Introduction to Quantum Phase Transitions

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Do We Need Quantum Mechanics to Understand Phase Transitions at Finite Temperature?

- Although quantum mechanics is essential to understand the existence of ordered phases of matter (e.g., superconductivity and magnetism are genuine quantum effects), it turns out that quantum mechanics does not influence asymptotic critical behavior of finite temperature phase transitions:

$\tau_c \sim \xi^z \sim |t|^{-\nu z}$ The decay time of temporal correlations for order-parameter fluctuations in dynamic (time-dependent) phenomena in the vicinity of critical point $\longrightarrow$ **critical slowing down**

$$i\hbar \frac{d\hat{A}}{dt} = [\hat{A}, \hat{H}]$$

In quantum systems static and dynamic fluctuations are not independent because the Hamiltonian determined not only the partition function, but also the time evolution of any obaservable via the Heisenber equation of motion

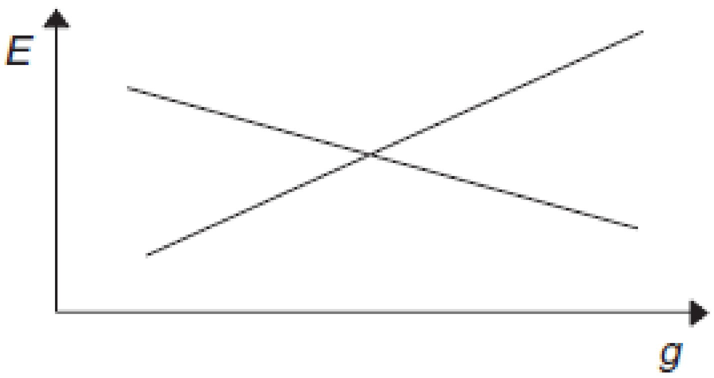
$E_c = \hbar/\tau_c \sim |t|^{\nu z}$ Thus, in quantum systems energy associated with the correlation time is also the typical fluctuation energy for static fluctuations, and it vanishes in the vicinity of a continuous phase transition as a power law

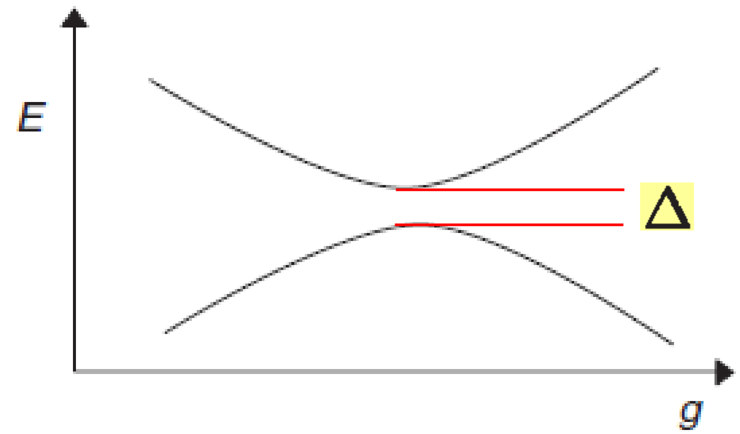
$E_c \ll k_B T_c$ This condition is always satisfied sufficiently close to T_c, so that quantum effects are washed out by thermal excitations and a purely classical description of order parameter fluctuations is sufficient to calculate critical exponents

- Phase transitions in classical models are driven only by thermal fluctuations, as classical systems usually freeze into a fluctuationless ground state at $T = 0$.
- In contrast, quantum systems have fluctuations driven by the Heisenberg uncertainty principle even in the ground state, and these can drive interesting phase transitions at $T = 0$.

Formal Definition of Quantum Phase Transitions

$$\hat{H}(g) = \hat{H}_0 + g\hat{H}_1,\ \ [\hat{H}_0, \hat{H}_1] = 0$$



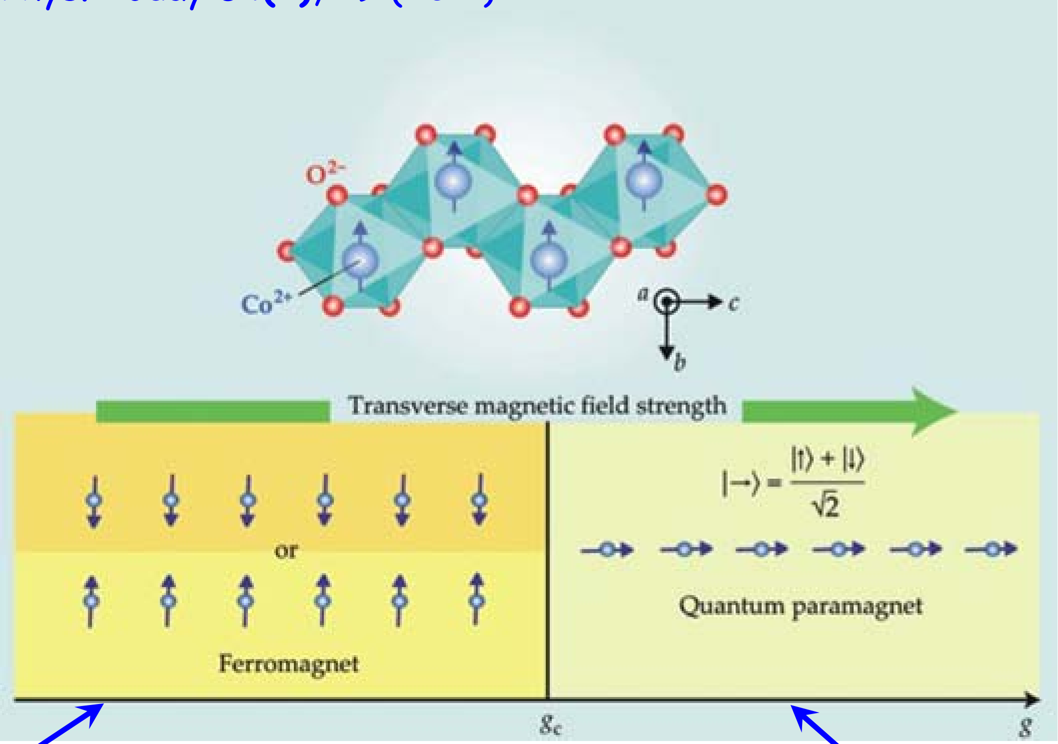


- An avoided level-crossing between the ground and an excited state in a **finite lattice** could become progressively sharper as the lattice size increases, leading to a **nonanalyticity** at $g = g_c$ in the **infinite lattice limit**.

- Any point of nonanalyticity in the ground state energy of the infinite lattice system signifies quantum phase transition.
- The nonanalyticity could be either the limiting case of an avoided level-crossing or an actual level-crossing.

Simple Theoretical Model I: Quantum Criticality in Quantum Ising Chain ($CoNb_3O_3$)

Phys. Today **64(2)**, 29 (2011)



Quantum Ising chain in transverse external magnetic field

$$\hat{H} = -J\sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - g\sum_i \hat{\sigma}_i^x$$

$$J > 0, g > 0$$

Each ion has two possible states:

$$\hat{\sigma}_z|\uparrow\rangle = +|\uparrow\rangle \qquad \hat{\sigma}_z|\downarrow\rangle = -|\downarrow\rangle$$

The first term in the Hamiltonian prefers that the spins on neighboring ions are parallel to each other, whereas the second allows quantum tunneling between the $|\uparrow\rangle$ and $|\downarrow\rangle$ states with amplitude proportional to g

$$|0\rangle = |\uparrow\rangle_1 \otimes |\uparrow\rangle_2 \cdots \otimes |\uparrow\rangle_N$$

or

$$|0\rangle = |\downarrow\rangle_1 \otimes |\downarrow\rangle_2 \cdots \otimes |\downarrow\rangle_N$$

$$\lim_{|x_i - x_j| \to \infty} \langle 0|\hat{\sigma}_i^z \hat{\sigma}_j^z|0\rangle = N_0^2$$

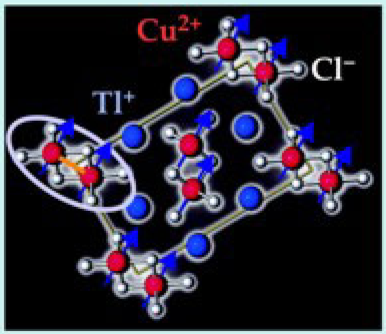
$$|0\rangle = |\rightarrow\rangle_1 \otimes |\rightarrow\rangle_2 \cdots \otimes |\rightarrow\rangle_N$$

