Emergence of Quantum Phases in Novel Materials

Instituto de Ciencia de Materiales de Madrid

Quantum Materials for Quantum Technologies (Q4Q)

Phase transitions

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More Is Different

Broken symmetry and the nature of the hierarchical structure of science.

P. W. Anderson

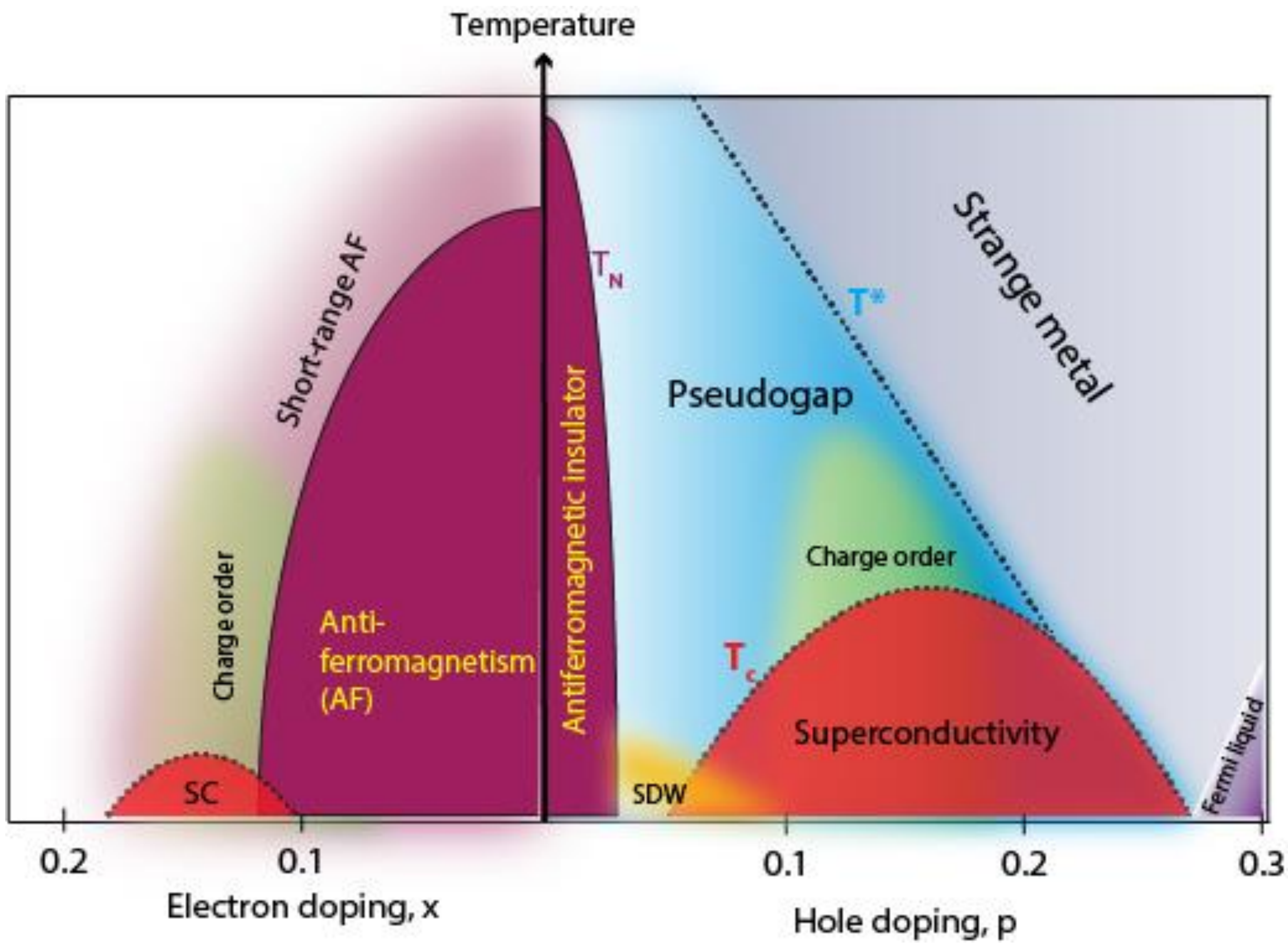
P. Anderson, Science'72

X	Y
solid state or many-body physics	elementary particle physics
chemistry	many-body physics
molecular biology	chemistry
cell biology	molecular biology
•	•
•	•
•	•
psychology	physiology
social sciences	psychology

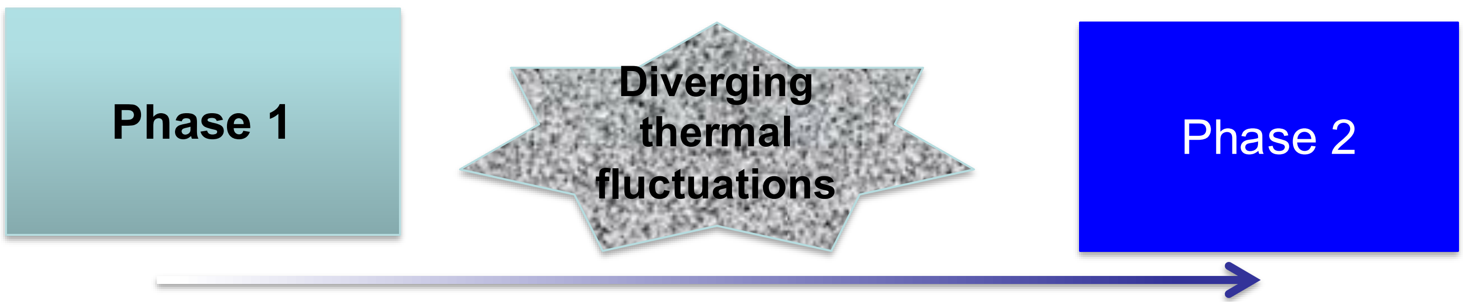
But this hierarchy does not imply that science X is "just applied Y." At each stage entirely new laws, concepts, and generalizations are necessary, requiring inspiration and creativity to just as great a degree as in the previous one. Psychology is not applied biology, nor is biology applied chemistry.

In my own field of many-body physics, we are, perhaps, closer to our fundamental, intensive underpinnings than in any other science in which non-trivial complexities occur, and as a result we have begun to formulate a general theory of just how this shift from quantitative to qualitative differentiation takes place. This formulation, called the theory of "broken symmetry," may be of help in making more generally clear the breakdown of the constructionist converse of reductionism. I will give an elementary and in-

Broken symmetry in the phase diagram full of CPT&QPT

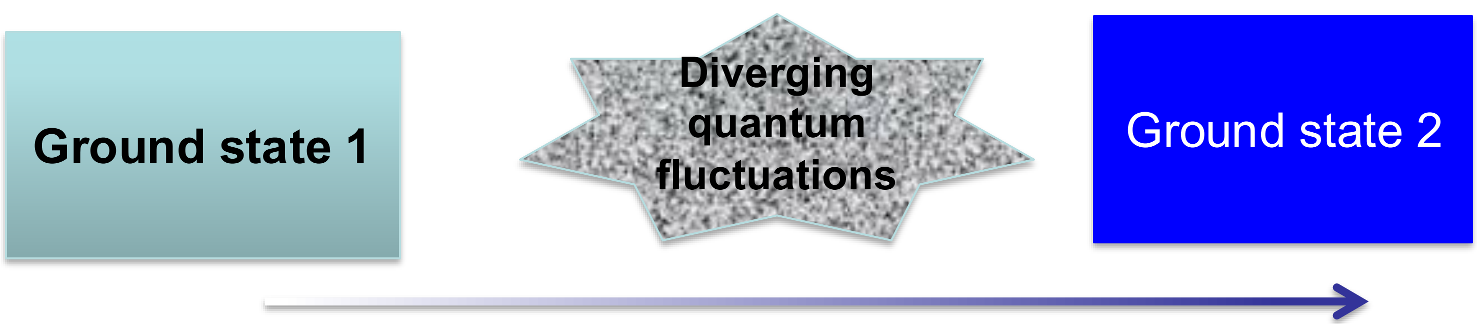


Classical phase transitions



Control parameter: temperature…

Quantum phase transitions



Control parameter: pressure, magnetic field…

Index for phase transitions

- How to describe phase transitions? Hamiltonian & effective theories. Symmetries
- Classical phase transitions
  - Landau theory and beyond
  - Microscopic theory. Example: Ising model
  - Micro-Macro bridge: Ising <-> Φ^4 theory
  - Criticality
  - Important theorems for continuous symmetry: Goldstone theorem, Mermin-Wagner Theorem, Kosterlitz-Thouless transition.
- Quantum phase transitions QPT
  - Quantum Ising model<-> Corresponding effective theory
  - Mapping QPT-CPT
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Hamiltonian description (micro scale, high energy, lattice…)

$$H(x_1,...,x_N)\psi_1(x_1)=E\psi_1(x_1)$$

$$\vdots$$

$$H(x_1,...,x_N)\psi_N(x_1)=E\psi_N(x_1)$$

$$H(x_1,...,x_N)=H_{eleckinetic}(x_1)+H_{elec,ion}(x_1,...,x_N)+H_{elec,elec}(x_1,...,x_N)+H_{ion}(x_1,...,x_N)$$

In principle we get ground state and excitations

Too many degrees of freedom! Even more for phase transitions
Simplification: Ising model (Spin)…, Hubbard model (spin and charge)… still complicated, even more for phase transitions

Effective theory (macro scale, low energy, continuum)

In the effective theory there are just the relevant degrees of freedom **ϕ** close to the phase transition

Example for effective action

$$S[\Phi] = \int dx^d \left[\frac{1}{2} (\nabla\Phi)^2 + \frac{r}{2}\Phi^2 + g\Phi^4 \right]$$

How to chose the relevant degrees of freedom?

Symmetry

Symmetry in Physics is the invariance of a physical law under transformations.

Symmetries form a group (O(n), SU(n)…)

For example, for the group O(3), the rotational group

$$\text{R is orthogonal if } \mathrm{RR}^T = 1$$

$$\text{If } \mathrm{R}_1, \mathrm{R}_2 \in \mathrm{O}(3) \quad \mathrm{R}_1\mathrm{R}_2 \in \mathrm{O}(3)$$

$$(\mathrm{R}_1\mathrm{R}_2)^T\,\mathrm{R}_1\mathrm{R}_2 = \mathrm{R}_2^T\mathrm{R}_1^T\mathrm{R}_1\mathrm{R}_2 = 1 \Rightarrow$$

R forms a group

Symmetries in condensed matter

Symmetry	System	Order parameter	Conjugate field	Physical example
Discrete				
Z_2/Ising	uniaxial FM	$\langle m_z \rangle$	h_z	
	uniaxial AF	$\langle m_{z,A} - m_{z,B} \rangle$	$h_{z,A} - h_{z,B}$	Rb_2NiF_4, K_2MnF_4
	order-disorder	$\langle n_A - n_B \rangle$	$\mu_A - \mu_B$	β-brass
	displacive	$\langle u_z \rangle$	f_z	$BaTiO_3$
	liquid-gas	$\langle n_L - n_G \rangle$	μ	many
Continous				
$O_2/U(1)$	easy-plane FM	$\langle \mathbf{m} \rangle$	$\mathbf{h}$	
	easy-plane AF	$\langle \mathbf{m}_A - \mathbf{m}_B \rangle$	$\mathbf{h}_A - \mathbf{h}_B$	
Internal: gauge symmetries	superfluid	$\langle \psi \rangle$	h_ψ	He_4
	smectic-C			Fig. 2.7.1
	hexatic-B	$\langle e^{6i\theta} \rangle$		Fig. 2.7.7
O_3	Heisenberg FM	$\langle \mathbf{m} \rangle$	$\mathbf{h}$	EuS, EuO, Fe, Ni
O_0	Heisenberg AF	$\langle \mathbf{m}_A - \mathbf{m}_B \rangle$	$\mathbf{h}_A - \mathbf{h}_B$	$RbMnF_3$
	SAW			polymer

Chaikin & Lubensky

Time-reversal symmetry: broken in ferromagnets, Chern insulator…

And more…can you think of an example?

