Basic Training QC Module.

Lect 1. Wed 04/15/2009.

Goal for the course.

Target level.

- What is QC
  - → Why is QC interesting
- What do we study at QC
- How do we study QC.

1) intelligent and fruitful conversation on the topic.

2) An eye for recognizing QC when you have it.

References for review.

RMP Colloquia: Continuous Quantum Phase Transitions
S. Sondhi, S.M. Girvin, J.P. Carini, D. Shahar
RMP $\underline{69}$, 315 (1997)

Quantum Phase Transitions, S. Sachdev

Example: triplon BEC in spin-dimer tuned by magnetic field
theory - review by Sachdev. arXiv:0401041 Sections 1-3.
experiment - Sebastian et al. Nature $\underline{441}$, 617 (2006)

Vol 441|1 June 2006|doi:10.1038/nature04732 nature

LETTERS

Dimensional reduction at a quantum critical point

S. E. Sebastian[1], N. Harrison[2], C. D. Batista[3], L. Balicas[4], M. Jaime[2], P. A. Sharma[2], N. Kawashima[5] & I. R. Fisher[1]

Phase Diagram

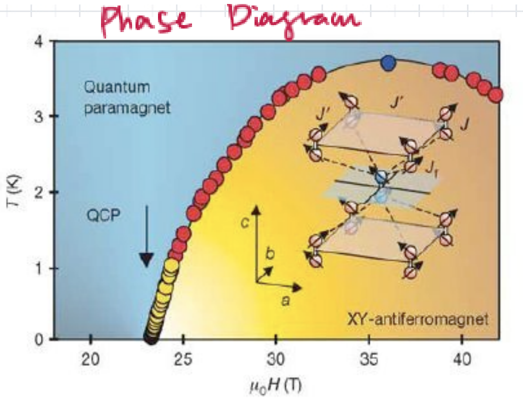
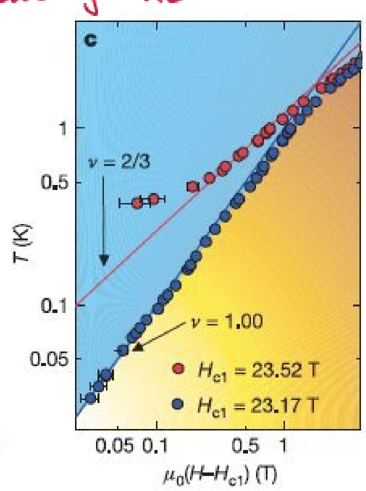


Figure 1 | Experimentally obtained phase boundary of $BaCuSi_2O_6$. The

Scaling and Critical exponents.



* Motivation for the choice of example.

i) Modern example.
ii) A motivated learning → research
iii) Material → experiment → mapping to known problem
iv) "Solvable example". QC without sign problem.

arXiv.org > cond-mat > arXiv:cond-mat/0401041v1

Condensed Matter > Strongly Correlated Electrons

Quantum phases and phase transitions of Mott insulators

Subir Sachdev

(Submitted on 6 Jan 2004)

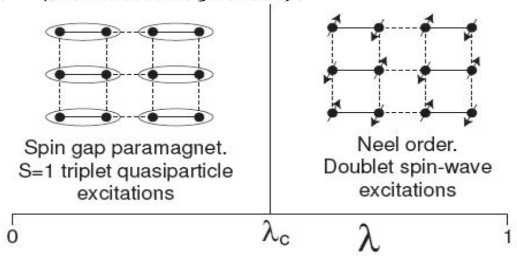


Fig. 4. Ground states of H_d as a function of λ The quantum critical point is at [28] $\lambda_c = 0.52337(3)$. The compound $TlCuCl_3$ undergoes a similar quantum phase transition under applied pressure [8].

