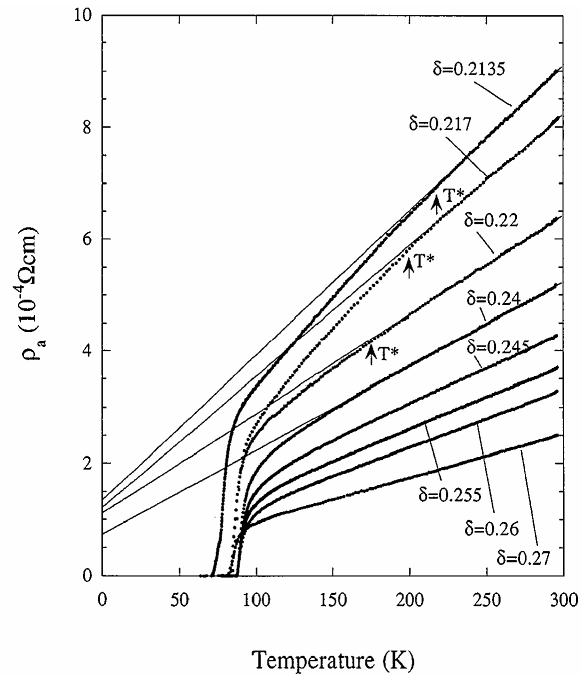
费米面不封闭，存在能隙

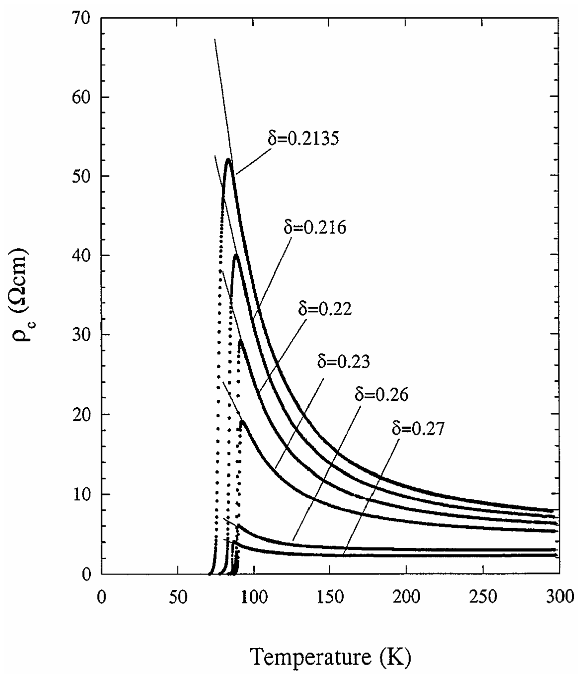


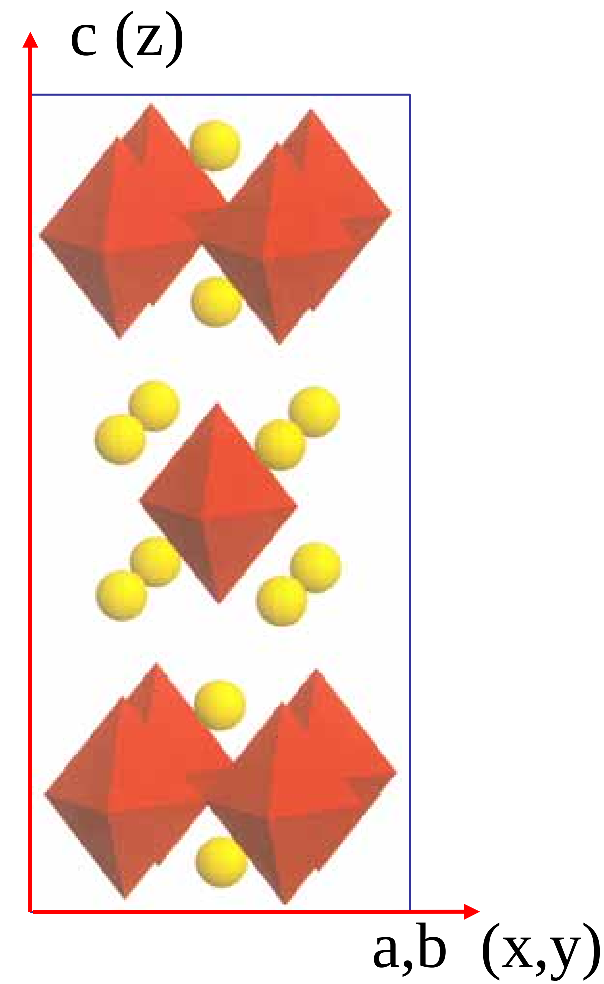
赝能隙现象：
- 正常相中出现的类似于超导能隙的现象
- 超导电子配对好像在相变之前就存在，但没有形成宏观相干