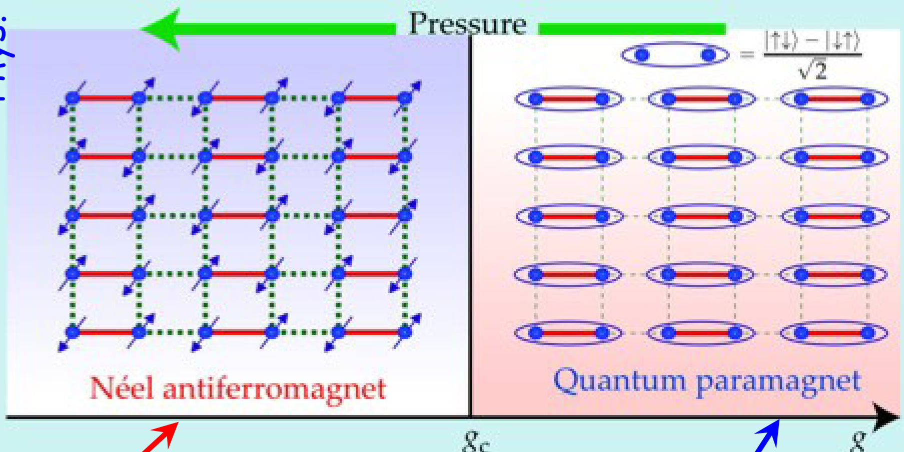
$$|\rightarrow\rangle_i = (|\uparrow\rangle_i + |\downarrow\rangle_i)/\sqrt{2}$$

$$\langle 0|\hat{\sigma}_i^z \hat{\sigma}_j^z|0\rangle \sim e^{-|x_i - x_j|/\xi}$$

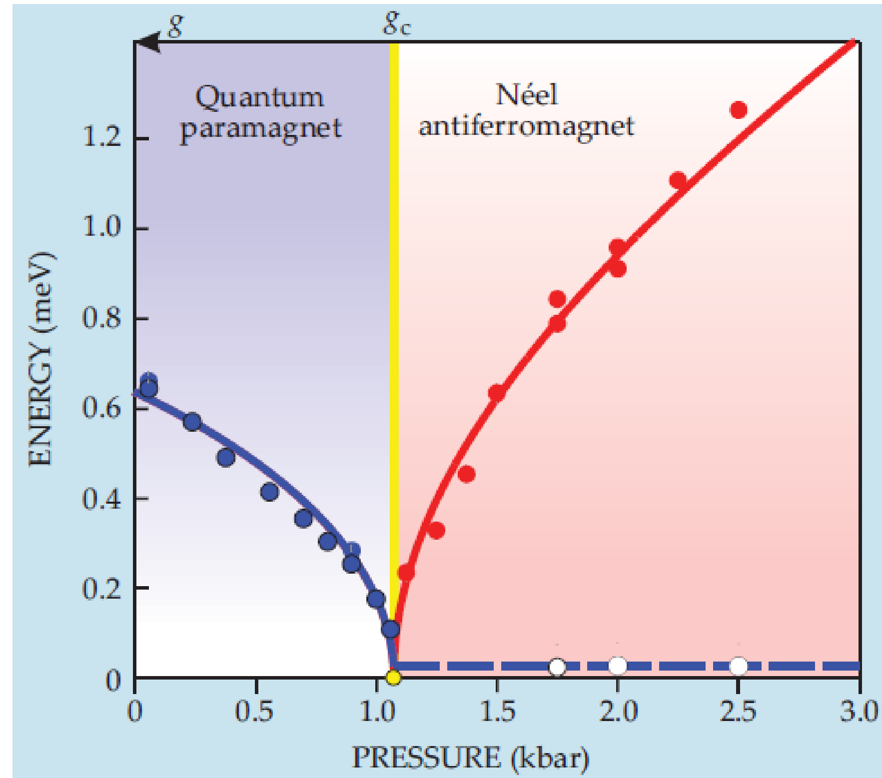
Simple Theoretical Model II: Quantum Criticality in Dimer Antiferromagnet ($TiCuCl_3$)

Phys. Today **64(2)**, 29 (2011)





Experiment: Phys. Rev. Lett. **100**, 205701 (2008)



- The two noncritical ground states of the dimer antiferromagnet have very different excitation spectra:

spin waves with nearly zero energy and oscillations of the magnitude of local magnetization

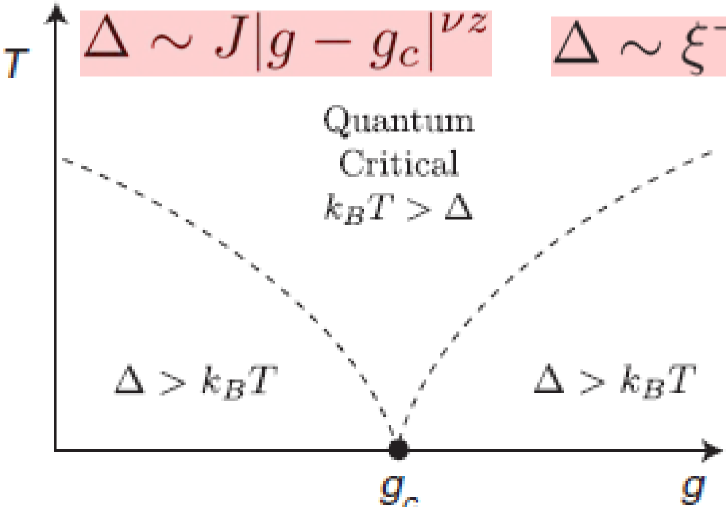
$$|0\rangle = \prod_i \otimes |s\rangle_i \qquad |s\rangle_i = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2} \qquad |t_1\rangle_i = |\uparrow\uparrow\rangle$$

$$|t_0\rangle_i = (|\uparrow\downarrow\rangle + |\uparrow\downarrow\rangle)/\sqrt{2}$$

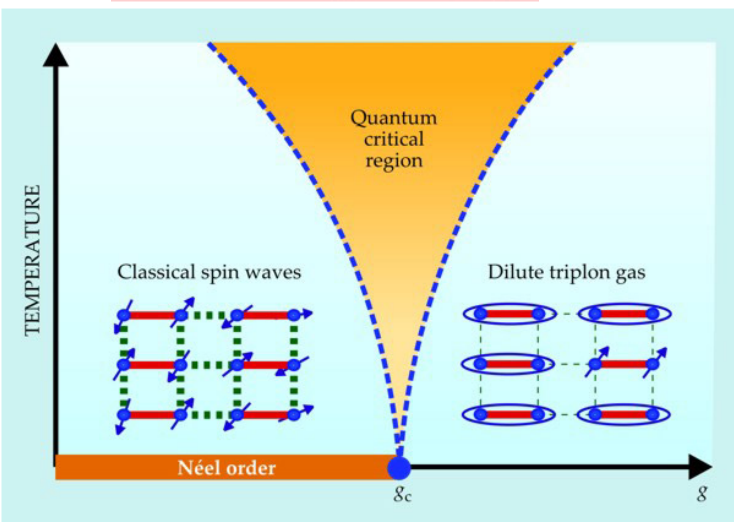
$$|t_m(\mathbf{k})\rangle = \frac{1}{\sqrt{N_d}} \sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} |t_m\rangle_i \prod_{j\neq i} \otimes |s\rangle_j \qquad |t_{-1}\rangle_i = |\downarrow\downarrow\rangle$$

How Quantum Criticality Extends to Non-Zero Temperatures

$\Delta \sim J|g - g_c|^{\nu z}$ $\Delta \sim \xi^{-z}$



$\xi^{-1} \sim \Lambda|g - g_c|^{\nu}$

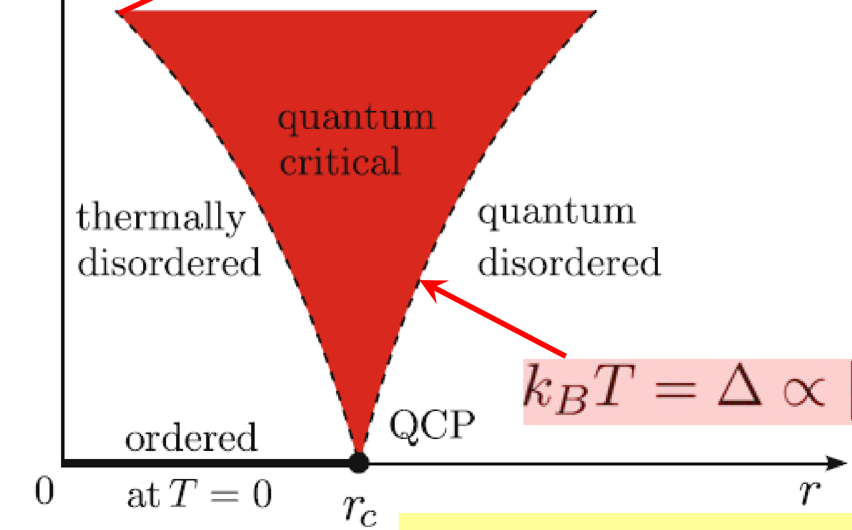


Phys. Today **64(2)**, 29 (2011)