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Landau theory

Phase 1

Diverging thermal fluctuations

Phase 2

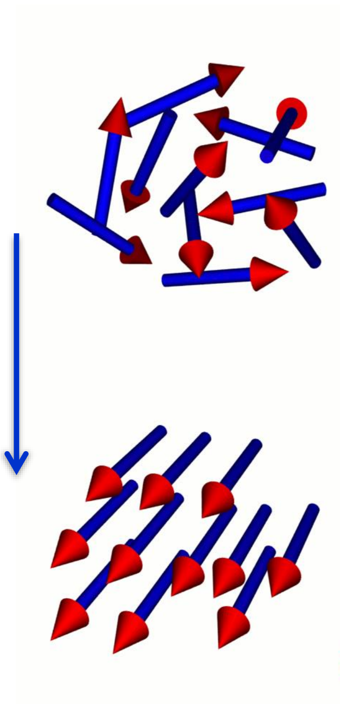
Control parameter: temperature

High symmetry (isotropic, homogeneous…),
Kinetic dominates over correlation, higher entropy

At Tc
Symmetry
breaking

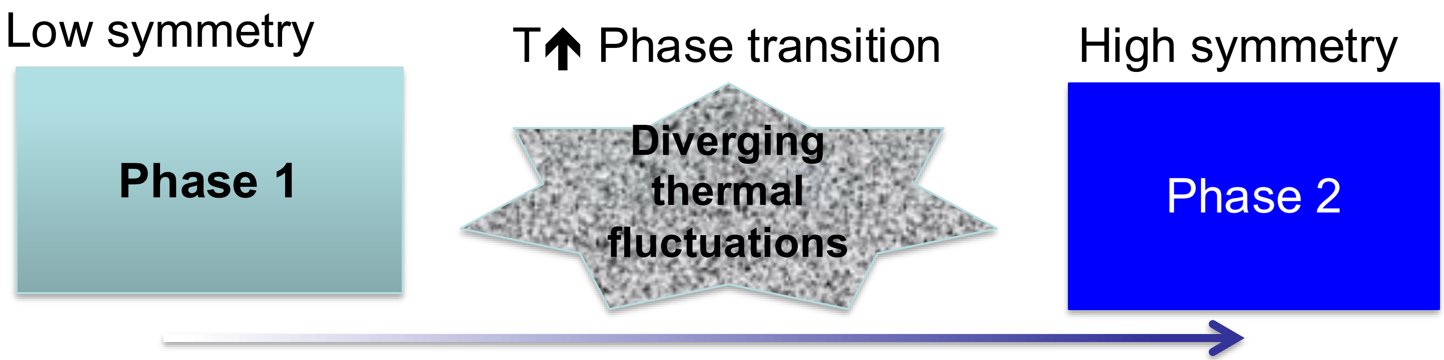
T ↓

Emergence
of FM phase



Lower symmetry (order), Correlation
dominates over kinetic energy,
Lower entropy, higher order

Landau Theory



Using these facts Landau proposed a theory (assumptions):

1. **Order parameter ϕ, <**$\langle\phi\rangle=0$ in the high symmetry phase and $\langle\phi\rangle\neq 0$ in the ordered phase with lower symmetry**. Symmetry breaking**. Ex magnetization (broken symmetry: spin rotation)
2. Free energy determined minimizing the following functional: $F = F_0(T)+F_L(T,\Phi)$ **ϕ controls the thermodynamic.**
3. Building of $F_L(T,\Phi)$: Φ small close to the phase transition, expand $F_L(T,\Phi)$ in powers of Φ respecting symmetries (Ex: $\Phi \to -\Phi$ discrete broken symmetry)

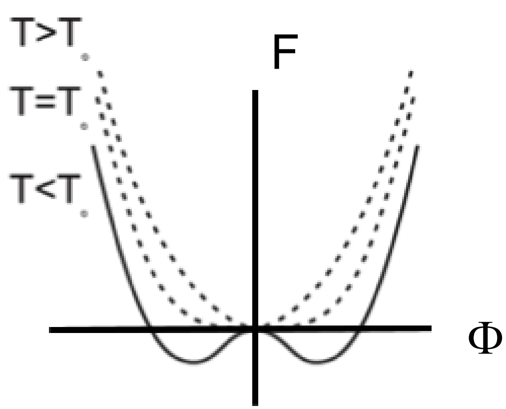
Landau Theory

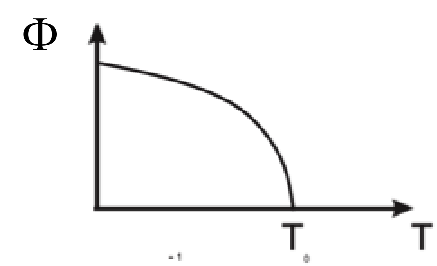
4. Non-trivial T dependence is in the lowest order signifying the competition between minimizing energy and increasing entropy, F=E-TS.

$$F(\Phi, T) = F_0(T) + V\left(\frac{1}{2} r_0 (T - T_c)\Phi^2 + g(T)\Phi^4\right)$$ Landau Functional

5. Minimizing the Landau functional over Φ we obtain the **mean field theory.**

$$\frac{\partial F}{\partial \Phi} = 0 \rightarrow r_0(T - T_c)\Phi + 4g(T)\Phi^3 = 0 \rightarrow \bar{\Phi} = \begin{cases} 0 & T > T_c \\ \left(\frac{-r_0(T - T_c)}{g}\right)^{1/2} & T < T_c \end{cases}$$





Contact with experiments: susceptibility

For example: magnetization:

Small (magnetic) perturbation

$$F[T,m]=\frac{r_0(T-T_c)}{2}m^2+g(T)m^4-hm...$$

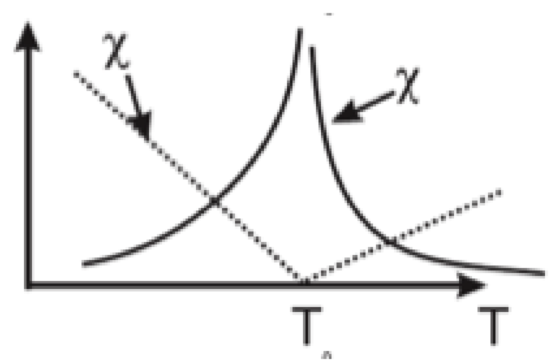
Linear response

χ Susceptibility:

$$\chi=\partial m\big/\partial h=\partial^2F\big/\partial h^2$$

$$\frac{\partial F[T,m]}{\partial m}=0 \Rightarrow \quad r_0(T-T_c)m+4g(T)m^3=h$$

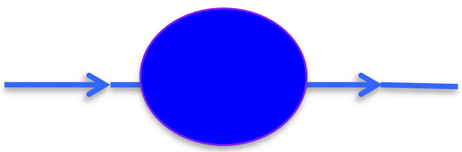
$$\chi_0^{-1}=\frac{\partial h}{\partial m}\propto r_0(T-T_c)$$



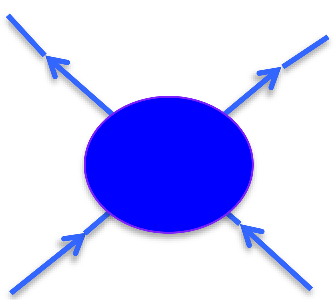
It diverges! Second order phase transition

Contact with experiments: Lineal response theory

Small (electromagnetic) perturbation $\longrightarrow$ Lineal response (Ex. $m=\chi H$)



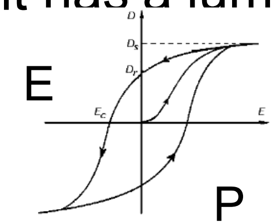
Response to one particle: thermodynamic quantities (specific heat, compressibility, magnetic susceptibility…), ARPES, STM,

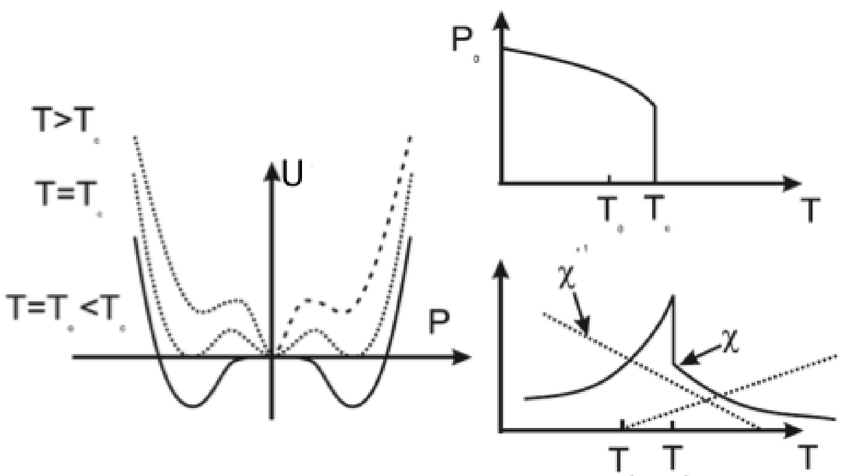


Response to two particles: transport (electric current, spin current, Hall current->Kubo formalism), spectroscopic techniques (Raman, X-ray, optical conductivity, neutron scattering…)

1st Order phase transitions

- The order parameter is not a continuous function of T but it has a jump. Susceptibility also with a jump.
- There can be phase separation (negative compressibility) and may exhibit hysteresis.
- Described by a Landau functional with more terms: cubic, sixth with negative fourth…





$$\alpha = \beta\left(T - T_0\right)$$

1st Order (γ<0)

$$U = \frac{\alpha}{2}P^2 + \frac{\gamma}{4}P^4 + \frac{\delta}{6}P^6 - EP$$

Ginzburg-Landau

Fluctuations around the mean field solution-> Getting closer to Criticality

Long-wavelengths fluctuations can be added in Landau theory fluctuations: $\phi(x)$ is slowly varying and one just keeps the gradient term

$$F_{GL}[T,\Phi] = \int dx^d \left(\frac{1}{2} c \left(\nabla \Phi \right)^2 + \frac{r}{2} \Phi^2 + g(T) \Phi^4 - h\Phi \ldots \right) \rightarrow$$

Ginzburg-Landau Functional: include fluctuations

$\Phi(x) \rightarrow$ ***local*** order parameter

A scale is introduced: ξ Correlation length at T>Tc

$$\xi^2 = \frac{c}{r_0 (T - T_c)}$$ □

ξ Diverges at T->Tc as ½ in mean field

For second order phase transitions the correlation length diverges as a power law at the critical point. At the transition point is infinite, implying that the thermodynamic properties Cv, χ, … also diverge

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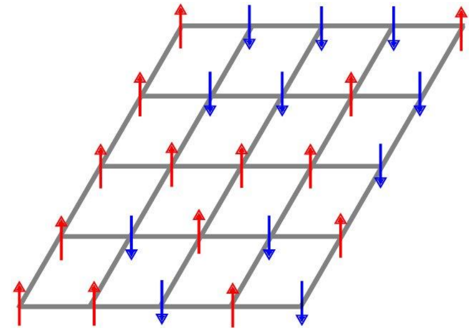
Spontaneous symmetry breaking in the Ising model



Ex: Consider the Ising model (S=±1)

$$H = -J \sum_{\langle ij \rangle} S_i S_j \qquad Z = \sum_{\{S_i\}} e^{-\beta H}$$

The hamiltonian possess a discrete symmetry-> Z_2 invariant (+1->-1) but in the ordered phase the ground state is not invariant-> Spontaneous symmetry breaking!

$$\langle m \rangle = \mu \sum_i \langle S_i \rangle = \frac{1}{Z} \sum_i \sum_{\{S_i\}} S_i e^{-\beta H} = 0!!!!$$

In fact it is impossible to observe a phase transition in a finite system

Solution -> ***Thermodynamic limit & extra field (h) in the Hamiltonian***

$$H = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i$$

$$\lim_{h \to 0} \lim_{N \to \infty} \langle m \rangle = \bar{m} \neq 0$$

Emergence of the FM phase

Limits cannot be interchanged!