低能熵缺失，状态数不守恒

高温超导体c轴电阻的反常



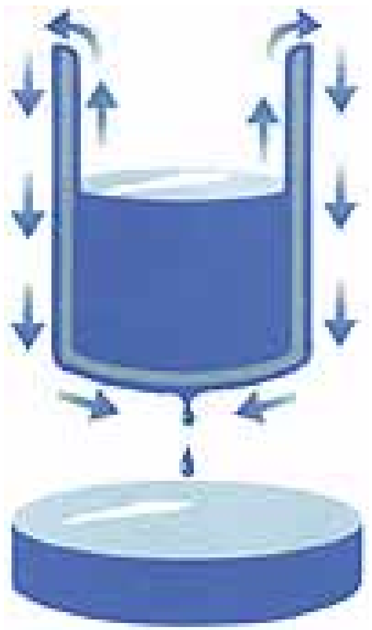




平面内电阻随温度降低而降低，典型的金属行为

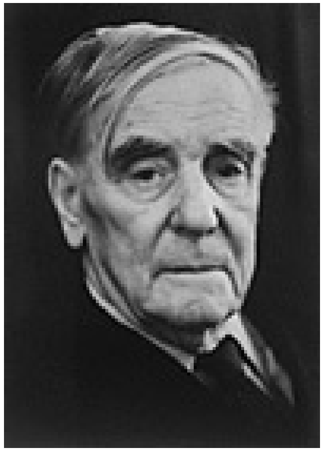
c轴方向电阻随温度降低而上升，典型的半导体行为

Superfluid $T \sim 4\ K$

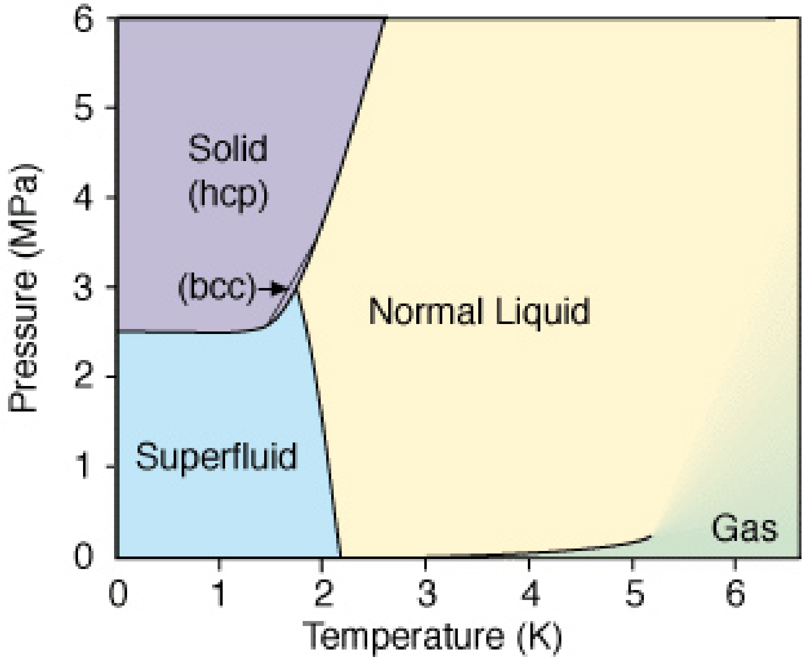


1938 Kapitsa discovered the superfluidity of ^{4}He --- first realization of Bose-Einstein Condensation

1940s Landau formulated the theory of ^{4}He superfluidity



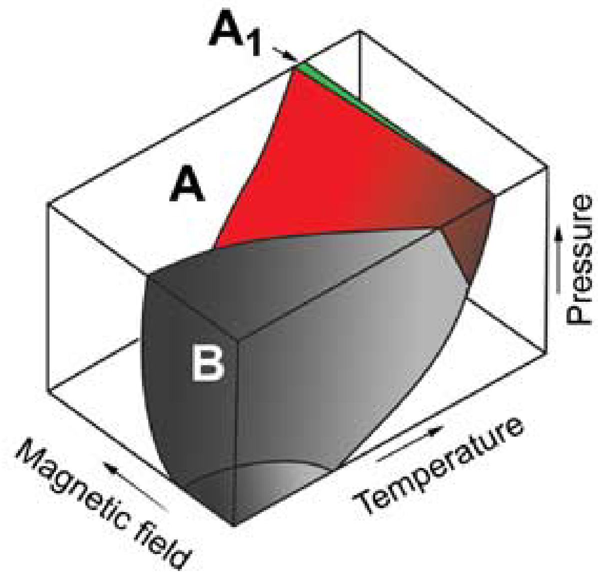
Pyotr L. Kapitsa 1938 (1978) Lev Landau 1941 (1962)