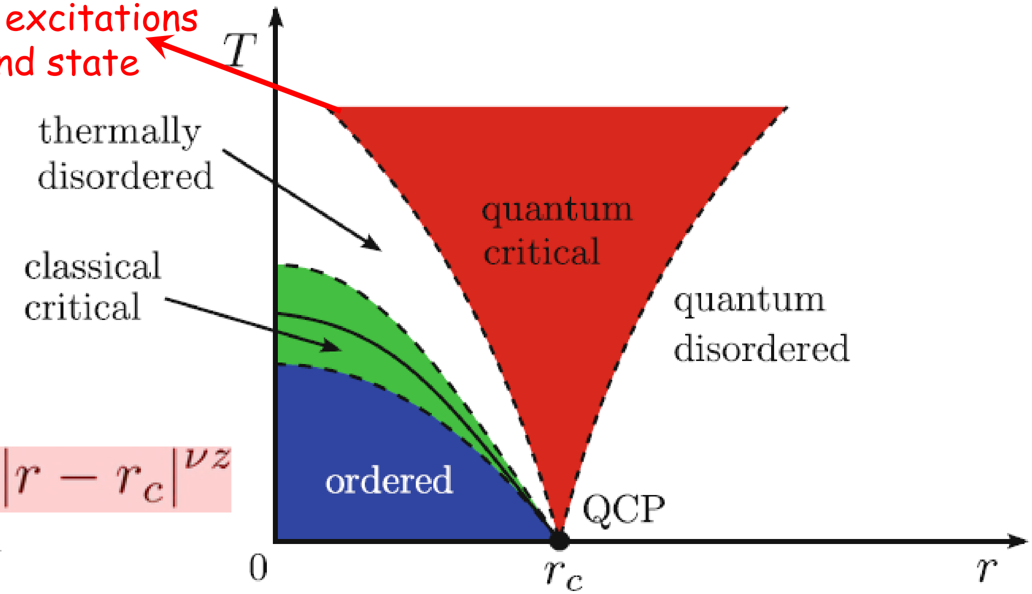
- In the blue region for small *g*, thermal effects induce spin waves that distort the Néel antiferromagnetic ordering.
- For large *g*, thermal fluctuations break dimers in the blue region and form quasiparticles called triplons. The dynamics of both types of excitations can be described quasi-classically.
- Quantum criticality appears in the intermediate orange region, where there is no description of the dynamics in terms of either classical particles or waves. Instead, the system exhibits the strongly coupled dynamics of nontrivial entangled quantum excitations of the quantum critical point g_c.
- Wavefunction at $g=g_c$ is a **complex superposition of an exponentially large** set of configurations fluctuating at all length scales → the critical point wavefunction, which cannot be written down explicitly, has long-range quantum entanglement which emerges for a very large number of electrons and between electrons separated at all length scales.

Scaling in the Vicinity of Quantum Critical Points

physics is dominated by thermal excitations of the quantum critical ground state



$$k_B T = \Delta \propto |r - r_c|^{\nu z}$$



$$Z = \int \mathcal{D}[\Phi] \exp\left\{ - \int_0^{1/T} d\tau \int d^D \mathbf{r} \mathcal{L}[\Phi(\mathbf{r},\tau)] \right\}$$

$\Phi(\mathbf{r},\tau)$ represents fluctuations of the order parameter and it depends on the imaginary time τ which takes values in the interval [0,1/T]; the imaginary time direction acts like an extra dimension, which becomes infinite for $T \to \infty$

$$T = 0: \quad f_{\mathrm{sing}}(G,h) = b^{-(D+z)} f_{\mathrm{sing}}(b^{y_g} G, b^{y_h})$$

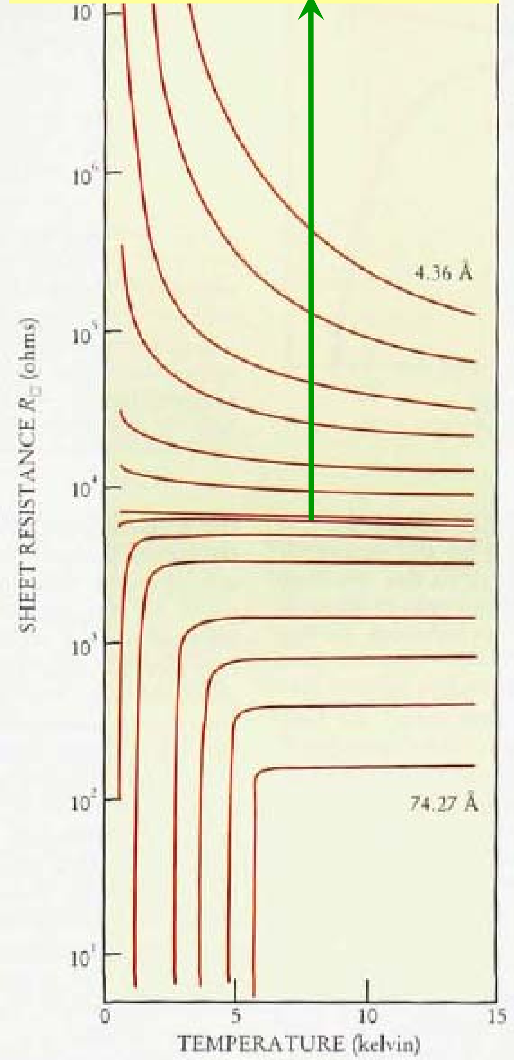
$$G = |g - g_c|/g_c$$

$$T > 0: \quad f_{\mathrm{sing}}(G,h,T) = b^{-(D+z)} f_{\mathrm{sing}}(b^{y_g} G, b^{y_h}, b^z T)$$

$$1/y_g = \nu$$

Example of Scaling Analysis: Superconductor-Insulator QPT in Thin Films

$R_c = h/4e^2 = 6450\ \Omega$



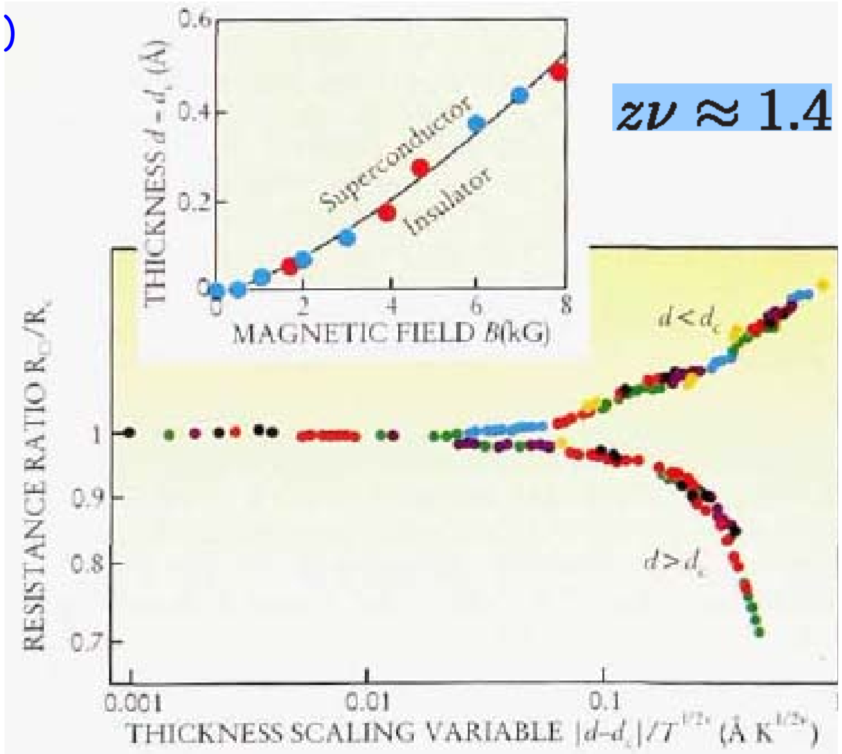
Phys. Today **51(11)**, 39 (1998)

The success of finite-size scaling analyses of the superconductor-insulator transitions as a function of film thickness or applied magnetic field provides strong evidence that $T = 0$ quantum phase transitions are occurring