Definitions: Correlation function

In Statistical Physics all the information is encoded in the partition function
The probability of finding the system in the microstate i with energy E_i is given in thermal equilibrium by the Boltzmann factor: $\exp(-E_i/k_BT)/Z$

$$Z = \sum_{\{S_i\}} e^{-\beta H} \Rightarrow$$ Generating function $$Z = e^{-\beta F} \Rightarrow F = -\frac{1}{\beta}\ln Z$$

$$H = -J\sum_{\langle ij\rangle} S_i S_j - \mu \sum_i B_i S_i$$

B_i -> fictitious (conjugate) field

$$\langle S_i\rangle = \frac{1}{Z}\sum_{\{S_i\}} e^{-\beta H} S_i = \frac{1}{(\beta\mu)}\left.\frac{\partial \ln Z}{\partial B_i}\right|_{B=0}$$

$$m = \mu\sum_i \langle S_i\rangle$$

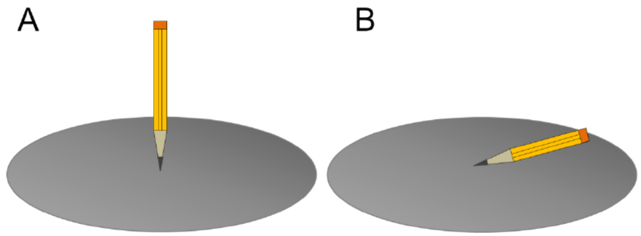
$$G_{ij} = \langle S_i S_j\rangle - \langle S_i\rangle\langle S_j\rangle = \frac{1}{(\beta\mu)^2}\left.\frac{\partial^2 \ln Z}{\partial B_i \partial B_j}\right|_{B=0}$$

Correlation function: measure how correlated is the system over a certain range of space

$$\chi = \frac{\partial m}{\partial B} = \frac{1}{\beta}\sum_{ij}\frac{\partial^2 \ln Z}{\partial B_j \partial B_i} = \beta\mu^2\sum_{ij}\langle S_i S_j\rangle - \langle S_i\rangle\langle S_j\rangle$$

Fluctuation-dissipation theorem:
χ -> response function Correlations can be measure!
At a phase transition χ diverges -> infinite fluctuations

In general: Spontaneous Symmetry Breaking SSB



G a symmetry group of the Hamiltonian H
Then SSB occurs if in the ground state (T=0) at the thermodynamic limit

$$\lim_{h \to 0} \lim_{N \to \infty} \langle m \rangle = \bar{m} \neq 0$$

When |i-j|->∞ (long wavelengths),

$G_{ij} = \bar{m}^2$ -> long-range ordered

observable not G-inv.-> The ground state is not invariant under G

$\bar{m}$: order parameter (of the new phase)

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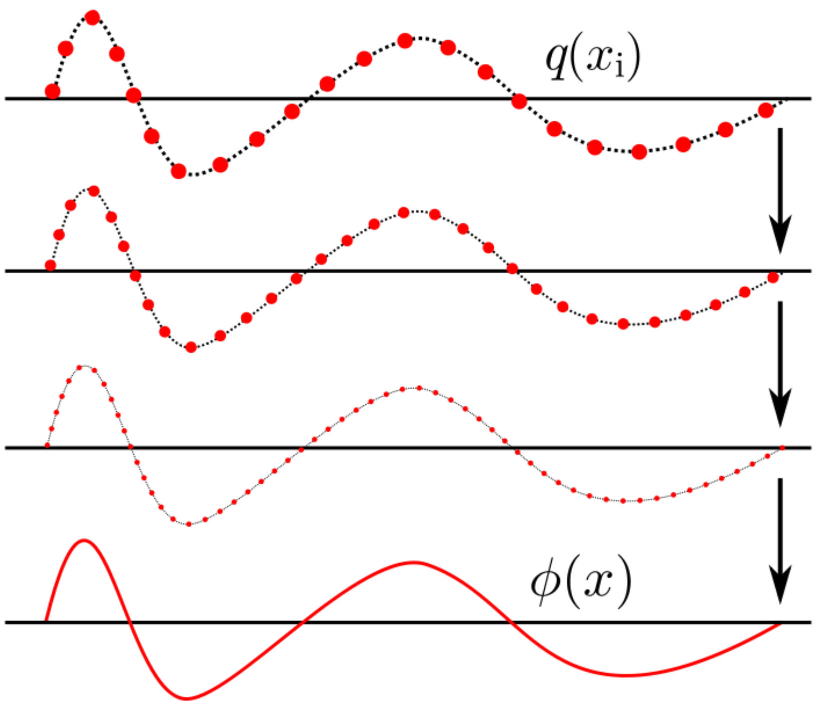
Definition: Continuum limit

Atland & Simons: Condensed Matter Field Theory



N->∞, V->∞ N/V-> finite

x_i=ai->x

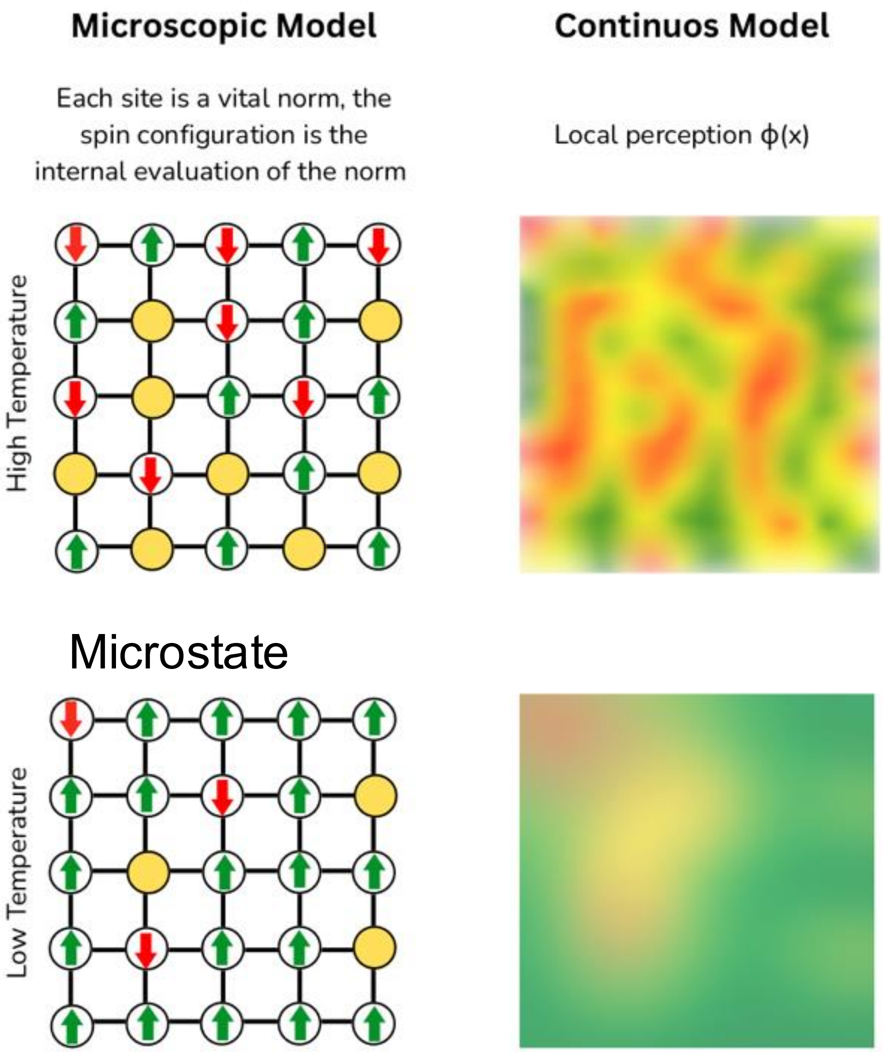
$$\sum_{i=1}^{N} \rightarrow \frac{1}{a}\int_0^L dx$$

$$\frac{\phi_{i+1}-\phi_i}{a} \rightarrow \frac{\partial\phi}{\partial x}$$

Φ(x) is a smooth function (**field**): relative fluctuations on atomic scales are weak-> ***Field theory***

Macro-Micro bridge

arXiv:2507.06041



Emergence of macroscopic patterns from microscopic degrees of freedom:

Intuition:

$$Z = e^{-\beta F} \approx e^{-\beta F_0} e^{-\min_{\{\Phi\}} \beta F_L[T,\Phi]}$$

Formal theory
Saddle point approach:

$$Z = e^{-\beta F} = \sum_{\{\mu\}} e^{-\beta H[\mu]} \approx e^{-\beta F_0} \int D\Phi \, e^{-F_{GL}[T,\Phi]/k_B T}$$

Formal connection with Landau Theory:

It can be shown that after a *Hubbard-Stratonovich* transformation the Ising model close to the phase transition transforms to the f^4 theory ($\Phi \ll 1$) in the continuum limit

Ising model (discrete)

Landau-Ginzburg functional or effective action (continuum)

$$H = -J \sum_{\langle ij \rangle} S_i S_j \qquad \xrightarrow[\text{Hubb-Strat Transform.}]{\text{Close to Tc}} \qquad S[\Phi] = \int dx^d \left[\frac{1}{2} (\nabla \Phi)^2 + \frac{r}{2} \Phi^2 + g \Phi^4 \right]$$

$$Z = \sum_{\{S_i\}} e^{-\beta H} \qquad\qquad Z = \int D\Phi \, e^{-S[\Phi]}$$

For 1D: $r \propto (1 - 2\beta J)$ $\quad g \propto J^2$ $\quad$ Macro parameters in function of micro!

r will change sign at T_c-> $k_B T_c$=2J The same result is obtained using mean field kTc=q J with q-> number of nearest neighbors. Mean field is equivalent to the saddle point approach:

$$\frac{\delta S[\Phi]}{\delta \Phi} = 0 \ \rightarrow \ \Phi_{MF}$$

To study fluctuations one must go beyond the saddle point approximation

Book: Atland&Simons

Fluctuations around mean field: approaching criticality

- ✓ Thermal fluctuations will tend to decrease Tc
- ✓ Validity of mean field: The amplitude of the fluctuations is small if the dimension of the system is larger than a critical dimension (d_c=4 for the Ising Universality class). This is stated by the Ginzburg criterion.

$$\frac{\Delta m^2}{m^2} = \frac{g}{6} r_0^{D/2-2} \left(T_c - T\right)^{D/2-2}$$

- ✓ Beyond mean field →renormalization group (a procedure to eliminate high energy states keeping only what affects the low energy physics).