Fermion Superfluid $T \sim 10^{-3}$ K

Early 1970s ^{3}He superfluidity was discovered

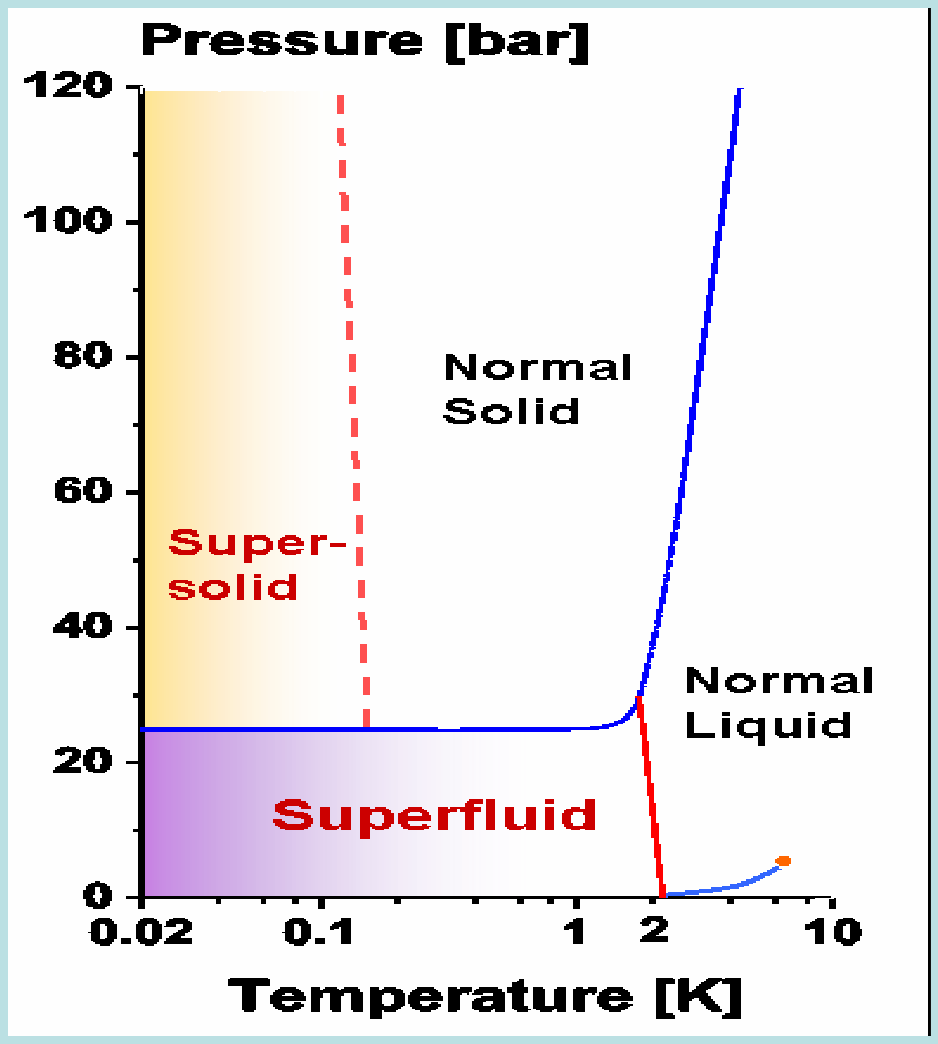
1996, 2003 Nobel prizes



自旋－轨道自发对称破缺

David M. Lee Douglas D. Osheroff Robert C.Richardson Anthony Leggett

Supersolid: intrinsic? Unsolved issue



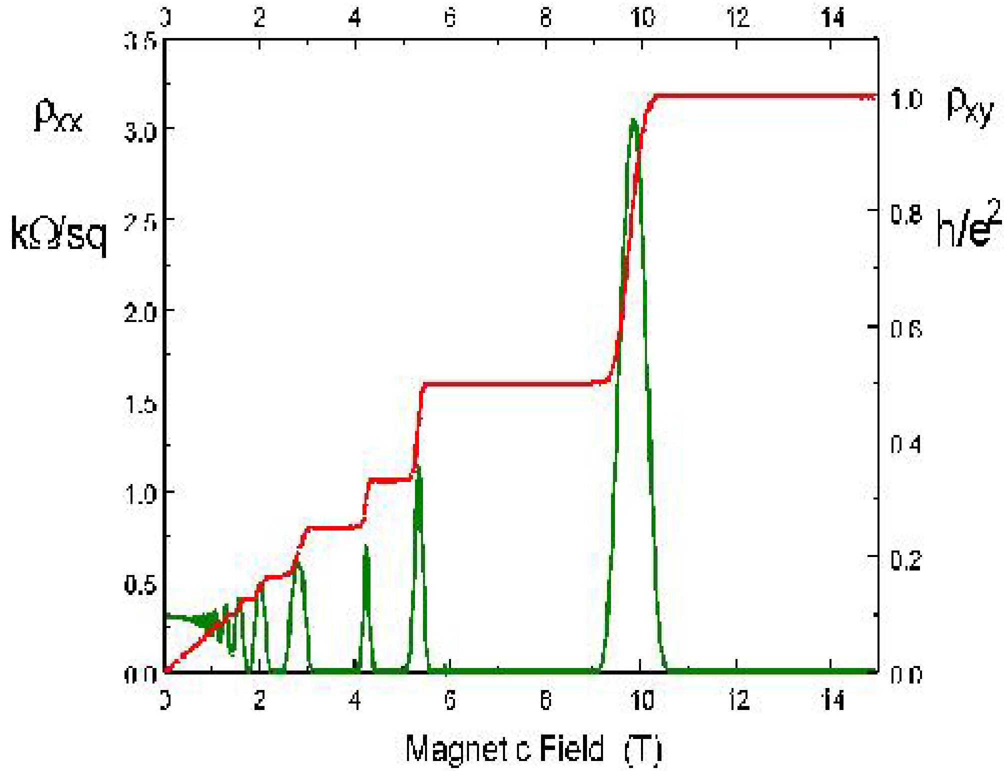
Moses H W Chan

2004 Penn State Univ

Quantum Hall Effect: novel Quantum state

Integer Quantum Hall Effect
1985 Nobel Prize

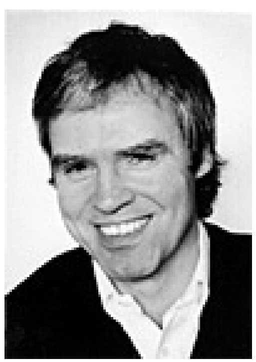
Klaus von Klitzing



Fractional Quantum Hall Effect $T \sim 10^{-2}\ K$

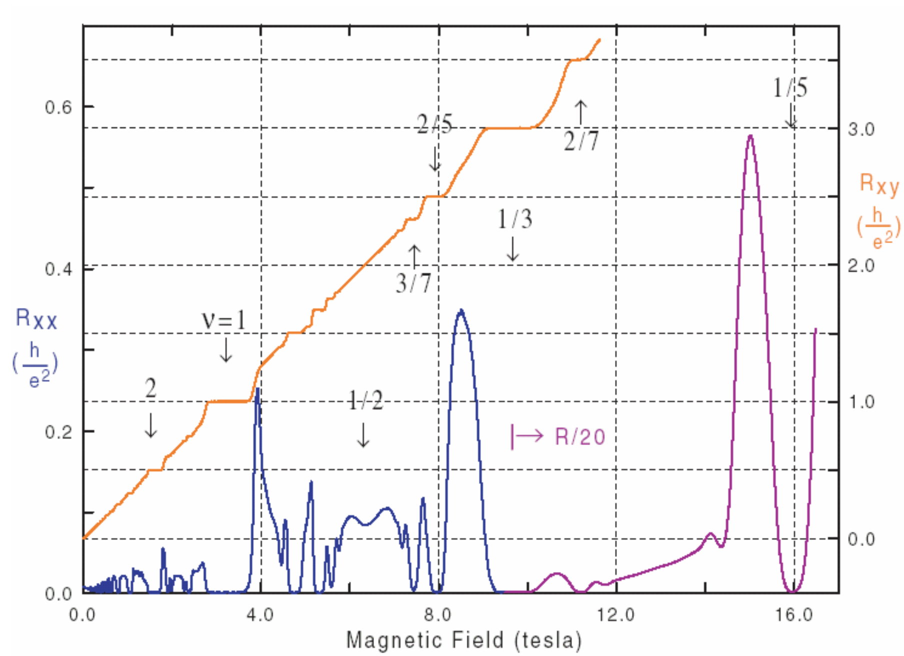
- Laughlin wave-function
- Fractional charge and fractional statistics
- Abelian and non-Abelian

Daniel C. Tsui

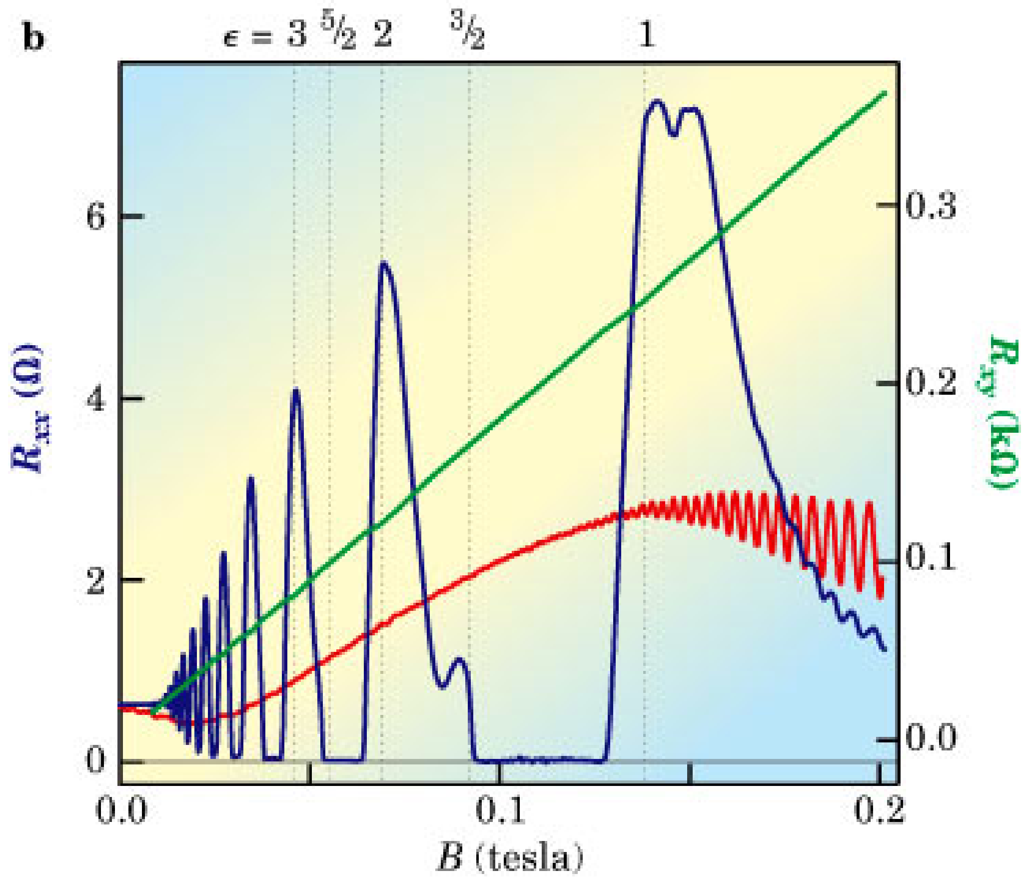


Horst L. Störmer
1998 Nobel Prize

Robert Laughlin



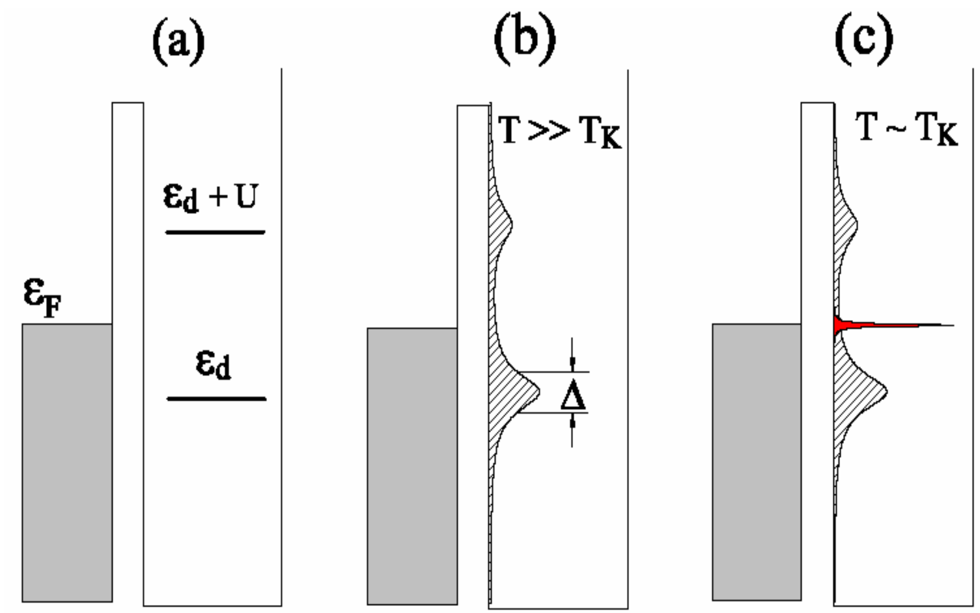
Microwave induced “zero-resistance state” --- a novel non-equilibrium transport state



RG Mani, JH Smet, K von Klitzing, et al., *Nature* **420**, 646 (2002);

MA Zudov, RR Du, et al., *PRL* **90**, 046807 (2003).