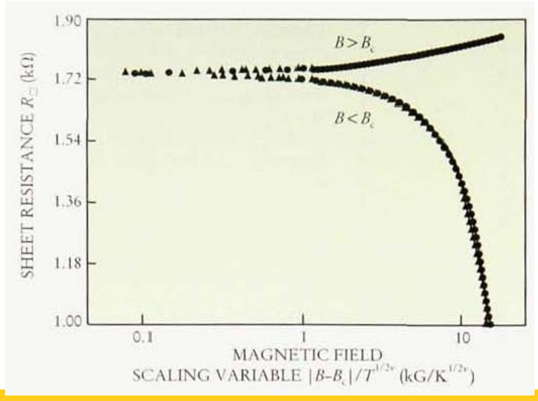
$$\xi \sim g^{-\nu} \qquad \xi_\tau \sim \xi^z$$

$$R_\square = R_c f\left(\frac{g}{T^{1/z\nu}}\right)$$

$$g = B \text{ or } g = d$$



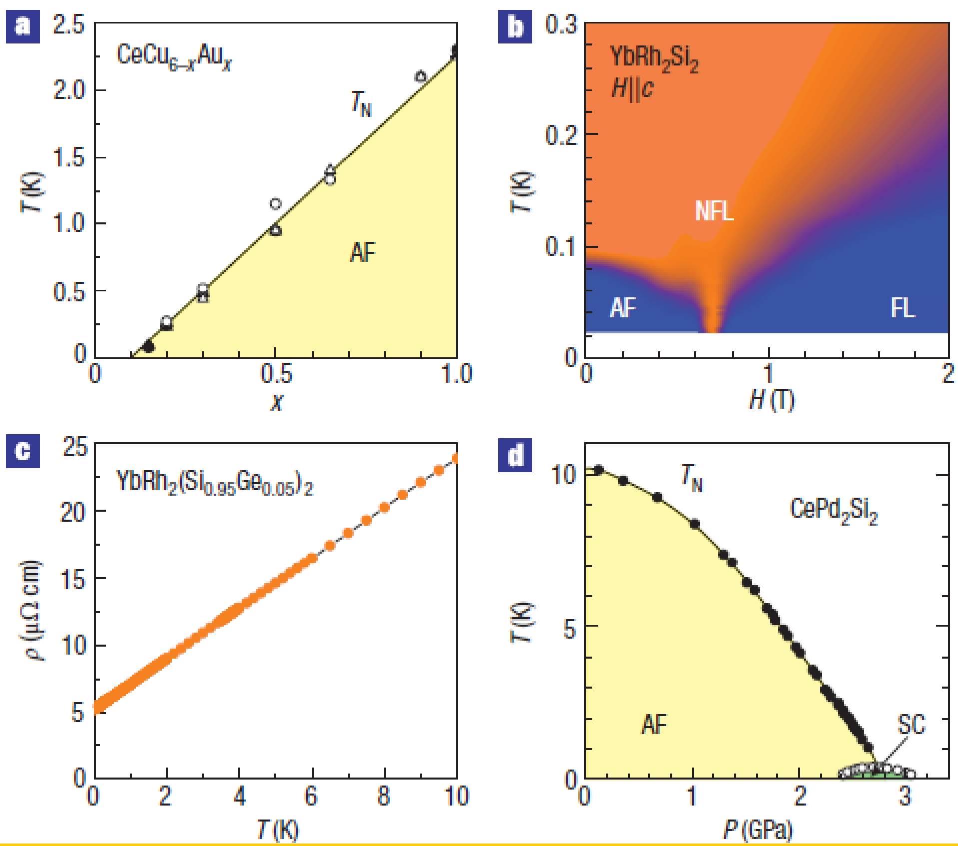
$z\nu \approx 1.4$



$z\nu \approx 1.36$

Experimental Example: Quantum Criticality in Heavy Fermion Materials

- Quantum criticality describes the collective fluctuations of matter undergoing a second-order phase transition at zero temperature.
- Heavy-fermion metals have in recent years emerged as prototypical systems to study quantum critical points.



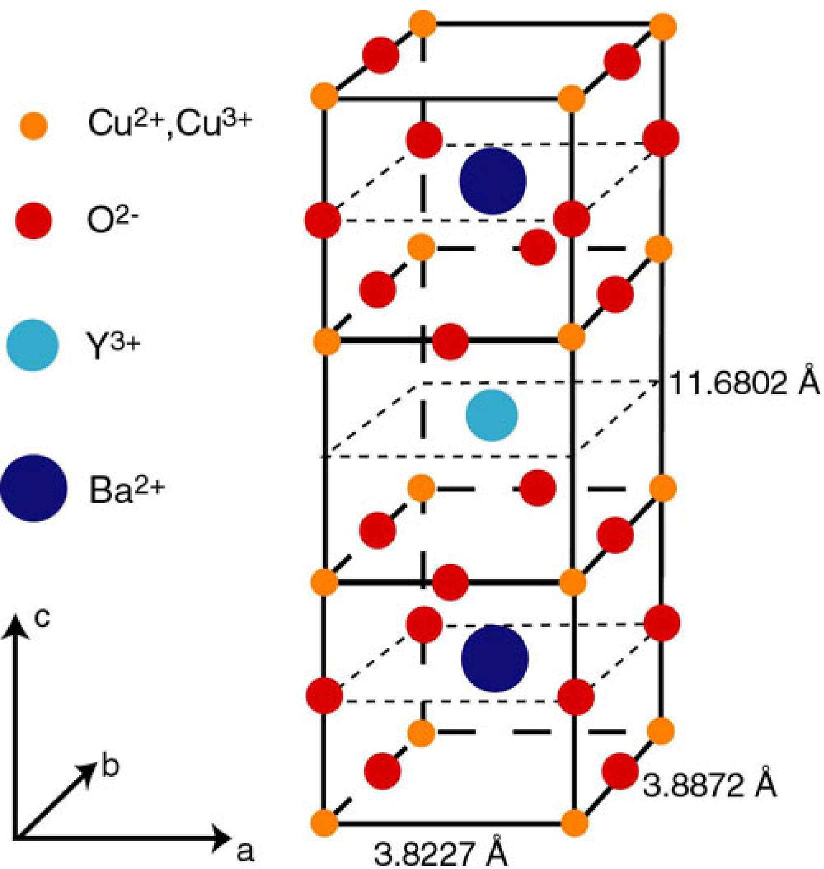
- Key characteristics of of both $CeCu_{5.9}Au_{0.1}$ and $YbRh_2Si_2$ is the divergence of the effective charge-carrier mass at the quantum critical point.

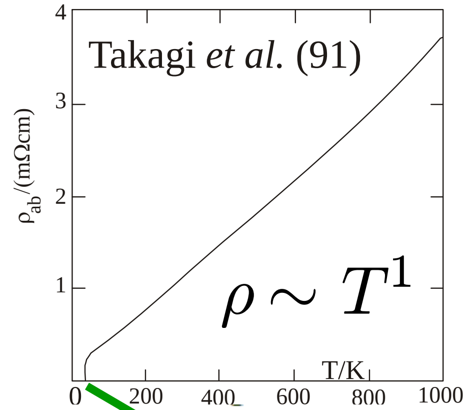
Figure 1 Quantum critical points in HF metals. **a**, AF ordering temperature T_N versus Au concentration x for $CeCu_{6-x}Au_x$ (ref. 7), showing a doping-induced QCP. **b**, Suppression of the magnetic ordering in $YbRh_2Si_2$ by a magnetic field. Also shown is the evolution of the exponent α in $\Delta\rho \equiv [\rho(T) - \rho_0] \propto T^\alpha$, within the temperature–field phase diagram of $YbRh_2Si_2$ (ref. 55). Blue and orange regions mark $\alpha = 2$ and 1, respectively. **c**, Linear temperature dependence of the electrical resistivity for Ge-doped $YbRh_2Si_2$ over three decades of temperature (ref. 55), demonstrating the robustness of the non-Fermi-liquid (NFL) behaviour in the quantum-critical regime. **d**, Temperature-versus-pressure phase diagram for $CePd_2Si_2$, illustrating the emergence of a superconducting phase centred around the QCP. The Néel (T_N) and superconducting (T_c) ordering temperatures are indicated by filled and open symbols, respectively[79].