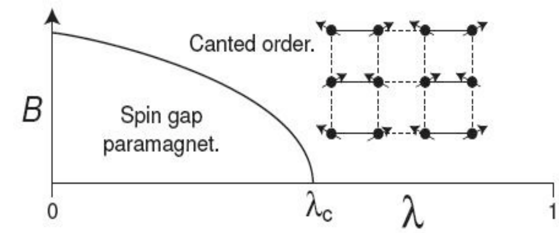


Fig. 5. Evolution of the phases of Fig 4 under a weak field B (magnetization

We consider the "coupled dimer" Hamiltonian [25]

$$H_d = J \sum_{\langle ij \rangle \in \mathcal{A}} \mathbf{S}_i \cdot \mathbf{S}_j + \lambda J \sum_{\langle ij \rangle \in \mathcal{B}} \mathbf{S}_i \cdot \mathbf{S}_j \qquad (1)$$

$$- \sum_j \mathbf{B} \cdot \mathbf{S}_j . \qquad (19)$$

and integrate out φ_z, then we obtain from (12), (22) the effective action for Ψ:

$$\mathcal{S}_\Psi = \int d^2 r d\tau \left[\Psi^* \partial_\tau \Psi + \frac{c_x^2}{2B} |\partial_x \Psi|^2 + \frac{c_y^2}{2B} |\partial_y \Psi|^2 - \mu |\Psi|^2 + \frac{u}{24B} |\Psi|^4 \right] . \qquad (24)$$

level of operation

1) I may aim for the state of slight confusion
just enough to tickle curiosity and invite you to think.

2) Questions/protests welcome. Being able to say "I'm confused" is an expression of confidence and route to learning

3) Assume command over QM and stat mech
(at least familiarity)

Outline.

Lect I I. Introduction

II. Quantum Statistical Mechanics & Quantum Field Theory

- Classical and Quantum Partition Functions
probability density & density matrix.
- Density matrix and path integral.

Lect 2. o Quantum → Classical mapping

(when it works → 4D Josephson junction array
(When it does not work. →

o Dynamics & Thermodynamics

Lect 3 III. Quantum Phase Transitions.

o Scaling at T=0

o Finite temperature

o Quantum to classical crossover

Lect 4. IV. How to identify QPT.

o Tuning Parameter
o Universality class ← scaling exponents
o Modeling
o Triplon condensation in spin-dimer compounds.

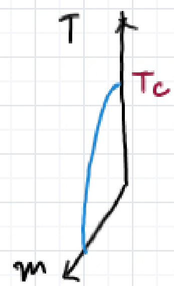
Lect 5. Field driven QPT in spin-dimer Hamiltonian.

Lect 6. Comparison with experiment.

I. Introduction

□ Quantum Phase Transitions (continuous)

○ Continuous PT (2nd order)



- Spontaneous symmetry breaking at $T = T_c$
- Ordered state for $T < T_c$
  - ↳ OP is nonzero
  - ⟺ Equilibrium state has lower symmetry than the effective Hamiltonian.

ex) $\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$

Symmetry op. $\sigma_i \to -\sigma_i \Leftrightarrow \mathcal{H} \to \mathcal{H}$ (def. of symm.)

But ordered state with $\frac{1}{N} \sum_i \langle \sigma_i \rangle = m$

transform to other ordered state

$\frac{1}{N} \sum_i \langle \sigma_i \rangle = -m$

- divergence/singularities in thermodynamic quantities
  C_v, χ
- diverging correlation length ξ.

correlation length defined in terms of correlation function

$$C(x) = \langle m(x) m(0) \rangle - \langle m(x) \rangle \langle m(0) \rangle \tag{1}$$

$$\propto e^{-x/\xi}$$

At C.P, divergence of ξ ⟺ correlation do not decay exponentially

$$C(x) \sim \frac{1}{x^{d-2+\eta_d}} \quad \text{only power law decay.} \tag{2}$$

- Divergence of ξ ⟺ absence of momentum scale.
  ⟺ scale invariance.