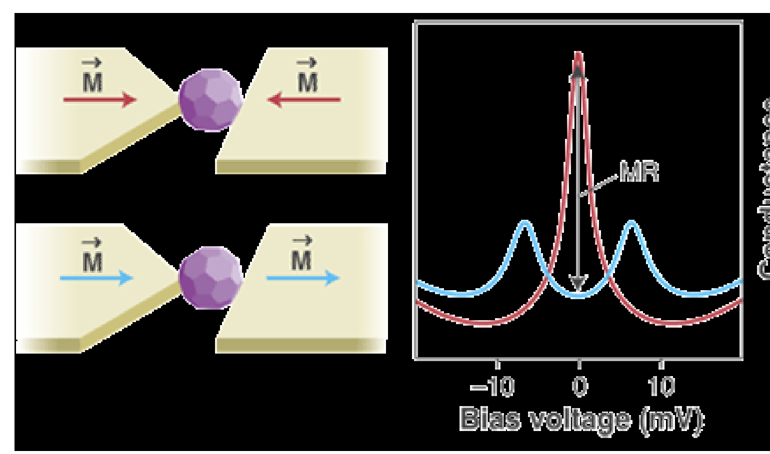
Kondo Effect: key for understanding many correlated effects



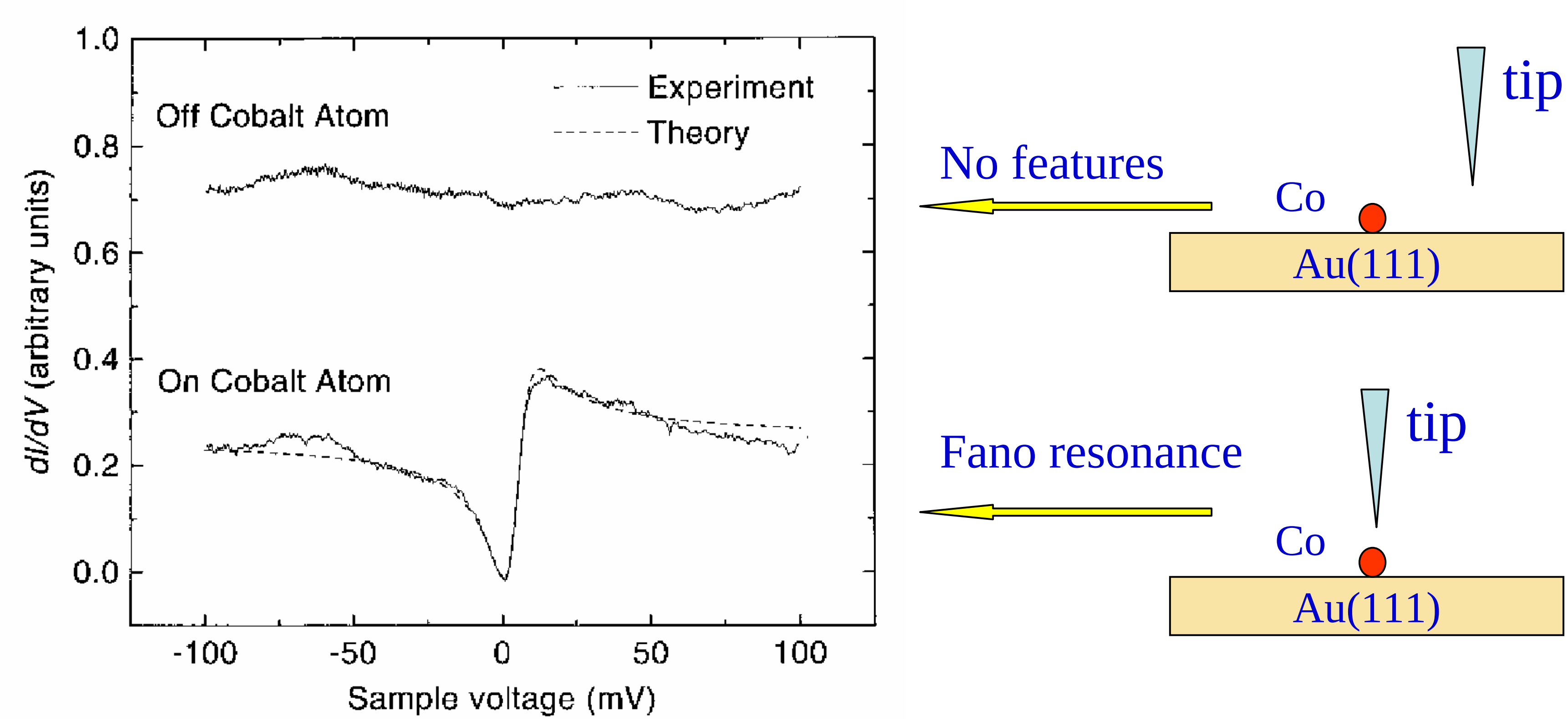
Kondo resonance

Kondo1964

磁性杂质与金属电子相互作用在费米面上产生一个杂质共振态



Experimental observation of Kondo Effect



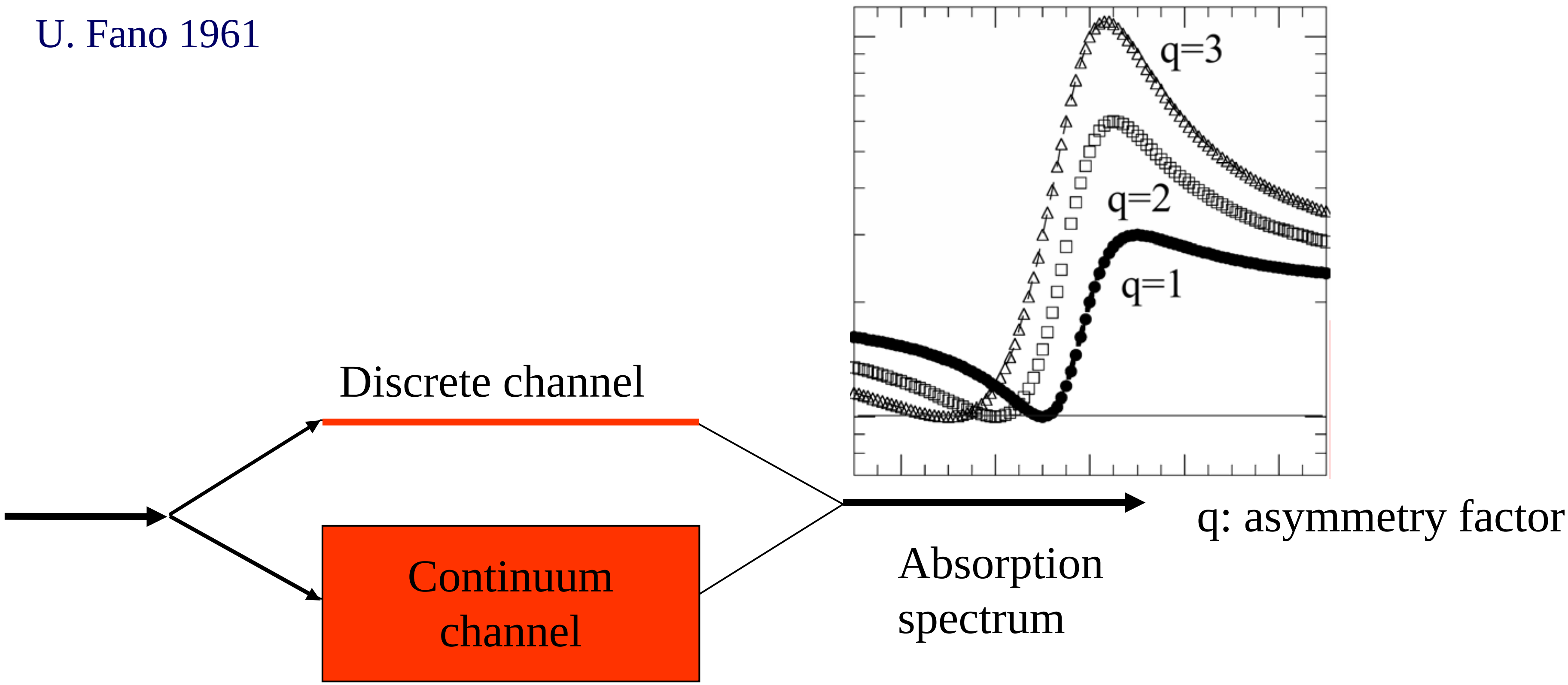
Kondo peak is observed, but it is not-symmetric!