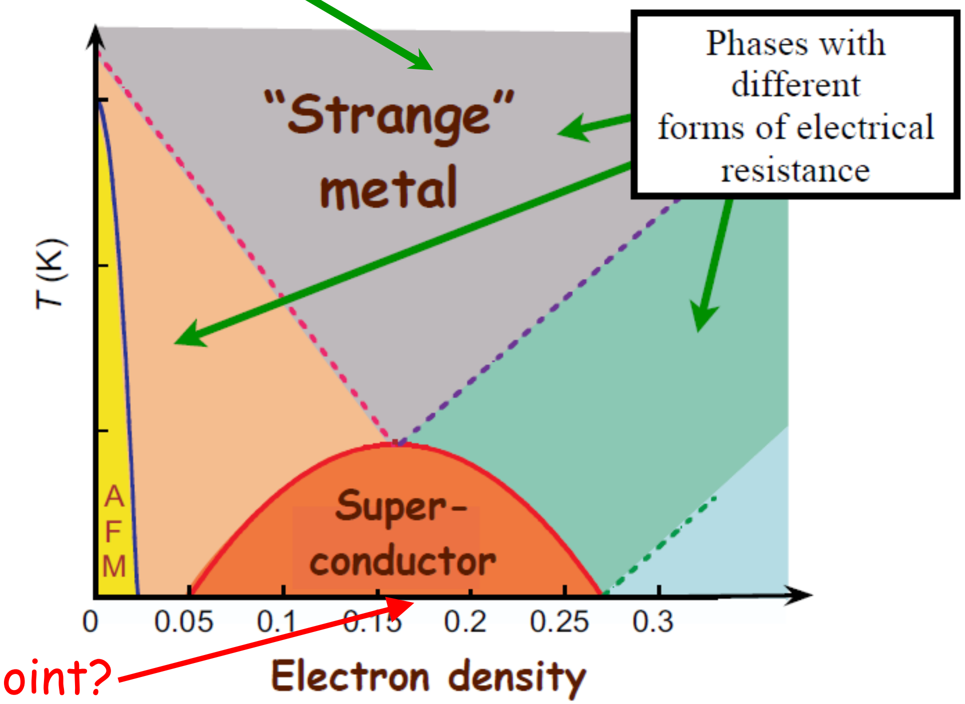
Nature Phys. **4**, 186 (2008)

Experimental Example: Quantum Criticality in High-Temperature Cuprate Superconductors

$YBa_2Cu_3O_{6+x}$

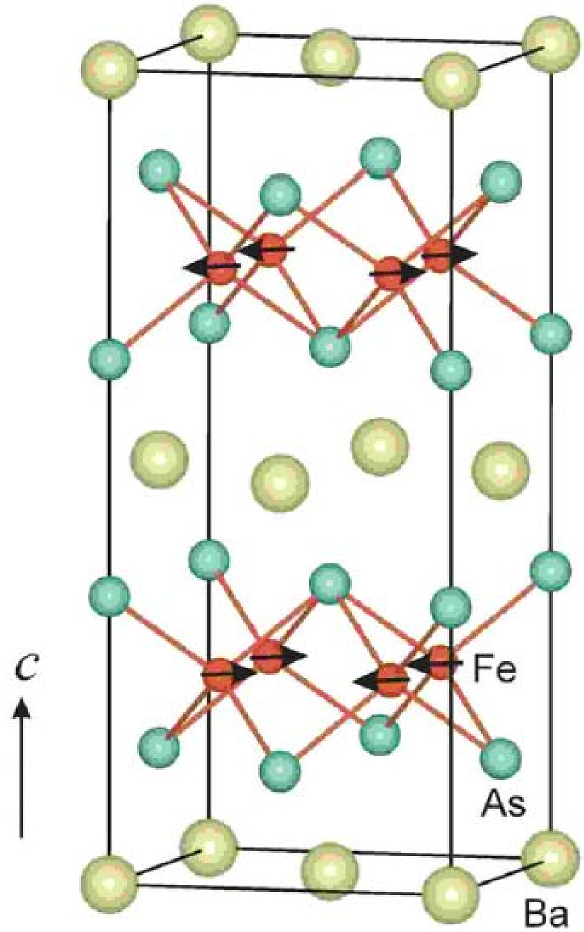


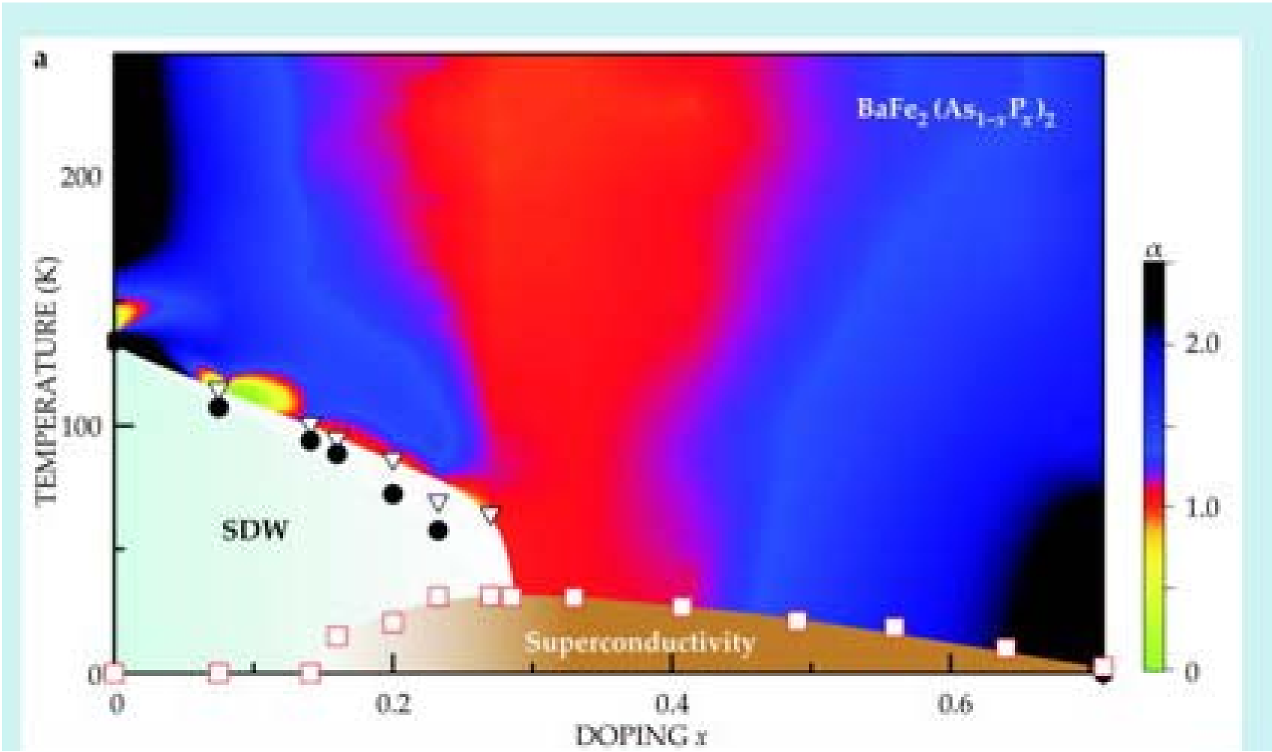




quantum critical point?