- Classic way to describe cont. P.T. is via
  LG free energy functional

$$\beta F[m] = \int d^d\vec{x} \; \frac{K}{2} (\vec{\nabla} m)^2 + \frac{t}{2} m^2 + u m^4 + \cdots \tag{3}$$

$$\beta F[\psi] = \int d^d\vec{x} \; \frac{K}{2} |\vec{\nabla} \psi|^2 + \frac{t}{2} |\psi|^2 + u |\psi|^4 + \cdots$$

for complex op. field $\psi(\vec{x})$

- Approach to criticality

$$t = \frac{T - T_c}{T} \tag{4}$$

- Universality class based on various exponents.

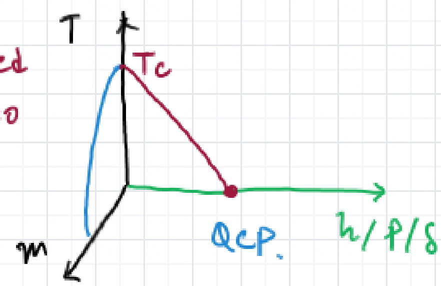
Q: What about T_c?

← Don't ask me. It is non-universal.

The fact that $T_c \neq 0$ means something.

→ There is an energy scale associated with All FINITE T_c transitions.

∘ Quantum Phase Transition



- Spontaneous symmetry breaking controlled by some other tuning parameter at $T=0$

- Quantum, in the sense the tuning parameter has to fight against system's tendency to order in the absence of entropic effect, via uncertainty principle : Quantum Fluctuation.

⇒ interaction vs quantum fluctuation
$U(x)$ ↔ quantum dynamics

- All finite temperature P.T's are classical.
  even when Q.M. is necessary for the existence of the order parameter.

  e.g. Ising Ferromagnet, Superfluid He^4, Superconductor.

  ∵ quantum fluctuations are unimportant at long distances sufficiently close to T_c.

$$\hbar \ll k_B T_c \cdot \xi^z \tag{5}$$

- Some (effective) Hamiltonian's are classical by design.
  ↔ all terms in the Hamiltonian commute with each other.

  e.g. $$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{6}$$

- For some Hamiltonians we ignore quantum fluctuation when dealing with classical limit.

  e.g. Heisenberg Model

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \left(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right) \tag{7}$$

$[S_x, S_y] = i\hbar S_z$ → in the large spin limit quantum fluct. ignored.

II. Quantum Stat Mech & QFT.

A. Classical vs Quantum Partition functions.

phonon's $\mathcal{H} = \sum_{\vec{k}} \left[\frac{1}{2m} |\tilde{p}(k)|^2 + \frac{1}{2} m \omega(k)^2 |u(k)|^2\right]$ (8)

$\tilde{p}(k)$: momentum, $u(k)$: displacement.

ignoring quantum uncertainty $[u(k), p(k)] = i\hbar$,

$$Z = \prod_{k} \int dp(\vec{k})\, du(\vec{k})\, \exp\left[-\beta \mathcal{H}(\tilde{p}(\vec{k}), \tilde{u}(\vec{k}))\right]$$

$$F = -k_B T \ln Z, \quad E = 3N\left(\tfrac{1}{2}k_B T + \tfrac{1}{2}k_B T\right) = 3Nk_B T.$$

With quantum effect

$$Z = \mathrm{Tr}\, e^{-\beta \hat{\mathcal{H}}}$$
$$= e^{-\beta E_0} \prod_{\vec{k}} \sum_{n_{\vec{k}}} e^{-\beta\hbar\omega(\vec{k}) n_k} \qquad n_k = 0, 1, 2 \cdots$$

Choosing the basis in which the density matrix is diagonal; the occupation # basis

$$= e^{-\beta E_0} \prod_{\vec{k},\alpha} \frac{1}{1 - e^{-\beta\hbar\omega_\alpha(\vec{k})}}$$

$$E^{\text{Debye}}(T) = -\frac{\partial \ln Z}{\partial \beta} = E_0 + \sum_{\vec{k},\alpha} \frac{\hbar v k}{e^{\beta\hbar v k} - 1}$$

$$c_V = \frac{dE}{dT} = k_B V \frac{2\pi^2}{5}\left(\frac{k_B T}{\hbar v}\right)^3 \propto N k_B \left(\frac{T}{T_D}\right)^3$$