V. Madhavan et al., Science 280, 567 (1998)

Fano Resonance

U. Fano 1961

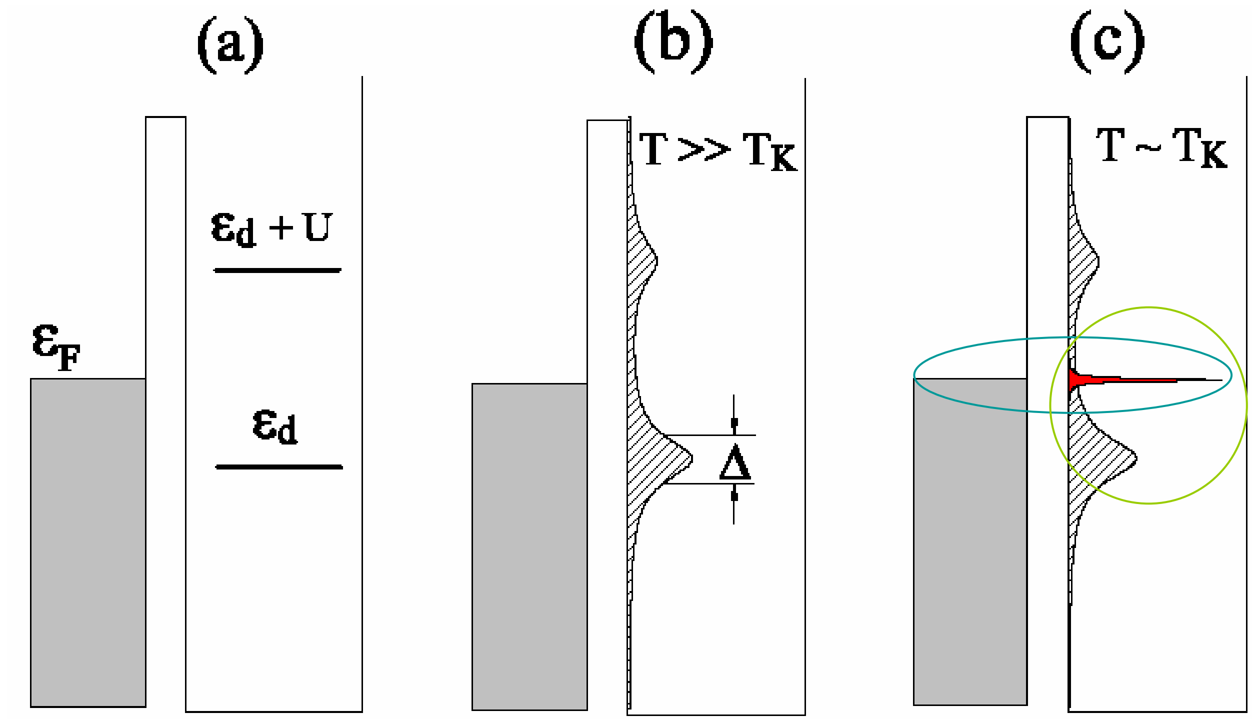
non-symmetric resonance led by the interference between a discrete level and a continuum