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Criticality

Criticality can be studied in the continuum limit: the correlation length is the only relevant length scale:

$$G(x,0) \sim e^{-x/\xi} \quad x \to \infty$$

Disorder phase
(Proper definition of ξ)

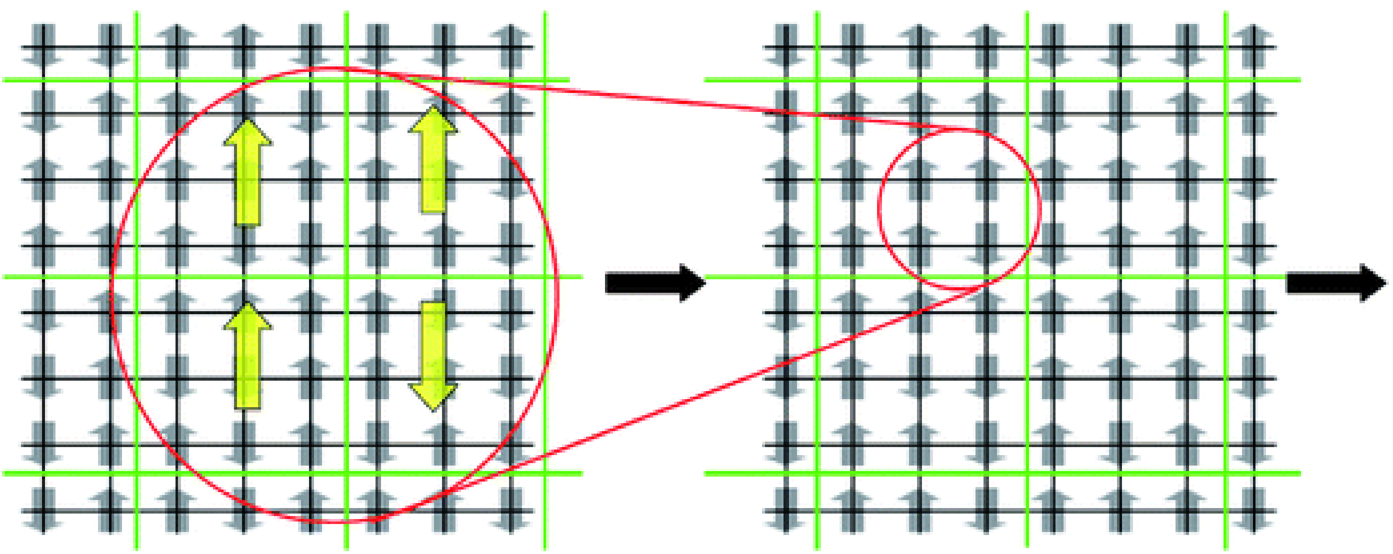
In the ordered phase:

In the disordered phase at long distances the correlation function:

$$\lim_{x \to \infty} G(x,0) = m^2$$

Ordered phase: Long range order

There must be a phase transition showing critical behavior.



G-> power law

ξ diverges-> criticality

Critical exponents

Experimentally, with scaling arguments, or with renormalization group it can be shown power law decay:

At the critical point
the correlation function -> $G(x) \sim \frac{1}{x^{D-2+\eta}}$ $G(k) \sim \frac{1}{k^{2-\eta}}$

Correlation length -> $\xi \equiv 1/\mathrm{r}^{\nu}$ $\mathrm{r} = \mathrm{r}_0(T - T_c)$

Using the fluctuation-dissipation theorem

$$\chi \approx |\mathrm{r}|^{-\gamma} = |\mathrm{r}|^{-\nu(2-\eta)}$$ -> experimentally

|, ⌇ and © … are critical exponents: set of different exponents characterizing the transition. They are *universal*.

Book: Le Bellac

Typical critical exponents:

Order parameter: $\psi \propto \{ \begin{matrix} (T_c - T)^{\beta} \\ h^{1/\delta} \end{matrix}$

Correlation length: $\xi \propto (T_c - T)^{-\nu}$

Susceptibility: $\chi \propto (T_c - T)^{-\gamma}$

Specific heat: $C \propto (T_c - T)^{-\alpha}$

Correlation function: $G_c^{(2)}(r) \sim \dfrac{1}{r^{d-2+\eta}}$ r large and T=Tc

Note that the Landau theory for an Ising model (or ϕ^4 theory) gives

β=1/2
ν=1/2
γ=1
α=0
$\delta = 3$

The exponents are related:
(only 2 are independent)

$$2 - \alpha = 2\beta + \gamma \qquad (2 - \eta)\nu = \gamma$$

$$2 - \alpha = \beta(\delta + 1) \qquad \nu d = 2 - \alpha$$

Universality

At T_c -> criticality, scale invariance, cooperative phenomena-> the properties (critical exponents) depend on

•Dimensionality of the space
•Dimensionality of the order parameter
•Symmetries of the local couplings
But not on the details of the interaction.

Ex: For the Ising model the square and the triangular lattice have the same critical exponents (at Tc the system is rotational invariance)

Ex: the solid and liquid or solid and gas transition (water, carbon dioxide…) belongs to the same universality class than the magnetic transition

Magnetic transition	$\longrightarrow$	Solid liquid/gas transition
Fluctuation magnetization	$\rightarrow$	fluctuating density
Order parameter m	$\longrightarrow$	density
Neutron scattering	$\longrightarrow$	light scattering
$M \propto (T_c - T)^\beta$		$\|\rho_L - \rho_g\| \propto \|T_c - T\|^\beta$

Better understood in the RG framework (fixed point)

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Continuous symmetry $\Phi = (\Phi_1(x), \Phi_2(x), ..., \Phi_n(x))$

$$\Phi^2 \to |\Phi|^2 = \sum_{i=1}^{N} \Phi_i^2$$

$$(\nabla\Phi)^2 \to |\nabla\Phi|^2 = \sum_{i=1}^{N} (\partial_x \Phi_i)^2$$

$$h\Phi \to \mathrm{h} \cdot \Phi$$

Congugate field

Important theorems:

- Goldstone theorem
- Mermin-Wagner theorem
- 2D->Korsterlitz-Thouless transition

Spontaneous symmetry breaking of a continuous symmetry: Goldstone Theorem

Low energy (long wavelength) excitations are possible in systems with continuous symmetry. The excitations are Goldstone Modes -> EMERGENT QUASIPARTICLES

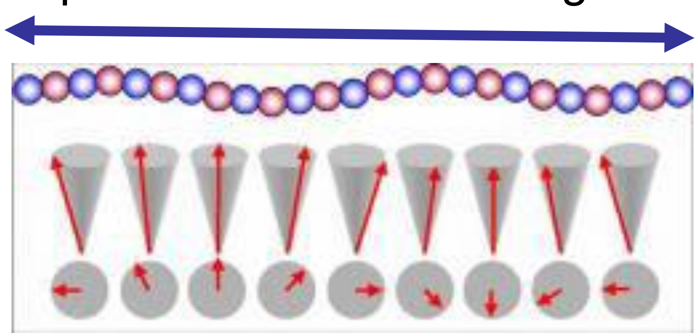
Example: Heisenberg model with S

$$H = -J\sum_{\langle ij \rangle} \vec{S}_i \; \vec{S}_j = -J\sum_{\langle ij \rangle} \cos\theta_{ij}, \; \vec{S}_i \in \mathrm{R}^3, \; \left|\vec{S}_i\right| = 1$$

$$E \sim J(1-\cos\theta) \sim J\theta^2 \qquad (\text{for small } \theta)$$

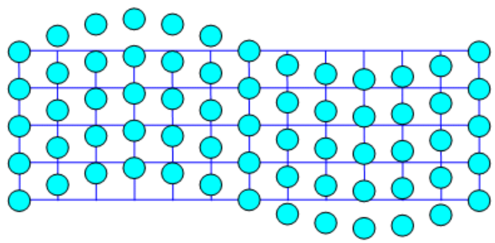
The cost of this energy can be vanishingly small

Spin waves with wavelength λ: magnons



Other goldstone modes

✓In a crystalline solid: acoustic phonons
E ~|q|.

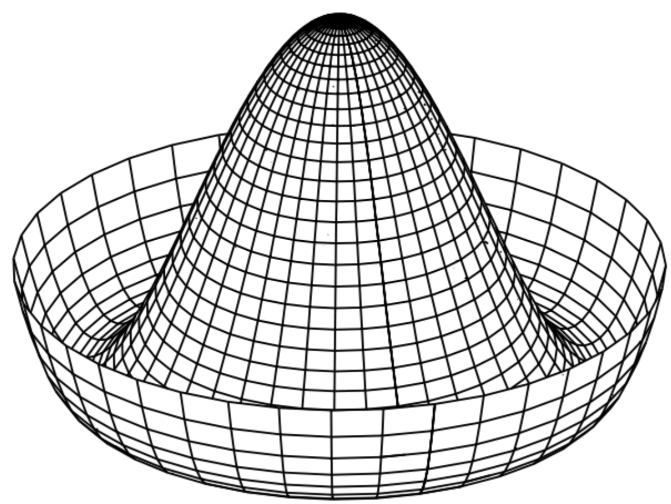


✓ In a superfluid (neutral fluid), Bogoliubov modes.

ϕ^4 theory, Φ complex U(1) symmetry

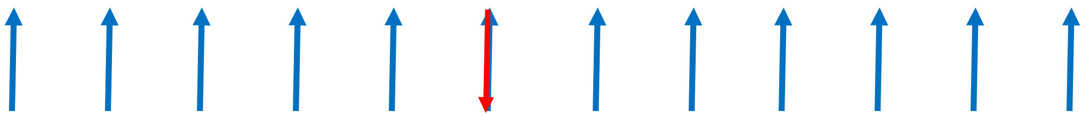
$$F = \left(\partial_\mu \phi\right)\left(\partial^\mu \phi^*\right) + m^2 \phi^* \phi + \lambda \left(\phi^* \phi\right)^2$$

$$\phi \to e^{i\Lambda}\phi \qquad\qquad -V(\phi)$$



No Goldstone modes

The Ising model has discrete symmetry:
E~J (domain wall) every excitation costs finite energy



A charged fluid (superconductor) develops a gapped spectrum:
Anderson-Higgs mechanism due to the electromagnetic field.

Mermin-Wagner theorem

(Phase transitions and dimensionality)

Mermin, N. D. & Wagner, H. *Phys. Rev. Lett.* **17**, 1133–1136 (1966).

Goldstone modes gives rise to large fluctuation effects in low dimensions

In general if we have:

- Spontaneous symmetry of a continuous group (i.e. not applicable to Ising model)
- Short range forces

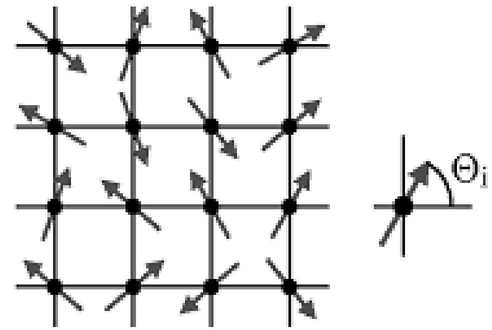
Then there is no phase transition (associated with a long range order!) for dimension $d \leq 2$ (for $T > 0$).