Experimental Example: Quantum Criticality in Iron-Based Pnictide Superconductors

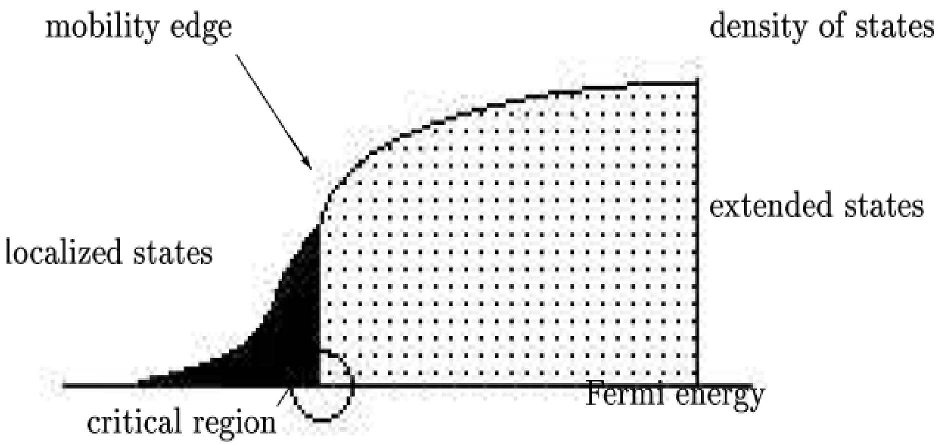


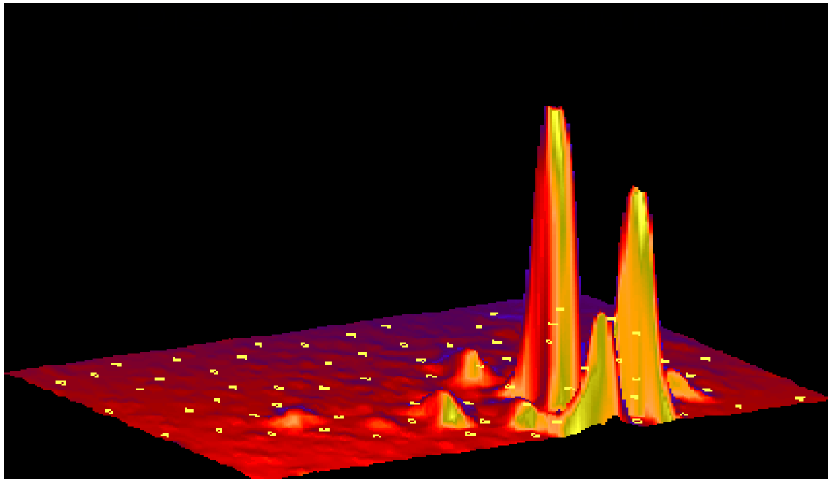


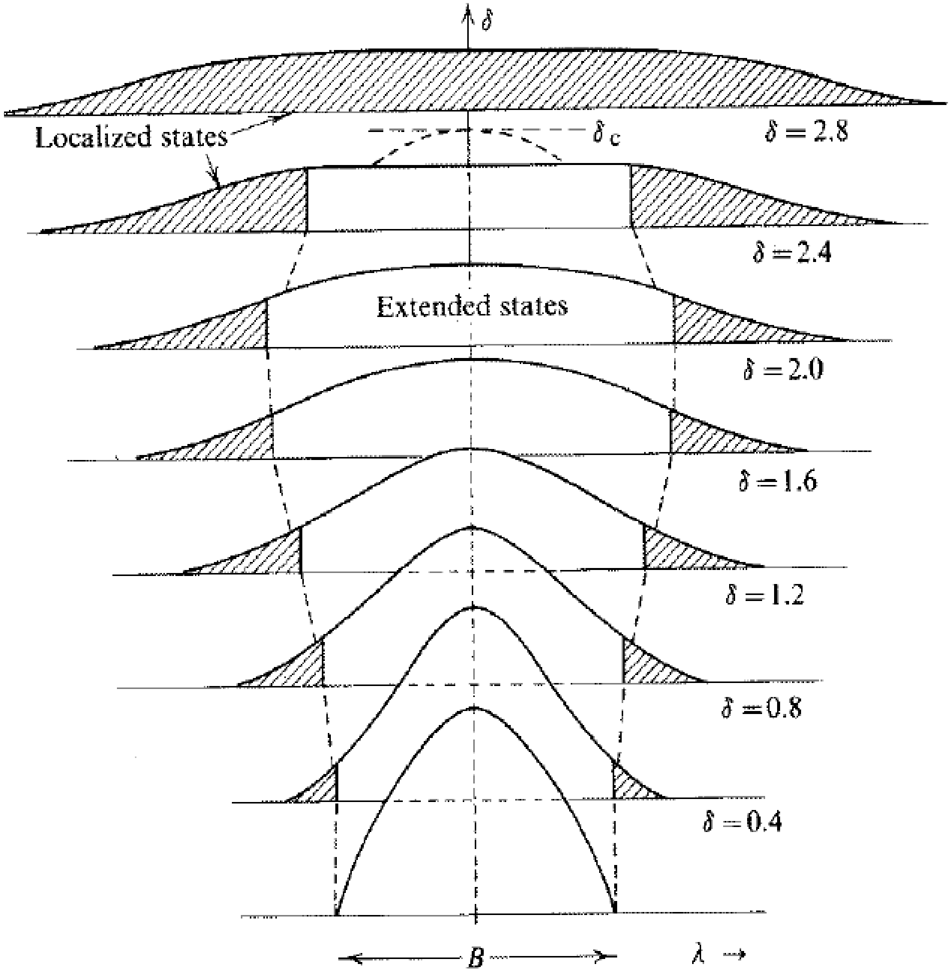
Historical Example: Anderson Localization

$$\hat{H} = \sum_{n} \varepsilon_{\mathbf{m}} |\mathbf{m}\rangle\langle\mathbf{m}| + \sum_{\langle\mathbf{m},\mathbf{n}\rangle} t_{\mathbf{mn}} |\mathbf{m}\rangle\langle\mathbf{n}|$$

$$\delta = W/B \ (\mathrm{B-bandwidth})$$







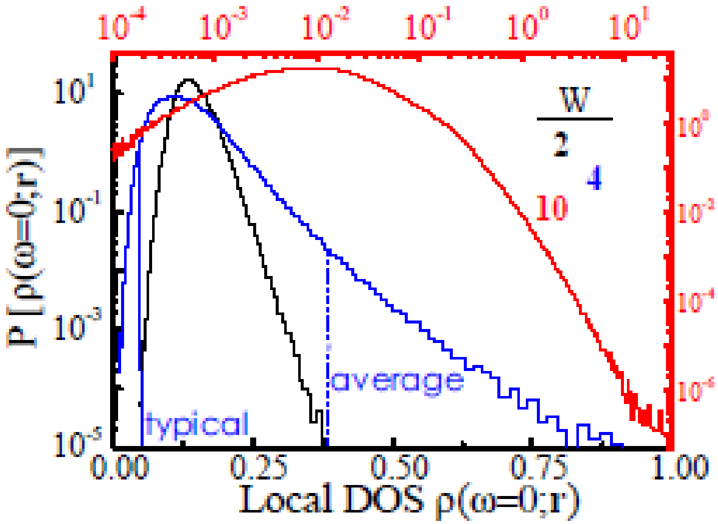
Order Parameter and Scaling in Anderson Localization

EUROPHYSICS LETTERS

Europhys. Lett., **62** (1), pp. 76–82 (2003)

Typical medium theory of Anderson localization: A local order parameter approach to strong-disorder effects

V. Dobrosavljević[1], A. A. Pastor[1] and B. K. Nikolić[2]



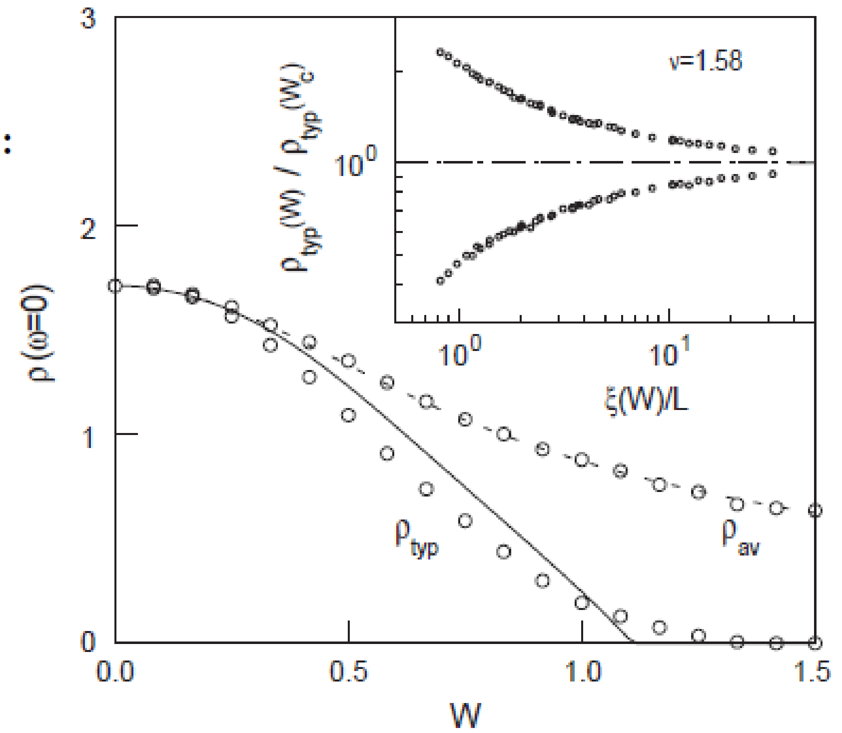
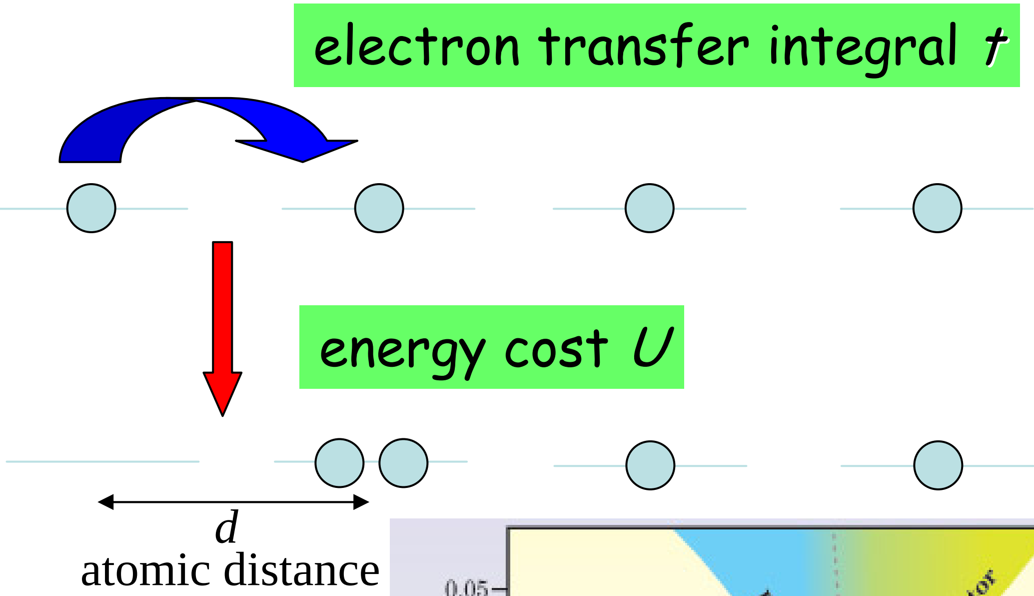