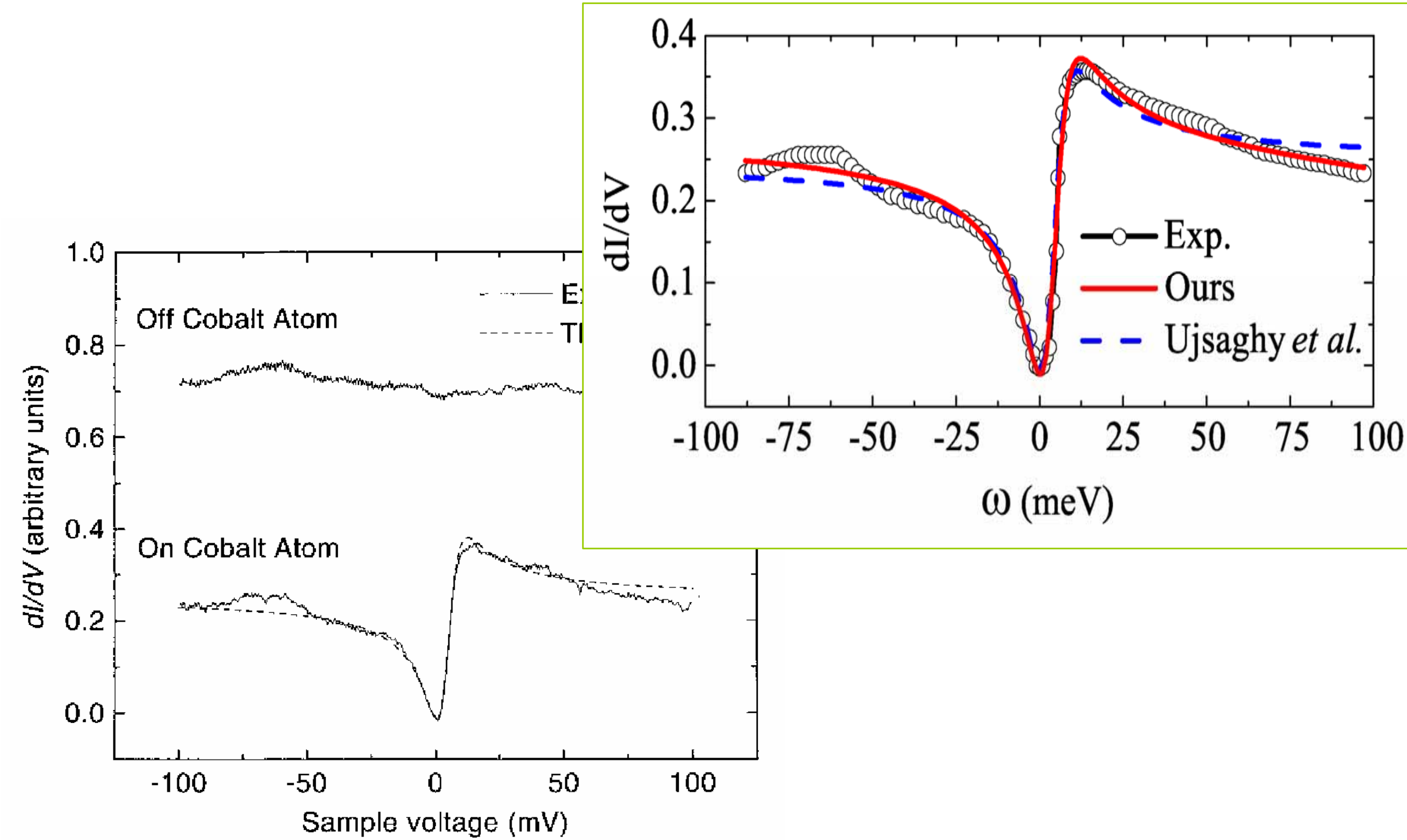
Two Kinds of Interference Channels

HG Luo, T Xiang, XQ Wang, ZB Su, L Yu, PRL 92 (2004) 256602

- Kondo共振态与导电电子的干涉
- Kondo共振态与展宽的杂质能级的自干涉



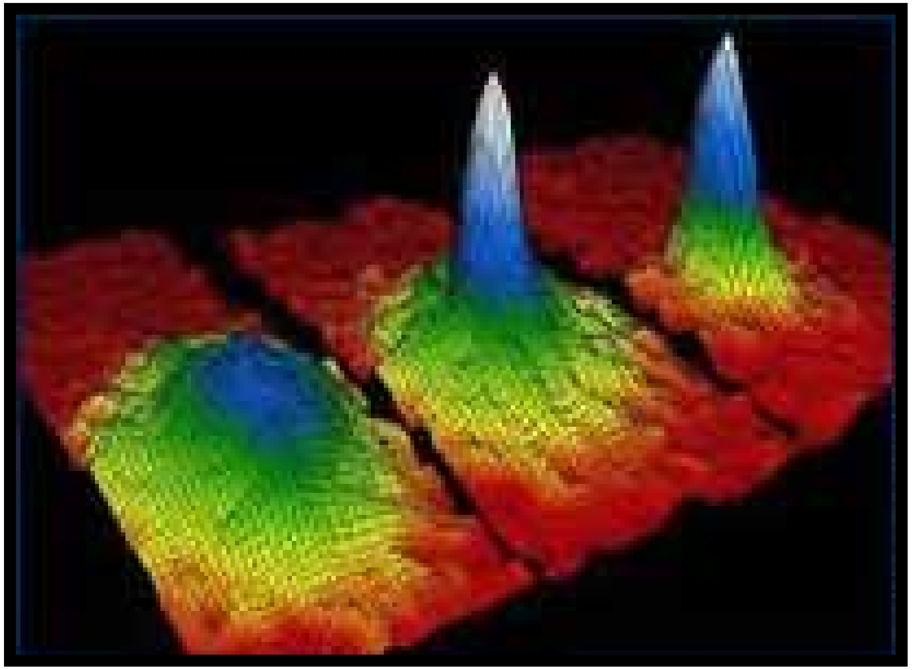
Comparison with Experimental Data



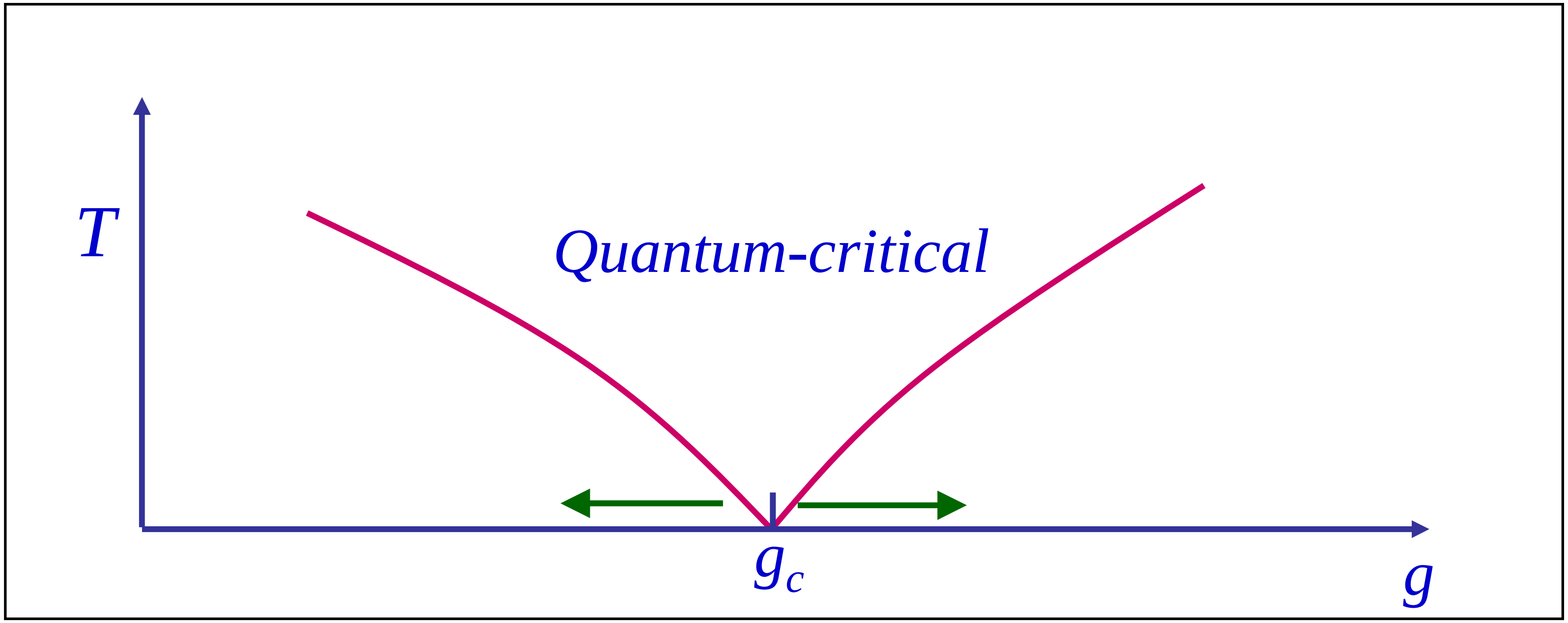
Bose-Einstein Condensation of diluted cold atoms

A technical breakthrough, stimulate the unification of quantum optics and condensed matter physics

2001 Nobel Prize



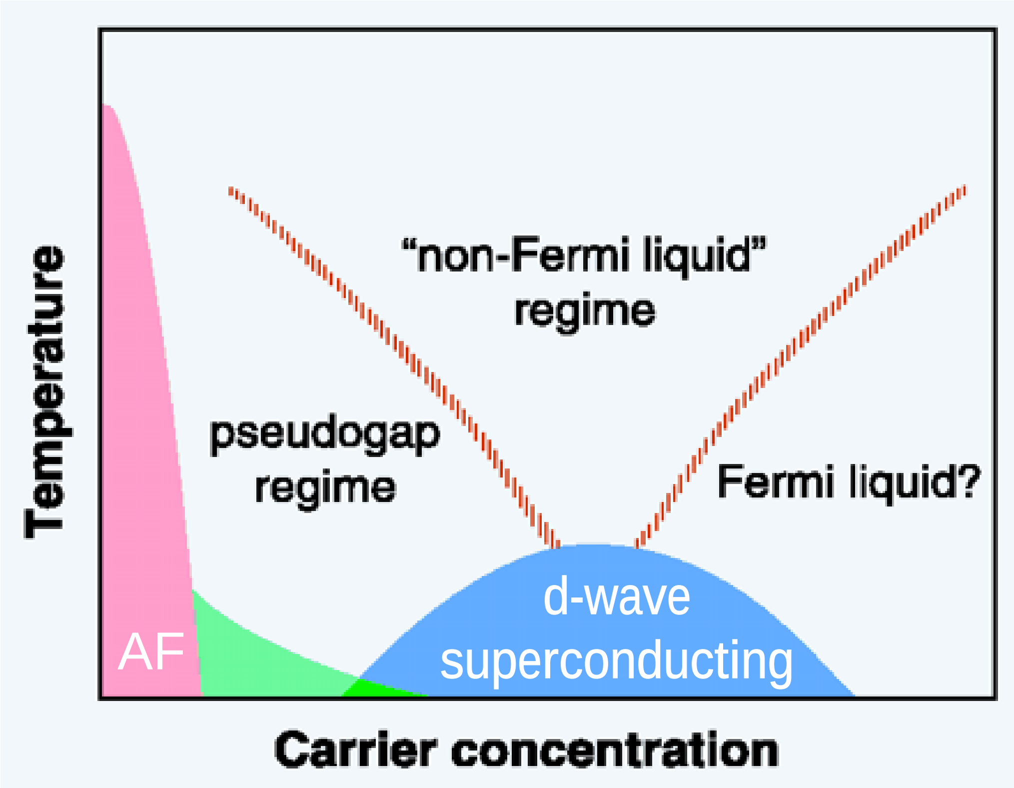
T = 0K ：Quantum Phase Transition



- 基态性质作为控制参数g的函数有奇异性，临界点是物质的新态，没有元激发！
- 强关联量子系统不同基态（呈展态）间的竞争
- 临界涨落控制整个量子临界区的动力学行为

Quantum Criticality in High-Tc Cuprates

Is the non-Fermi liquid behavior discovered in high-Tc a quantum critical phenomenon?