The special case of d=2 and D=2: the Kosterlitz-Thouless transition

The XY model (D=2) in 2dim (d=2) has continuous symmetry U(1)/O(2), hence it cannot have a phase transition to a long-range ordered state (Mermin-Wagner).

$$S_i = (\cos\theta_i, \sin\theta_i)$$

$$H = -J\sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -J\sum_{\langle i,j\rangle} \cos(\theta_i - \theta_j)$$



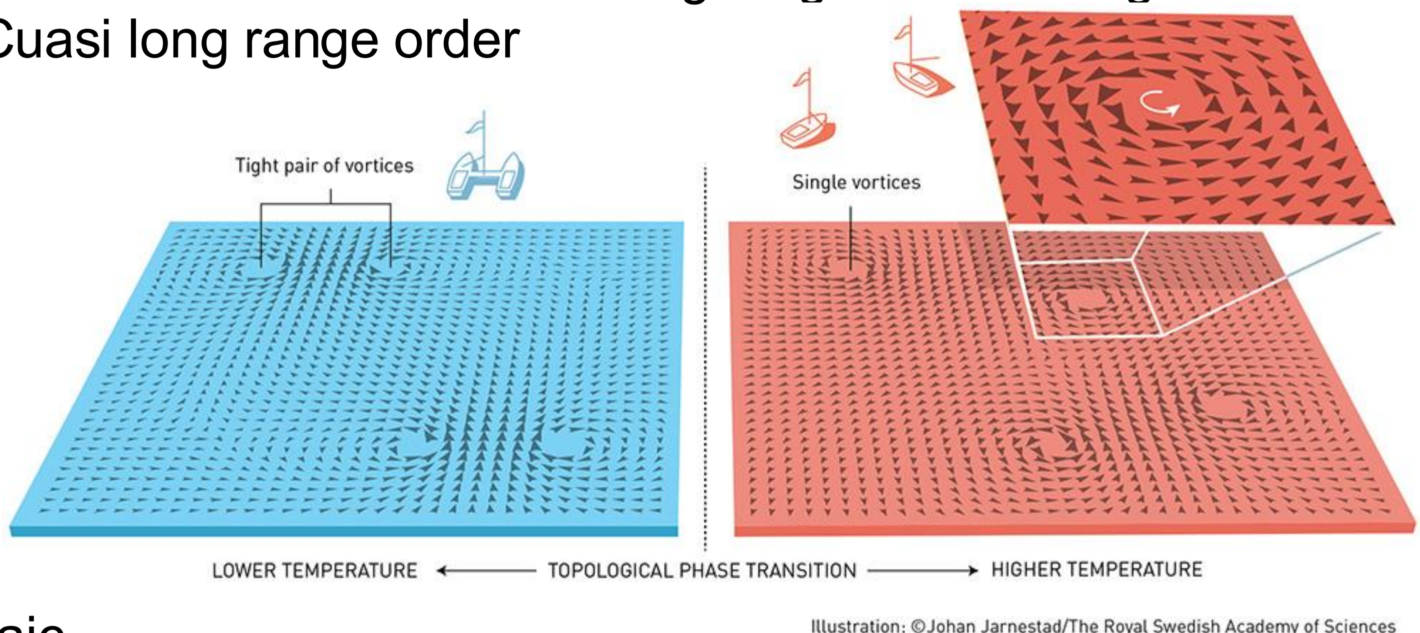
Berezinskii (1970), Kosterlitz and Thouless (1972) demostrated that the system undergoes a phase transition (though not long range ordered, there is not symmetry breaking).

The special case of d=2 and D=2: the Kosterlitz-Thouless transition

Solution: vortices (topological defects) that contribute to the entropy.

Low T:vortex-antivortex binding HighT: Unbinding vortices

Cuasi long range order



Algebraic decay!

$$G(x,0) \approx \left(\frac{a}{|x|}\right)^{\frac{b}{\beta}} \quad x \to \infty$$

$$G(x,0) \sim e^{-x/\xi} \quad x \to \infty$$

XY universality class: Topological defects (Coulomb charges in 2D, dislocations in 2D crystals, vortices in 2D superconductors ($Y \sim e^{iq}$) or superfluids…)

Quantum phase transitions

Quantum phase transitions

QPT: T=0

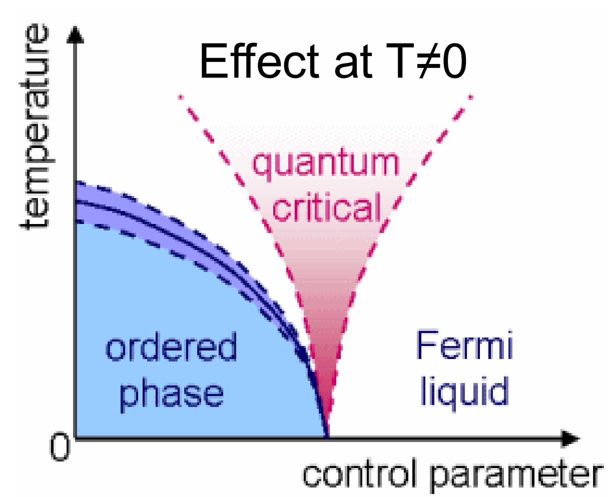
Ground state 1 — **Diverging quantum fluctuatios** — Ground state 2

Control parameter: pressure, magnetic field…

Quantum fluctuations are driven by the Heisenberg uncertainty principle

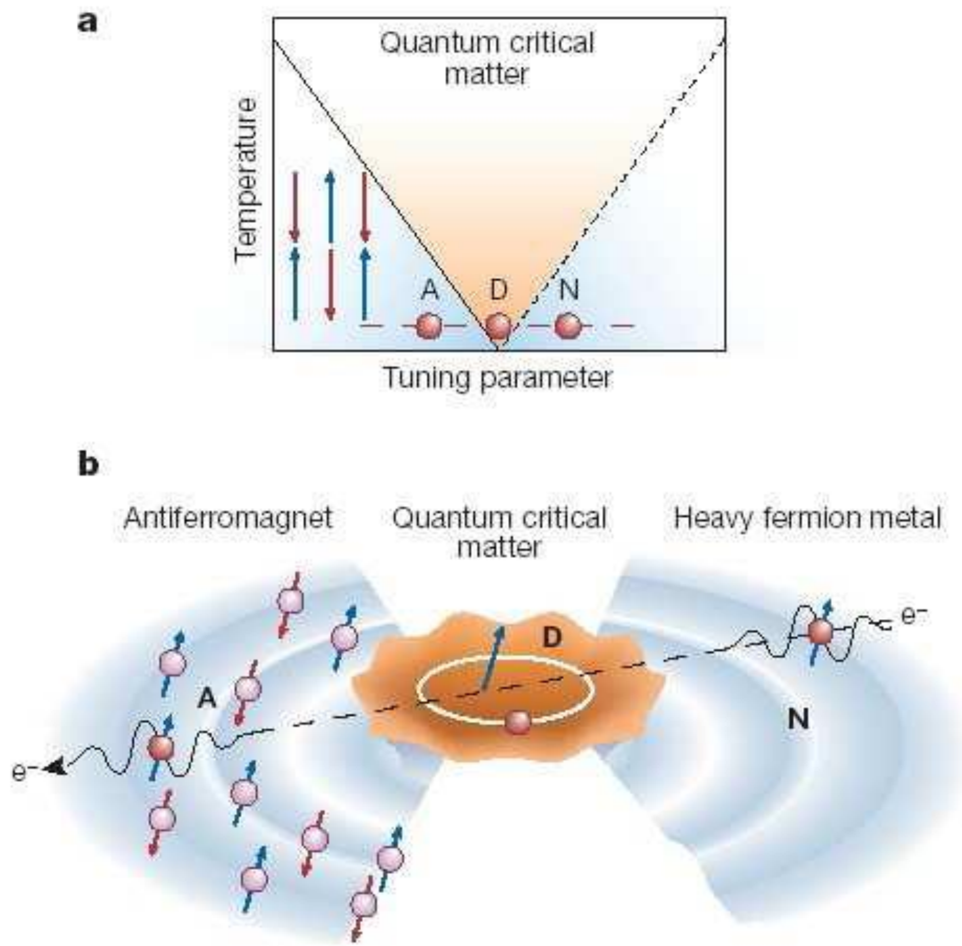
$$H(g) = H_0 + gH_1$$

- Transition at g_c (a point of non-analyticity of the ground state).
- The nature of the correlations in the ground state changes qualitatively at g_c.



g

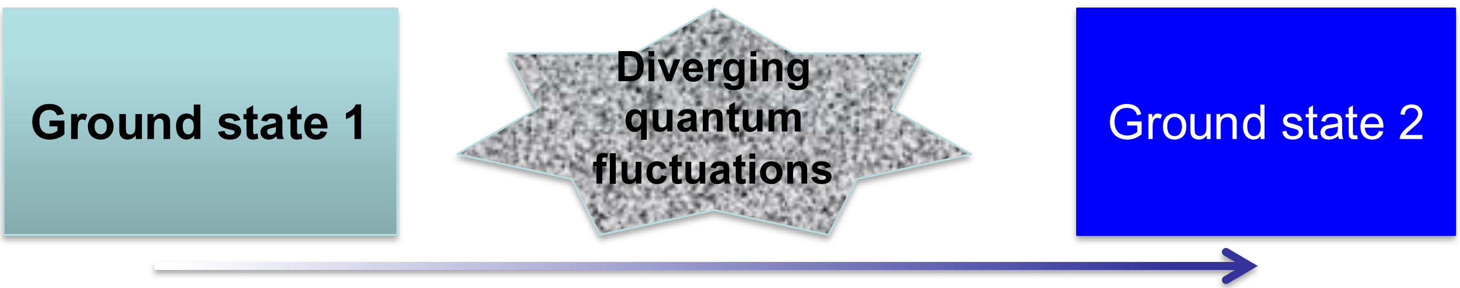
Non Fermi liquid behavior



P. Coleman & A. Schofield, Nat.'05

Quantum phase transitions

QPT: T=0



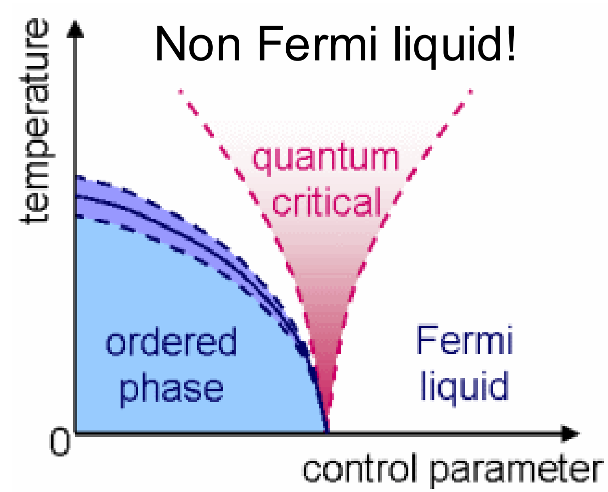
Control parameter: pressure, magnetic field…

QPT have consequences at T≠0.

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

$$\left.\begin{aligned}\tau_\varphi &\sim \xi^{z} = |g-g_c|^{-\nu z}\\ \Delta &\sim |g-g_c|^{\nu z}\end{aligned}\right\}\text{New! } \tau_\varphi,\ z$$

2nd order QPT:



g

z is the dynamical exponent, Δ is the gap

τ_φ is the coherence time, time over which the wave function retains its memory of its phase: it diverges at a QPT

Example: Quantum Ising model

Ising model in a transverse field

$$H = -Jg\sum_i \hat{\sigma}_i^x - J\sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z$$

$$\hat{\sigma}_i^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{\sigma}_i^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{\sigma}_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

For g=0 -> Ising model $\sigma_i^z=1,-1$ $|\uparrow\rangle$, $|\downarrow\rangle$ -> *Ordered phase*

For $g\neq 0$ σ_i^x-> off diagonal-> quantum mechanical tunneling $|\uparrow\rangle \to |\downarrow\rangle$ -> *Disordered phase*

This model can describe real systems such as $LiHoF_4$ where it has been identified a QCP

Example: Quantum Ising model T=0, g>>1 limit

Ising model in a transverse field

$$H = -Jg\sum_{i}\hat{\sigma}_i^x - J\sum_{\langle ij\rangle}\hat{\sigma}_i^z\hat{\sigma}_j^z$$

Limits:

g>>1 1st term dominates: quantum paramagnetic (QPM)

$$|0\rangle = \prod_i |\rightarrow\rangle_i$$

$$|\rightarrow\rangle_i = \left(|\uparrow\rangle_i + |\downarrow\rangle_i\right)/\sqrt{2} \qquad (-1)$$

$$|\leftarrow\rangle_i = \left(|\uparrow\rangle_i - |\downarrow\rangle_i\right)/\sqrt{2} \qquad (1)$$

$$|i\rangle = |\leftarrow\rangle_i \prod_{j\neq i} |\rightarrow\rangle_j$$

The system is totally uncorrelated. 1st excitations (gap=Δ)

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

Example: Quantum Ising model T=0, g<<1 limit

Ising model in a transverse field

$$H = -Jg\sum_{i} \hat{\sigma}_i^x - J\sum_{\langle ij\rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z$$