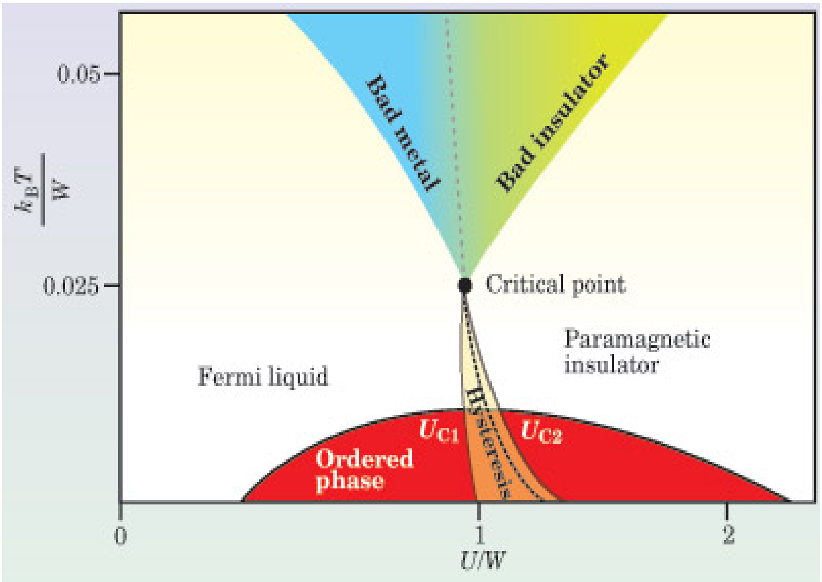
Fig. 1 – Typical and average DOS as a function of disorder W, for a three-dimensional cubic lattice at the band center ($\omega = 0$). Results from exact numerical calculations (circles) are compared to the predictions of TMT (for TDOS, full line) and CPA (for ADOS, dashed line). Finite-size scaling of the numerical data in the critical region $W = 1.17$–1.58, and sizes $L = 4$–12 is shown in the inset, where $\rho_{\text{typ}}(W,L)/\rho_{\text{typ}}(W_c,L)$ is plotted as a function of $\xi(W)/L$, and $\xi(W) = 0.5|(W_c - W)/W_c|^{-\nu}$ is the correlation length in units of the lattice spacing. The numerical data are consistent with $\beta = \nu = 1.58$.

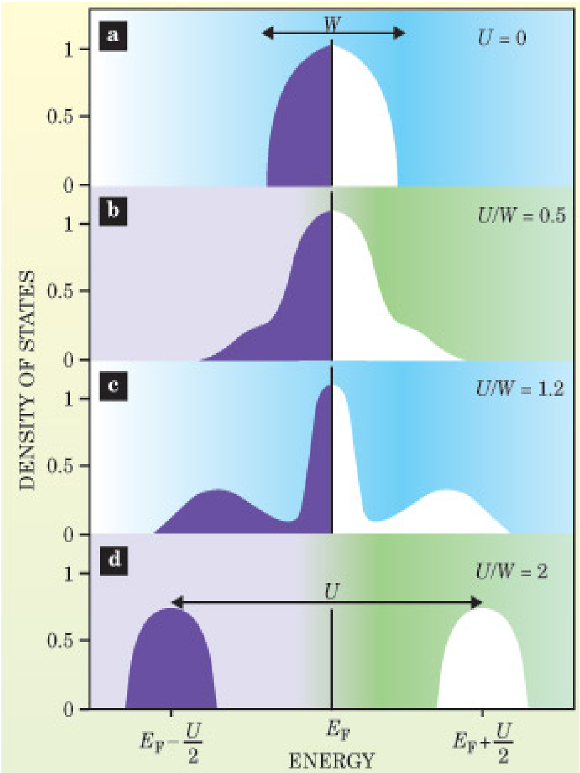
Historical Example: Mott-Hubbard Metal-Insulator Transition



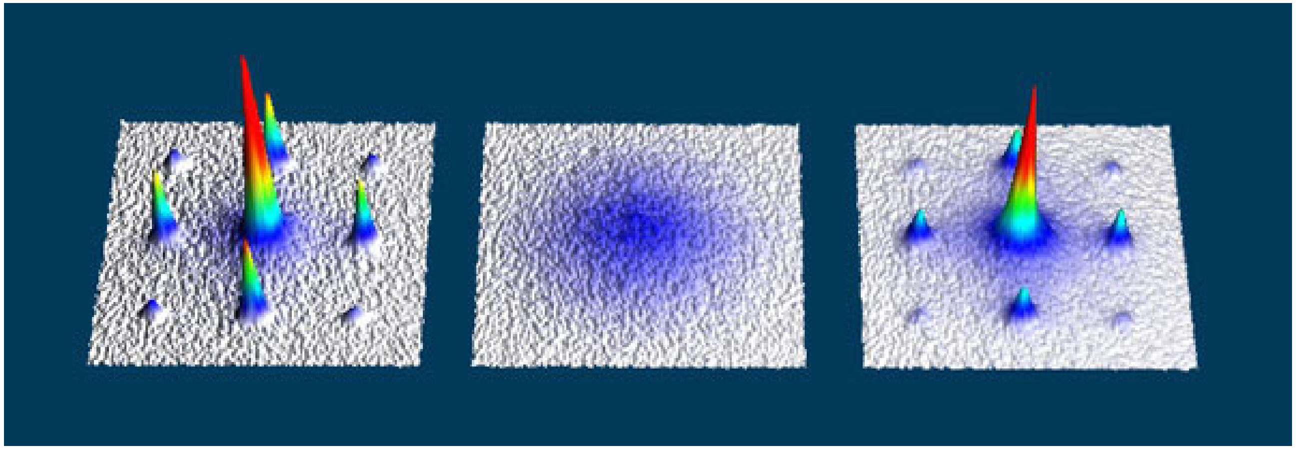
$d \to \infty$ (atomic limit with no kinetic energy gain): insulator

$d \to 0$: possible metal as seen in alkali metals



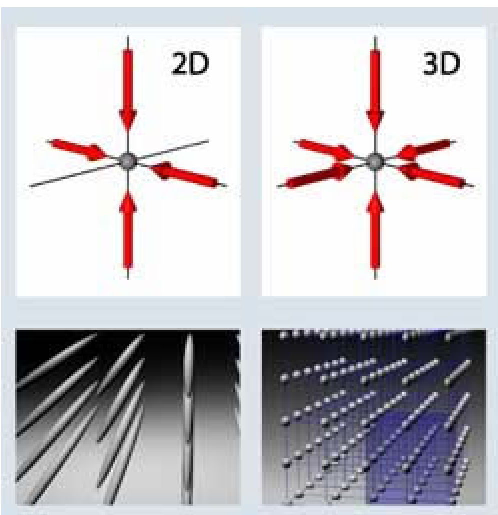


Experimental Example: Superfluid-Mott Insulator QPT in a Gas of Ultracold Atoms

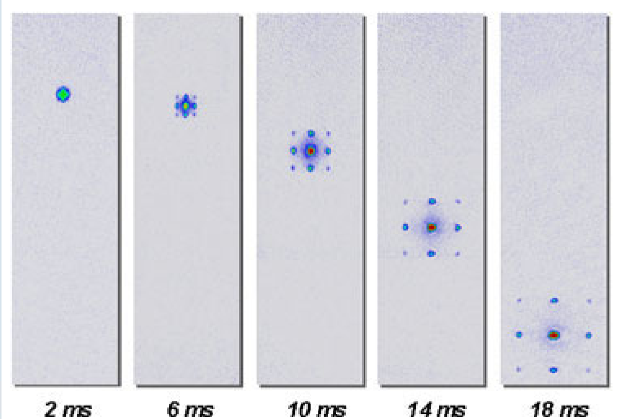


Superfluid state with coherence → Mott insulator state without coherence → superfluid state after restoring the coherence

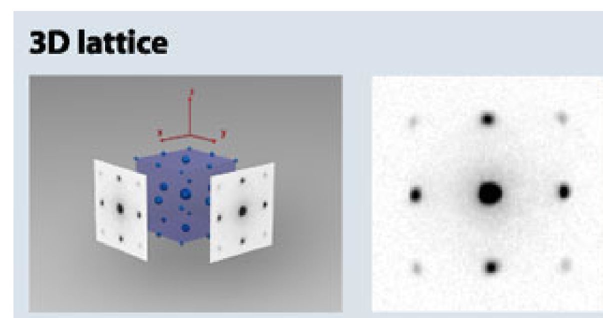
Nature **415**, 39 (2002)



Switch off the optical lattice beams, so that the localized wavefunctions at each lattice site can expand and interfere with each other. They form a multiple matter wave interference pattern which reveals the momentum distribution of the system.