Mott Transition

- Standard Model:

  Odd number of electrons: metal

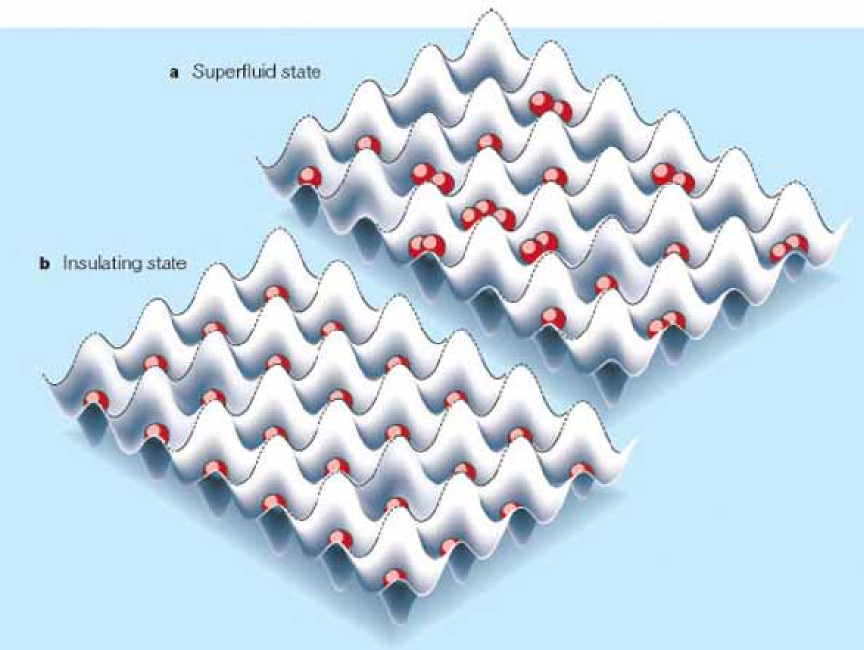
  Even number of electrons: insulator

  But many materials (eg La_2CuO_4) that are expected to be metals are actually insulators

- Is the Mott transition really intrinsic, not a result of the ordering of other parameters (eg AFM)?

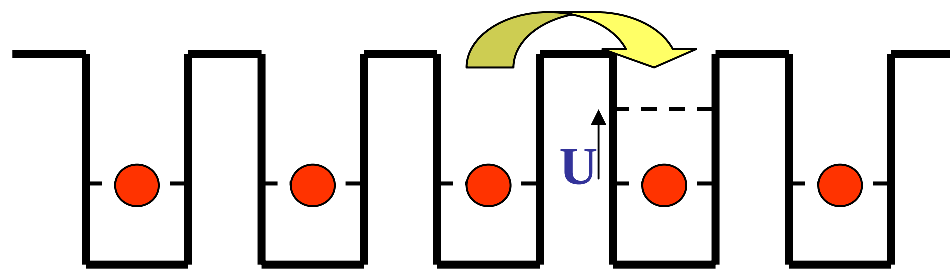
- What is the equation describing the Mott Transition? Is there any order parameter?

Optical Lattice



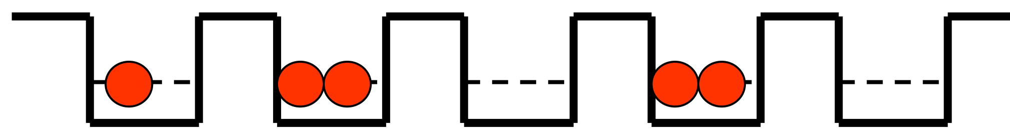
Mott绝缘态： t << U

库仑排斥U大于粒子的动能 t



超流凝聚态：t >>U

库仑排斥U小于粒子的动能 t

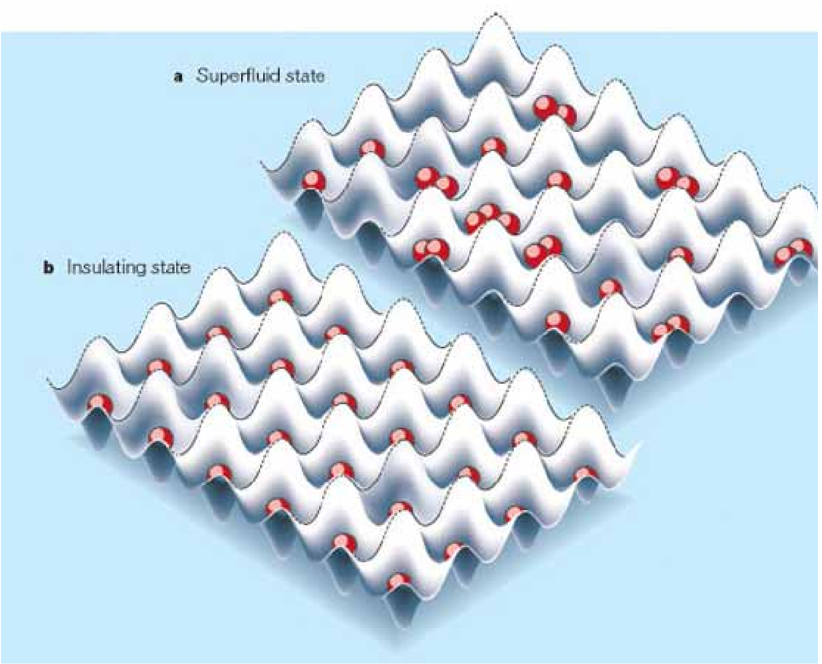


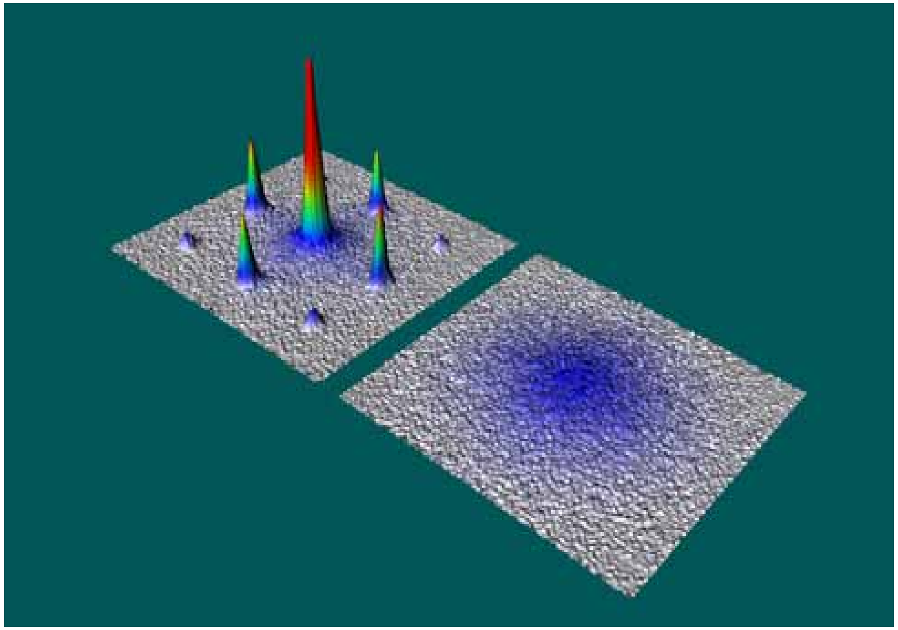
Tools of Quantum Optics

Problems of Condensed Matter

$T \sim 10^{-6}$ K

Accurately controlled Quantum Phase Transition
--- Superfluid-Insulator Transition





M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, *Nature* **415**, 39 (2002).