Limits:

g<<1   2nd term dominates: Z_2 symmetry: Magnetic long range order (MLRO)

$$|\rightarrow\rangle = \prod_i |\rightarrow\rangle_i \quad \text{or} \quad |\uparrow\rangle = \prod_i |\uparrow\rangle_i$$

Excitations (gap=Δ): domain walls: turning on g will mix up and down spins but still Z_2 symmetry.

$$|\rightarrow\rangle|\rightarrow\rangle|\uparrow\rangle|\uparrow\rangle|\uparrow\rangle|\rightarrow\rangle|\rightarrow\rangle$$

Only in the thermodynamic limit:

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

M=1 if g=0

Example: Quantum Ising model T=0, Quantum phase transition

Ising model in a transverse field

$$H = -Jg\sum_i \hat{\sigma}_i^x - J\sum_{\langle ij\rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z$$

Limits:

g>>1 $\quad \langle 0|\hat{\sigma}_i^z \hat{\sigma}_j^z|0\rangle \sim e^{-|x_i - x_j|/\xi}$

g<<1 $\quad \lim_{|x_i - x_j| \to \infty} \langle 0|\hat{\sigma}_i^z \hat{\sigma}_j^z|0\rangle \sim M^2$

At g=g_c we have a QPT, we expect ξ diverges and G goes as a power law

It is possible to calculate the exact spectrum using a Jordan-Wigner transformation (mapping between spin ½ degrees of freedom and spinless fermions). The result is:

$$\varepsilon(k) = 2J(1 + g^2 - 2g\cos k)^{1/2}$$ Δ=2J|1-g|-> g =1 QCP!!

g>1 exp. law

g<1 long range

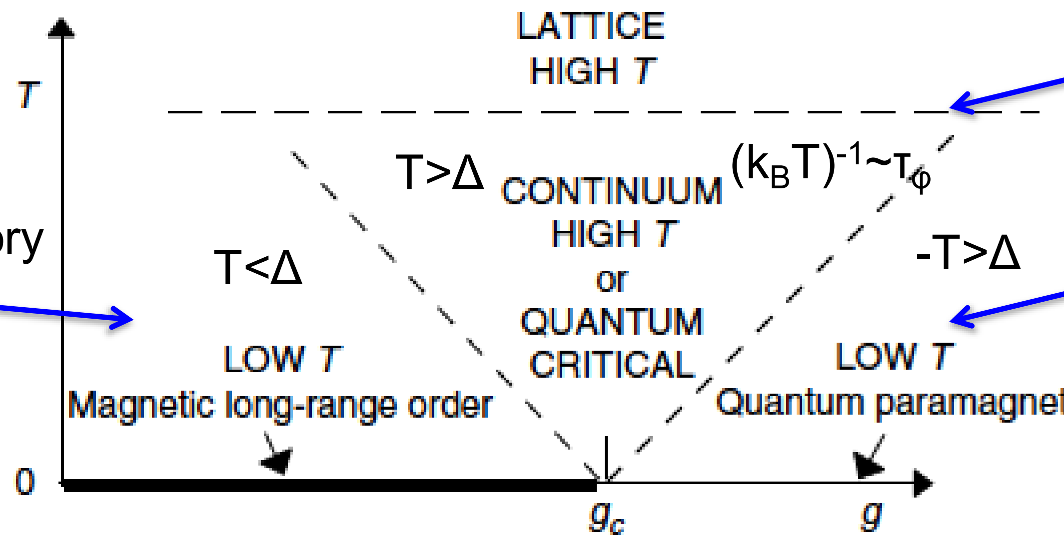
$$\varepsilon(k \to 0, g = 1) = 2J(2 - 2(1 + \frac{1}{2}k^2))^{1/2} = 2J|k|$$ **Excitations without gap!**

Example: Quantum Ising model Phase diagram: Exact solution

z=1

$|\Delta|, T \sim |g-g_c|$

Effective theory with DW QP



T~J

Effective theory with flipped spins QP

	Low T (magnetically ordered) quasi-classical particles –domain walls	T Continuum high (quantum critical)	Low T (quantum paramagnetic), quasi-classical particles –flipped spins
ξ	$\left(\frac{\pi c^2}{2\Delta T}\right)^{1/2} e^{\Delta/T}$	$\frac{4c}{\pi T}$	$\frac{c}{\lvert\Delta\rvert}$
τ_φ	$\frac{\pi}{2T} e^{\Delta/T}$	$\frac{\cot(\pi/16)}{2T}$	$\frac{\pi}{2T} e^{\lvert\Delta\rvert/T}$

relaxational

Sachdeev: Quantum phase transitions

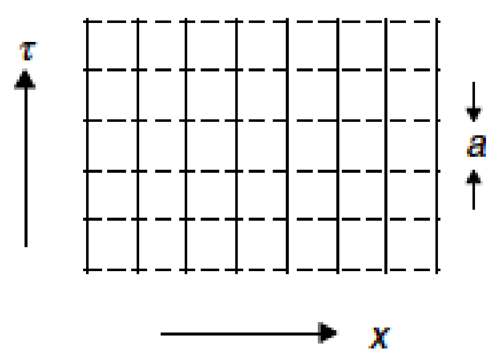
Quantum classical mapping

$$Z = \sum_{\{S_i\}} e^{-\beta H} \qquad H = H_{kin} + H_{pot}$$

In a classical system $[H_{kin}, H_{pot}]=0$ thus $Z=Z_{kin}Z_{pot}$ and statics and dynamics are decoupled -> Effective time-independent theories in D dimensions.
In a quantum system **$[H_{kin},H_{pot}]\neq 0$** thus **statics and dynamics are coupled.** $\phi(x,\boldsymbol{\tau})$. The operator $e^{-H/kT}$ looks like $e^{-H\tau}$

$1/kT= \tau=-it/\hbar$-> Mapping

D (>1 dimensional classical)=d (dimensional quantum)+z
These models belong to the same universality class



z measures the anisotropy between x-dim and t-dim

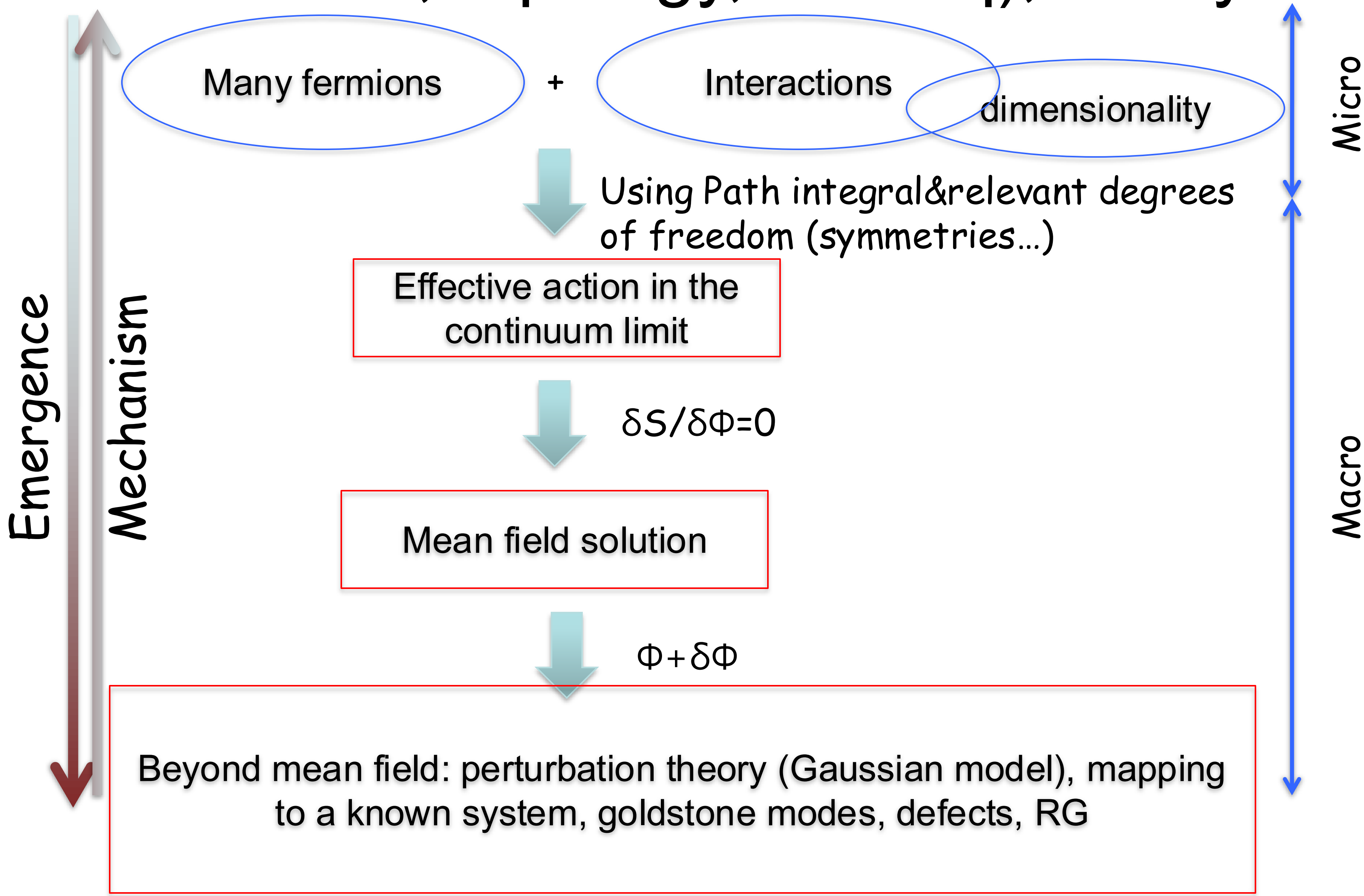
Are QPT(d+z) different from CPT(D)?

- The Quantum-Classical mapping yields quantum correlation functions that are in imaginary time. The analytical continuation to real time is highly non-trivial.
- It emerges a new time scale: the coherence time τ_{φ} (not present in the classical analog)
- Berry physics
- Emergence of the quantum critical region

Classical Phase Transitions	Quantum Phase Transitions
• CPT are points or sets of points in the phase diagram which are singularities in the free energy as a function of T. SSB mechanism. 1^{st} and 2^{nd} order. •Thermal fluctuations arises from the competition between S and E •Kinetic and Potential energy are decoupled. (z no special role) •The critical exponents characterize the CPT • At Tc the correlation length diverges	• QPT are points or sets of points non-analytic as a function of a non thermal parameter. SSB mechanism. 1^{st} and 2^{nd} order. •Quantum fluctuations arises from the competition between different ground states. •Kinetic and Potential energy are coupled, •z characterized the transitions together with the other critical exponents. •At Tc the coherent time and the correlation length diverges •Quantum critical region (NFL)

Quantum classical mapping:
D (>1 dimensional classical)=d (dimensional quantum)+z
(it has its limitations)

Condensed Matter Field Theory (Hubbard-like, topology, non-eq), life systems



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- Le Bellac: Quantum and Statistical Field Theory
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- Fradkin: Field Theories of Condensed Matter Systems
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¡Gracias!