The sharp and discrete peaks observed directly prove the phase coherence across the entire lattice



Theoretical Explanation of Superfluid-Mott Insulator QPT in a Gas of Ultracold Atoms

Bose-Hubbard Hamiltonian for periodic lattice potential

$$H = -J\sum_{\langle i,j\rangle} \hat{a}_i^{\dagger}\hat{a}_j + \sum_i \varepsilon_i \hat{n}_i + \frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i - 1)$$

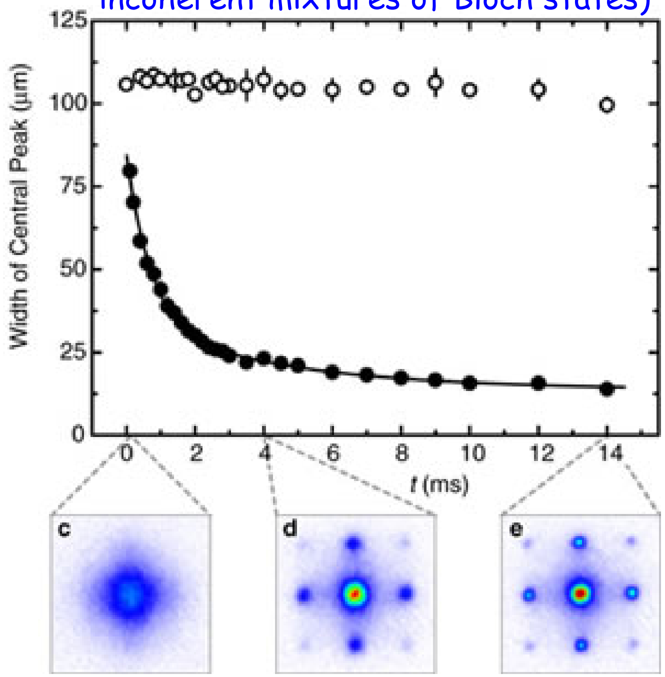
Tunnel matrixelement J:

$$J = -\int d^3x\, w(x-x_i)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{lat}(x)\right)w(x-x_j)$$

On-site interaction energy U:

$$U = \frac{4\pi\hbar^2 a}{m}\int d^3x\, |w(x)|^4$$

Experimental proof for the Mott insulator phase rather than statistically dephased superfluid state (i.e., incoherent mixtures of Bloch states)



Greiner Lab, http://greiner.physics.harvard.edu

$U/J < g_c$

kinetic energy term dominates:

Weakly interacting bosonic gas

-> Superfluidity

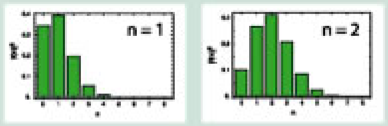
- Atoms are **delocalized** over the entire lattice

$$|\Psi_{SF}\rangle \propto \left(\sum_{i=1}^{M}\hat{a}_i^{\dagger}\right)^N |0\rangle$$

- Coherence, manybody state can be described by a **macroscopic wavefunction**

$$\langle a_i\rangle \neq 0$$

- **Coherent state**
  Superposition with a Binomial atom number distribution per lattice site
  -> number fluctuations



- **Gapless excitation spectrum**

$U/J > g_c$

interaction energy term dominates:

Strongly corrolated bosonic system

-> Mott insulator

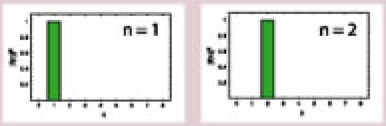
- Atoms are completely **localized** to lattice sites

$$|\Psi_{Mott}\rangle \propto \prod_{i=1}^{M}(\hat{a}_i^{\dagger})^n |0\rangle$$

- No coherence, no macroscopic wavefunction

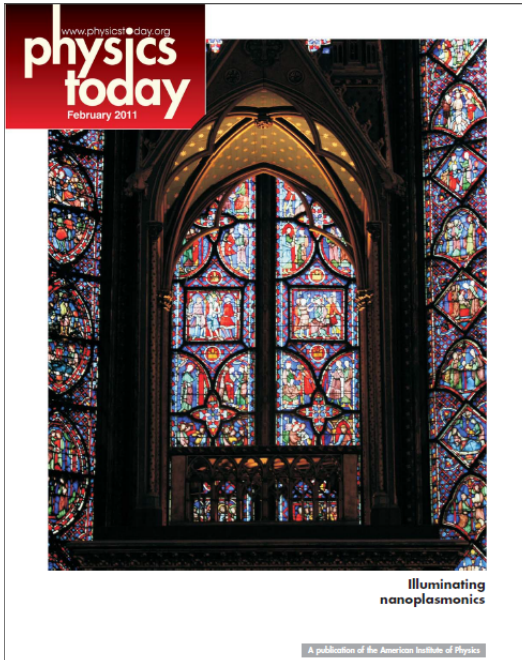
$$\langle a_i\rangle = 0$$

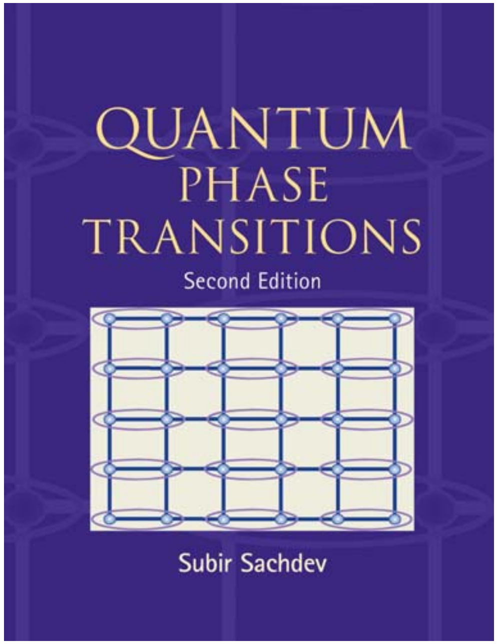
- **Fock state**
  with a vanishing number fluctuation per lattice site



- **Excitation spectrum has an energy gap** $\Delta = U$

References





REVIEW ARTICLE | FOCUS

Quantum criticality in heavy-fermion metals

Quantum criticality describes the collective fluctuations of matter undergoing a second-order phase transition at zero temperature. Heavy-fermion metals have in recent years emerged as prototypical systems to study quantum critical points. There have been considerable efforts, both experimental and theoretical, that use these magnetic systems to address problems that are central to the broad understanding of strongly correlated quantum matter. Here, we summarize some of the basic issues, including the extent to which the quantum criticality in heavy-fermion metals goes beyond the standard theory of order-parameter fluctuations, the nature of the Kondo effect in the quantum-critical regime, the non-Fermi-liquid phenomena that accompany quantum criticality and the interplay between quantum criticality and unconventional superconductivity.

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point (QCP)[2,3]. The quantum-critical state is distinct from the phases on both sides, and is expected to show features in its physical properties that are universal. Moreover, it will contain emergent low-energy excitations that are highly collective, thereby representing a quantum state of matter with properties that are necessarily different from those of any weakly interacting system.

It was not until recent years that QCPs were experimentally observed[4,5]. Particularly clear-cut examples have come from heavy-fermion (HF) metals, rare-earth-based intermetallic compounds in which the effective charge-carrier masses are hundreds of times the bare-electron mass. Accompanying the large effective

feature article

Quantum criticality

Subir Sachdev and Bernhard Keimer

A phase transition brought on by quantum fluctuations at absolute zero may seem like an abstract theoretical idea of little practical consequence. But it is the key to explaining a wide variety of experiments.

Subir Sachdev is a professor of physics at Harvard University in Cambridge, Massachusetts. **Bernhard Keimer** is a director of the Max Planck Institute for Solid State Research in Stuttgart, Germany.

2 MARCH 2012 VOL 335 SCIENCE

Observation of Quantum Criticality with Ultracold Atoms in Optical Lattices

Xibo Zhang,* Chen-Lung Hung, Shih-Kuang Tung, Cheng Chin*

Quantum criticality emerges when a many-body system is in the proximity of a continuous phase transition that is driven by quantum fluctuations. In the quantum critical regime, exotic, yet universal properties are anticipated; ultracold atoms provide a clean system to test these predictions. We report the observation of quantum criticality with two-dimensional Bose gases in optical lattices. On the basis of in situ density measurements, we observe scaling behavior of the equation of state at low temperatures, locate the quantum critical point, and constrain the critical exponents. We observe a finite critical entropy per particle that carries a weak dependence on the atomic interaction strength. Our experiment provides a prototypical method to study quantum criticality with ultracold atoms.