Why Challenging

Emergent quantum phenomena are mainly caused by the collective motions of electrons, correlations among electrons are important

In nearly 99% case, we can only solve rigorously a problem of *Harmonic Oscillators*

Perturbation is the only tool we have to attack a many-body problem. But the correlated effect is non-perturbative!

New concepts and new methods are desired!

How to face the challenge

- Capture key physics from experimental observations: physical intuition
- Theoretical modeling: power of theoretical analysis
- “First principle” calculations: determine basic parameters

Theoretical Methods

- Analytical: perturbation from a right starting point
  - Green's Functions (Shao-Jing Qin)
  - Path Integral and Mean Field Theory (Yue Yu)
  - Equations of Motion (truncation approach)

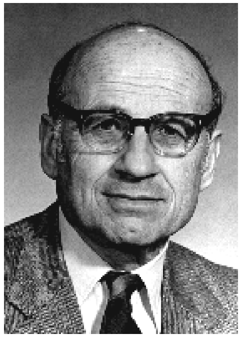
- Numerical: object oriented
  - Density Functional Theory (single-particle)
  - Quantum Monte Carlo (minus sign problem)
  - Density Matrix Renormalization Group
  - Dynamical Mean-Field Theory (∞ D)

Density Functional Theory

- First principle: no input parameters
- Basis of materials design
- Good only for weakly coupled systems:

  in real calculations, LDA or other approximations has to be taken
- Correlated effects cannot be correctly and fully treated

指数墙问题幽灵不散！

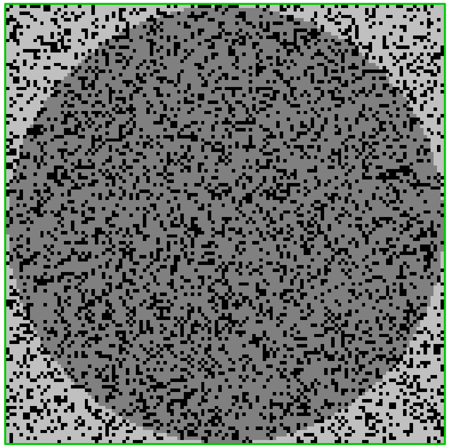


Walter Kohn

面对纷繁呈展的世界，物理学家始终在做着还原的梦:

从最基本的量子力学原理和电子间的库仑相互作用出发，计算和分析各种呈展量子现象

Quantum Monte Carlo



- Random sampling (integration)
- Detailed balance

  $$P(x)r(x \rightarrow x') = P(x')r(x' \rightarrow x)$$

- Metropolis algorithm:

  If P(x') > P(x) accept move

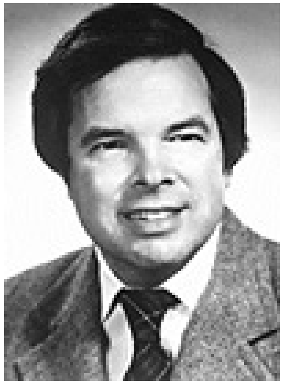
  If P(x') < P(x) accept with probability

  $$r(x \rightarrow x') = P(x') / P(x)$$

- Minus Sign Problem:

  fermions P(x) can be negative

克服指数墙的约束：密度矩阵重正化群



Kenneth K. Wilson
1982 Nobel 物理奖

重正化群与标度不变性

数值重正化群

数值重正化群的基本出发点：

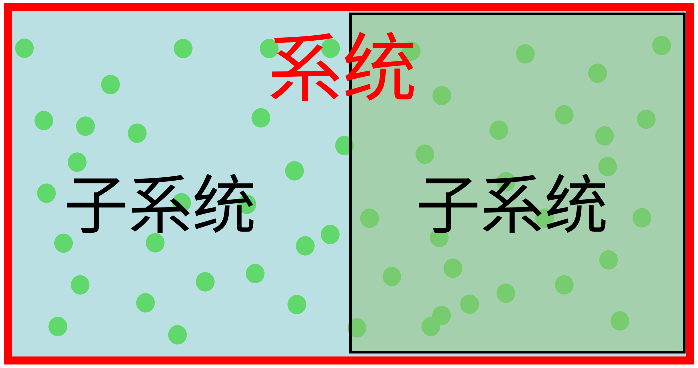
在研究低能物理性质时，高能量状态的贡献很小，因此我们可以用有限个基矢来近似表达一个无限大自由度(或Hilbert空间)的状态

核心问题：

如何判别哪个基矢重要，哪个不重要

密度矩阵重正化群（DMRG）

如何确定每个自由度对
目标状态贡献的大小？



物理实验：外加一个扰动，测系统的反应

例如：加电流，测电压，确定电阻　R = V / I

DMRG实验：无外界扰动，用系统的一部分作为探针（约化密度矩阵）去探测另一部分所处的状态

$$\rho_s = Tr_e \left| \psi_{s \oplus e} \right\rangle \left\langle \psi_{s \oplus e} \right|$$

密度矩阵重正化群（DMRG）

研究一维多体量子体系最精确的方法
能精确计算各种基态、热力学和动力学量

<u>1D S=1 Heisenberg模型</u>

	基态能量	能隙	粒子数
量子蒙特卡罗	-1.4015(5)	0.41	10^2
严格对角化	-1.40148(2)	0.41049(2)	10^1
DMRG	-1.401484038971(4)	0.41050(2)	∞

近年来的新进展：多体含时Schordinger方程的求解

有望突破的方向：高维量子系统和量子化学计算，与量子Monte Carlo方法的结合

Dynamical Mean Field Theory

- Reduce the quantum many body problem to a one site or a cluster of sites, in a medium of non interacting electrons obeying a self consistency condition.

- Instead of using functionals of the density, use more sensitive functionals of the one electron spectral function.

- Perspective: Combine with LDA

Dynamical Mean Field Theory

- Freeze the spatial fluctuation, consider only the local quantum fluctuation
- Map a lattice model onto a quantum impurity model of electrons in a medium of non-interacting electrons obeying a self consistency condition
- Instead of using functionals of the density, use more sensitive functionals of the one electron spectral function.
- Perspective: Combine with LDA

Dynamical Mean Field Theory

- Hubbard model

$$H = -t\sum_{\langle ij\rangle} c_{i\sigma}^{+} c_{j\sigma} + U\sum_{i} n_{i\uparrow} n_{i\downarrow}$$

- Single-site action

$$S_{eff} = -\int_0^{\beta} d\tau d\tau' \sum_{\sigma} c_{0\sigma}^{+}(\tau) G_0^{-1}(\tau - \tau') c_{0\sigma}(\tau') + U\int_0^{\beta} d\tau n_{0\uparrow} n_{0\downarrow}$$

- Self-consistent equation

$$G_0^{-1}(i\omega_n) = i\omega_n + \mu - \Sigma(i\omega_n)$$