Gaussian approximation

We can do perturbation theory starting from the MF solution:

$$S[\Phi] = \int dx^d \left(\frac{1}{2} c(\Box\Phi)^2 + \frac{r}{2}\Phi^2 + g\Phi^4 \right) \quad \frac{\delta S[\Phi]}{\delta \Phi} = 0 \;\rightarrow\; \Phi_{MF} \equiv 0 \quad \Phi = \Phi_{MF} + \varphi$$

perturbation

Gaussian approximation (T->Tc from above)

$$S_{Gaussian}[\Phi] = \int dx^d \left(\frac{1}{2} c(\Box\varphi)^2 + \frac{r}{2}\varphi^2 - h\varphi \right) \rightarrow G(k) = (r + ck^2)^{-1} \rightarrow \chi_0 = G(0) = 1/r$$

1 loop perturbative expansion: $\chi^{-1} = r - \Sigma = r + \frac{g}{2} \Box \frac{dk'^d}{(2\pi)^d} \frac{1}{r + k'^2}$

Observation:

- fluctuations make Tc smaller ($r=r_0(T-T_{cMF})$)
- UV divergence for d>3 (short distance)
- Infrared divergence for d≤2!!!! **(small momenta or large distance!) We will speak more about this later.**

Solution: Renormalization group

Renormalization group (Wilson)

Perturbative approach.
Systematically eliminate the high energy modes of the system keeping only the low energy physics

$$S[\Phi]=\int dx^{d}\left[\frac{1}{2}(\nabla\Phi)^{2}+\frac{r}{2}\Phi^{2}+g\Phi^{4}\right] \qquad Z=\int D\Phi\, e^{-S[\Phi]}$$

$$\Phi=\Phi_{H}+\Phi_{L}$$

$$\Phi_{H}=\Phi(k),\quad \text{for}\quad \Lambda s<k<\Lambda\ \ (\text{slow modes})\qquad \Lambda\rightarrow\ \text{cutoff}$$

$$\Phi_{L}=\Phi(k),\quad \text{for}\quad \Lambda<k<\Lambda/s\quad (\text{high modes})\quad s<1\quad (\text{eventually } s\rightarrow 0)$$

$$Z=\int D\Phi_{L}D\Phi_{H}\ e^{-S[\Phi_{L}+\Phi_{H}]}=\int D\Phi_{L}e^{-S'_{\Lambda}[\Phi_{L}]}$$

Integration over high modes

$$S'_{\Lambda}[\Phi_{L}]=\int d^{D}x\sum g_{i}\theta_{i}[\Phi_{L}]=\int d^{D}x\ r'\Phi_{L}^{2}+g'\Phi_{L}^{4}\rightarrow\text{effective action}$$

$[\theta_{i}]=s^{\delta_{i}}$ Expanded in terms of local operators

Renormalized values

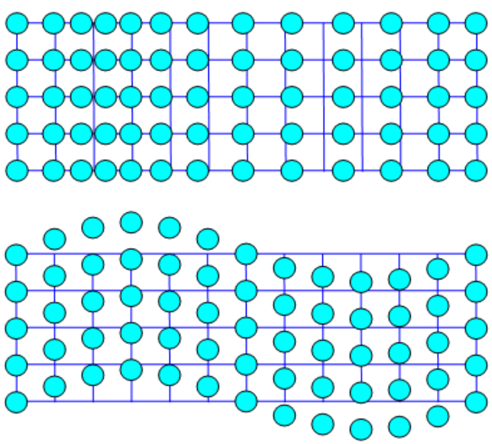
Scaling analysis δ_i

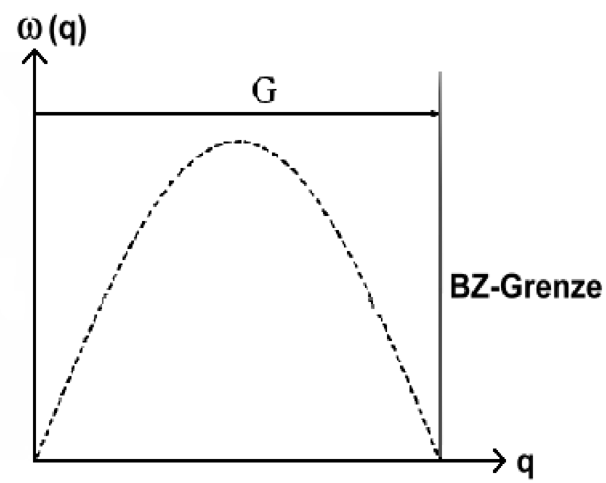
- <0 g_i' grows -> relevant ->
- =0 g_i' marginal -> ?-> RG prescription
- >0 g_i' decreases -> irrelevant

Goldstone modes: phonons

Remark: order parameter (density) modulated with wave-vector Q
$\det G^{-1}(Q) = 0$ (before: special case Q = 0)

Consider $\rho(q) \Rightarrow$ order parameter $\rho(Q)$ (Q: reciprocal lattice vector)
Question: Are the sound waves Goldstone modes?
$\lim_{q\to 0} \omega(q) = 0$: but at q=0! (usual sound waves that appear in liquids and solids)
Goldstone Modes: "Umklapp" or transverse phonons at q =Q





Goldstone modes are zero modes of G^{-1}
But not all the zero modes of G^{-1} are Goldstone modes because they do not correspond to a broken symmetry

Hubbard model

$$H = -t \sum_{\substack{\langle \vec{r},\vec{r}\,'\rangle \\ \sigma=\uparrow,\downarrow}} \left(c_\sigma^\dagger(\vec{r})c_\sigma(\vec{r}\,') + \mathrm{h.c.}\right) + U \sum_{\vec{r}} n_\uparrow(\vec{r}) n_\downarrow(\vec{r})$$

$$\vec{S}(\vec{r}) = \frac{1}{2} c_\sigma^\dagger(\vec{r}) \vec{\tau}_{\sigma\sigma'} c_{\sigma'}(\vec{r})$$

$$H = -t \sum_{\langle \vec{r},\vec{r}'\rangle} c_\sigma^\dagger(\vec{r})c_\sigma(\vec{r}\,') + \mathrm{h.c.} - \frac{2}{3} U \sum_{\vec{r}} \left(\vec{S}(\vec{r})\right)^2$$

Broken symmetry in condensed matter systems: Hubbard model

Example: Hubbard model in path integral representation. Continuum.

$$Z = \int D\bar{\Psi} D\Psi \, \mathrm{e}^{-S[\bar{\Psi},\Psi]} \qquad \Psi \rightarrow \text{fermionic coherent state}$$

$$S[\bar{\Psi},\Psi] = \int d\tau d\vec{r}\, \bar{\Psi}_{\sigma}(\tau,\vec{r})(\partial_{\tau} - \mu)\Psi_{\sigma}(\tau,\vec{r}) + H[\bar{\Psi},\Psi]$$

$$H_{\text{int}}[\bar{\Psi},\Psi] = \int d\tau d\vec{r}\, \bar{\Psi}_{\sigma}(\tau,\vec{r})\vec{\tau}_{\sigma\sigma'}\Psi_{\sigma'}(\tau,\vec{r})\, \vec{S}(\tau,\vec{r})$$

Introducing a bosonic field: $\vec{\Phi}(\tau,\vec{r}) \rightarrow \vec{S}(\tau,\vec{r})$

To arrive to Seff (Landau functional) we do the Hubbard-Strat. transformation where the interacting term is decoupled at the expense of the introduction of a bosonic field

$$e^{\frac{u_{spin}}{2}(\bar{\Psi}\vec{\tau}\Psi)^2} = \int D\Phi e^{-\frac{\vec{\Phi}^2}{2u_{spin}} + \bar{\Psi}\vec{\tau}\Psi\vec{\Phi}}$$

What channel should we use (FM, AF, SC, CDW, dDW…)? Hints from mean field, other techniques, experiments…

SDW in the Hubbard model

Let's chose to study the AF phase

- Observation: Hubbard Hamiltonian-> SU(2) spin invariance (continuous symmetry) but the AF ground state breaks this symmetry->we expect Goldstone modes (SDW).
- Integrating fermions out.

$$Z=\int D\bar{\Psi}D\Psi\, e^{-\int \bar{\Psi}G^{-1}\Psi}=\det(G^{-1}) \qquad G^{-1}=G_0^{-1}-\Sigma(\Phi)$$ Dyson equation

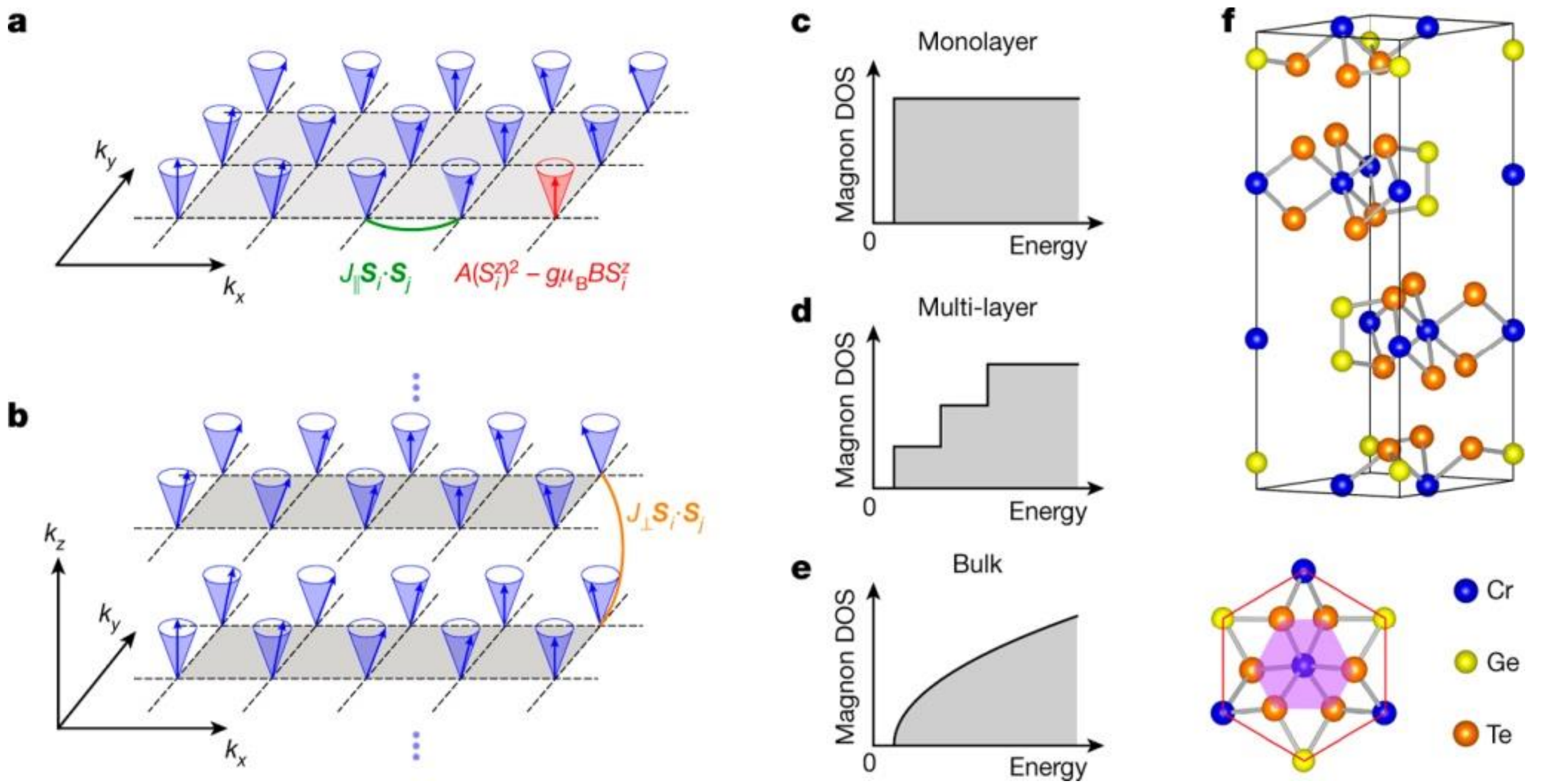
- Effective action (Landau functional): $Z=\int D\Phi\, e^{-S_{eff}[\Phi]}$

$$S_{eff}[\Phi]=\frac{1}{2u_{spin}}\Phi^2-Tr\log(1-G_0\Sigma(\Phi^2)) \qquad Tr\log(1-G_0\Sigma(\Phi^2))=\sum_n\frac{1}{n}(Tr(G_0\Sigma(\Phi)))^n$$

- Saddle point approximation and arrive to the AF mean field solution. The higher the spin the better for the mean field solution (semi-classical approximation)
- Gaussian fluctuations: the fluctuation $\delta\Phi(r,t)$ is small, slowly varying (compared with $\tau=1/\Delta$) and smooth (compared to $\xi^2=v_F/\Delta$).
- **The 3D Hubbard model has *two* gapless transverse spin waves π and a massive (gapped) longitudinal amplitude mode σ.**

Fradkin book

Schematics of spin-wave excitations in two and three dimensions

- 

Cr2Ge2Te6

C Gong *et al.* *Nature* 1–5 (2017) doi:10.1038/nature22060

Example: Quantum Ising model Continuum limit

Continuum limit

$$H = E_0 + \int dx \left[\frac{c}{2} \left(\Psi^+ \frac{\partial \Psi^+}{\partial x} - \Psi \frac{\partial \Psi}{\partial x} \right) + \Delta \Psi^+ \Psi \right]$$

$$\Delta = 2J(1-g) \qquad c = 2Ja \qquad \Delta > 0 \text{ MLRO}; \ \Delta < 0 \quad \text{QPM}$$

Δ, c macroscopic parameters, J and g microscopic parameters

Lagrangean path integral

$$Z = \int D\Psi D\Psi^+ \exp\left(-\int_0^{1/T} d\tau \, dx \, \mathcal{L} \right)$$

$$\mathcal{L} = \Psi^+ \frac{\partial \Psi}{\partial \tau} + \left[\frac{c}{2} \left(\Psi^+ \frac{\partial \Psi^+}{\partial x} - \Psi \frac{\partial \Psi}{\partial x} \right) + \Delta \Psi^+ \Psi \right]$$

This Lagrangean contain the required universal theory

The temporal term arises from the fact that different t slices do not commute-> term responsible of the **quantum fluctuations**

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This Lagrangean contain the required universal theory

The temporal term arises from the fact that different t slices do not commute-> term responsible of the **quantum fluctuations**

Example: Quantum Ising model Scaling transformation->QCP

$$\mathcal{L} = \Psi^{+}\frac{\partial \Psi}{\partial \tau} + \left[\frac{c}{2}\left(\Psi^{+}\frac{\partial \Psi^{+}}{\partial x} - \Psi\frac{\partial \Psi}{\partial x}\right) + \Delta\Psi^{+}\Psi\right]$$

$\varepsilon(k) = (\Delta^2 + c^2 k^2)^{1/2}$ Δ is the gap and c the velocity of the excitation

Scaling transformation: a-> lattice spacing, Λ=π/a k<<Λ: to get the long distance behavior we eliminate the short distances degrees of freedom, Dimensionless rescaling factor e^{-l}<1 ->Eliminate modes with k between Λ and Λe^{-l}. We complete the rescaling with:

$$x' = xe^{-l}$$

$\tau' = \tau e^{-zl} \rightarrow$ *z determines the relative rescaling factor of space and time*

In this case z=1

$$\Psi' = \Psi e^{l/2}$$

At the QCP, Δ=0, $\mathcal{L}$ is invariant under a scaling transformation-> all the correlators are invariant under the scaling transformation

Example: Quantum Ising model Scaling transformation: Temperature

If $\Delta \neq 0$ -> S not scale invariant unless $\Delta' = \Delta e^{l}$ scale-> invariant

$$\frac{d\Delta}{dl} = \Delta \qquad \dim \Delta = 1 \qquad \Delta$$ Grows: relevant perturbation

Recall $\Delta \sim |g-g_c|^{z\nu}$, since $z=1$ -> $\nu=1$ and $\xi \sim |g|^{-1}$

$\beta \sim t$ **dimT=z=1 relevant!** $\xi \sim |T|^{-1}$

The correlation function for $g>1$: information of space fluctuations and quantum fluctuations

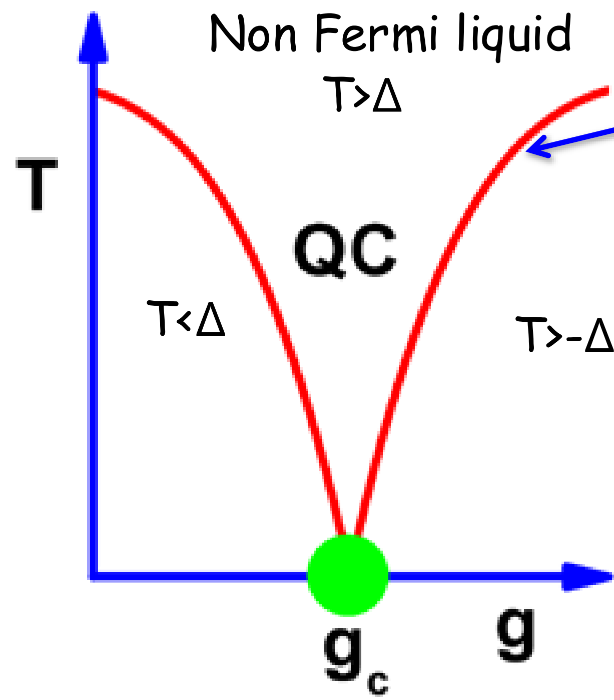
$$G(x,0) \sim e^{-|x|/\xi} \qquad \xi$$

$$G(0,t) \sim e^{-|t|/\tau_{\varphi}} \qquad \tau_{\varphi} \quad \square$$

From here we calculate the coherence time: time over which the wave function retains phase memory.

Phase diagram in a Condensed Matter System

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



Crossovers that separate regions with different scattering length and different coherent time

In the Non Fermi liquid region quantum and thermal fluctuations are equally important

QPT and fermions

The quantum critical behavior depends crucially on whether order parameter fluctuations can couple to the low energy fermionic excitations

• Gap$\neq$0-> the order parameter fluctuations are the low energy excitations

• Gap=0-> there are order parameter fluctuations and low energy fermions that can be coupled. Integrating out fermions can lead to divergences. *The theory is under construction*. It also can happens for d-wave superconductors.

Non Fermi liquid behavior

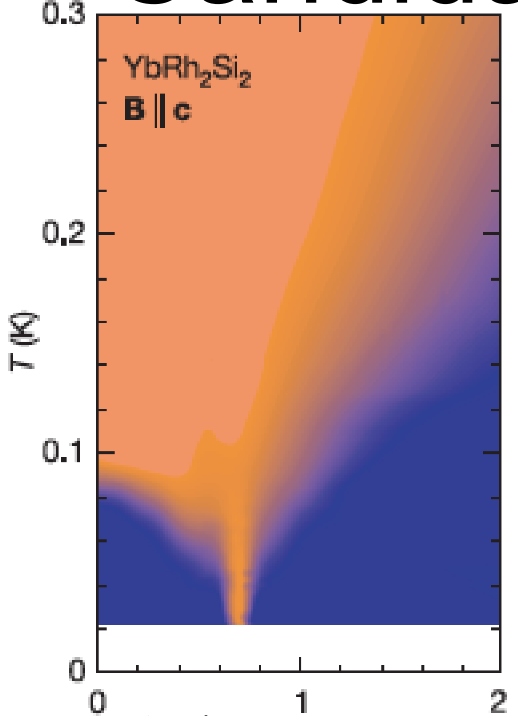
The non-Fermi liquid behavior can be understood with the quantum-classical mapping:
In classical systems:

$$G(k) \sim \frac{1}{k^{2-\eta}}$$

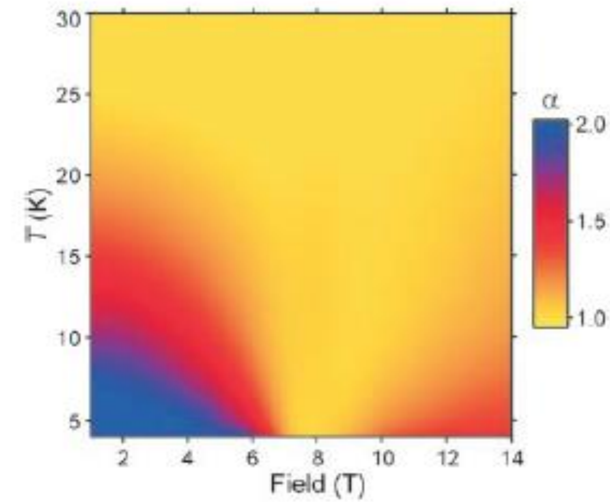
In quantum systems:

$$G(k,\omega) \sim \frac{1}{(k^2 + (\omega + i\delta)^2)^{\frac{2-\eta}{2}}} \rightarrow$$ Branch cut! Non-Fermi liquid behavior

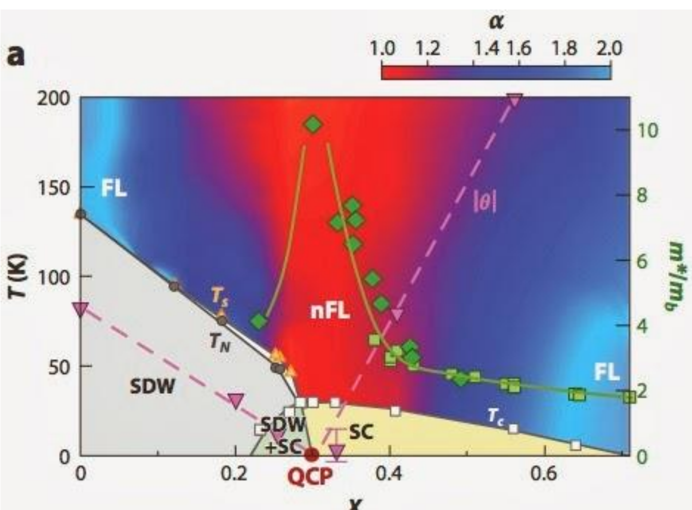
Candidates to Quantum Critical points



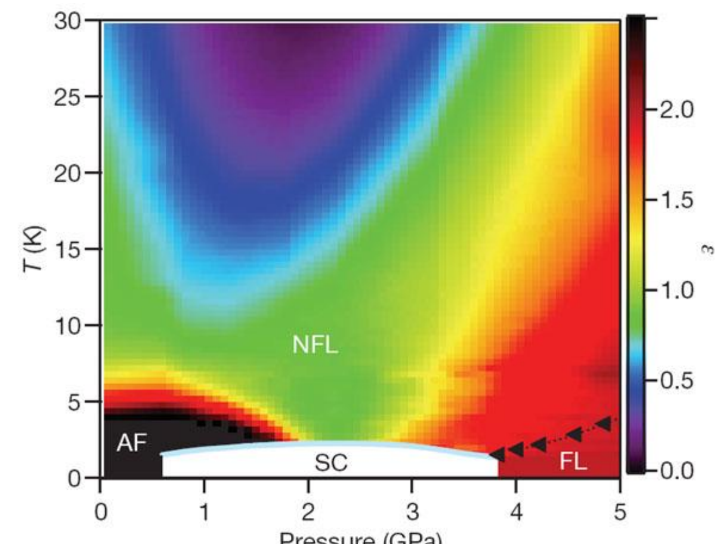
YbRh$_2$Si$_2$ Custers, Lett to Nat.'03



$Sr_3Ru_2O_7$; Grigera, Science'01



$BaFe_2(As_{1-x}P_x)_2$; Analytis, Nat.Phys.'14



CeRhIn$_5$; Park, Nat'08

Summary and outlook

- Effective field theories for phase transitions are built to describe phase transitions and deal with fluctuations.
- Connection to statistical mechanics and field theory in high energies
- It includes concepts of topology and geometry
- Functional-integral based approach that gets the most of mean field, mapping, perturbative methods and RG.
- It can be generalized to non-equilibrium systems in condensed matter