A set of lectures on Quantum Phase Transitions

: transitions between distinct GROUND STATES

in a quantum Hamiltonian

$\exists$ terms that do not commute

Lect 1. The standard lore

: work out your muscle through a concrete example of

quantum paramagnet – Neel order transition. (Homework problem)

Lect 2. New probes and new reality.

$\downarrow$ STM $\downarrow$ Inhomogeneity

$\exists$ QPT in the presence of disorder ?

Lect 3. What if there is no order parameter ?

: Topological QPT.

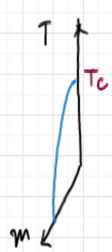
} Research problems!

Lecture 1. The Standard Lore.

I. Introduction: Quantum Phase Transitions (continuous)

Reading suggestion: RMP 69, 315 (1997)
Sondhi, Girvin, Carini, Shahar

o Continuous PT (2nd order)



- Spontaneous symmetry breaking at $T = T_c$
- Ordered state for $T < T_c$ (OP is nonzero)

  $\Leftrightarrow$ Equilibrium state has lower symmetry than the effective Hamiltonian.

  ex) $H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$ symmetry op $\sigma_i \to -\sigma_i \Leftrightarrow H \to H$ (def. of symm.)

  But an ordered state to the other ordered state

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

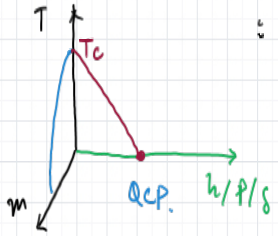
- divergence/singularities in thermodynamic quantities C_v, χ
- diverging correlation length ξ. $\Leftrightarrow$ absence of momentum scale. $\Leftrightarrow$ Scale invariance.
- LG free energy functional

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

$t \equiv \frac{T - T_c}{T_c}$ tunes the distance to the CP.

$$\beta F[\psi] = \int d^d\vec{x} \; \frac{K}{2}|\vec{\nabla}\psi|^2 + \frac{t}{2}|\psi|^2 + u|\psi|^4 + \cdots$$ for complex op. field $\psi(\vec{x})$

∘ Quantum Phase Transition



: $T=0$ transitions between distinct GROUND STATES

in a quantum Hamiltonian

$\exists$ terms that do not commute

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

$\Rightarrow$ interaction vs quantum fluctuation
$U(x)$ $\leftrightarrow$ quantum dynamics

- All finite temperature PT's are classical even when Q.M. is necessary for the order parameter.

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

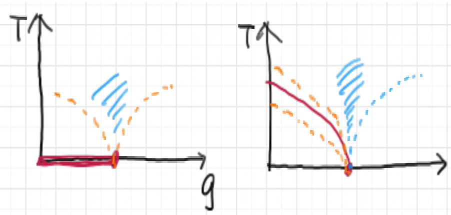
$\because$ quantum fluctuations are unimportant at long distances sufficiently close to T_c.

$$\hbar \ll kT \xi^z$$

- Some (effective) Hamiltonian's are classical by design. e.g. $\mathcal{H} = -J\sum_{\langle ij\rangle} \sigma_i \sigma_j$
- For some Hamiltonians we ignore quantum fluctuation the classical limit.

$\mathcal{H} = -J\sum_{\langle ij\rangle} (S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z)$, $[S_x, S_y] = i\hbar S_z$ ignored in the large S limit.

∘ The Standard Lore $d \to d+z$ and



1) $d \to d+z$

$\hat{\mathcal{H}} = \hat{K} + \hat{U}$ in d-dim space

do not commute

$[x, p] = i\hbar$, $[S_x, S_y] = i\hbar S_z$ ..
$[\phi(x), \Pi(x')] = i\hbar\,\delta(x-x')$

with QFT

$\langle 0|0\rangle = \int \mathcal{D}\phi\, e^{iS[\phi]}$

$S[\phi] = \int dt \int d\vec{x}\, \mathcal{L}[\phi(\vec{x})]$

$\mathcal{L}[\phi(x)] = \Pi_\phi \dot{\phi} - \mathcal{H}$

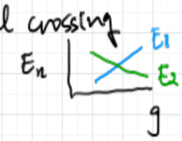
$S[\phi] \quad it = \tau, \quad S_E[\phi]$

with quantum stat mech

$Z = \mathrm{Tr}\,\hat{\rho} = \mathrm{Tr}\, e^{-\beta\hat{\mathcal{H}}}$ → the density matrix

choose your basis

i) If you know $\{|n\rangle\}$ such that $\hat{H}|n\rangle = E_n|n\rangle$, lucky you. QPT is just a level crossing



ii) If unlucky

$Z = \int \mathcal{D}\phi\, \langle\phi(x)|\, e^{-\beta\hat{H}}\, |\phi(x)\rangle$

Deal with $e^{-\beta(\hat{K}+\hat{U})} \neq e^{-\beta\hat{K}} e^{-\beta\hat{U}}$ by slicing up.

$\beta = N d\tau$, $N \to \infty$

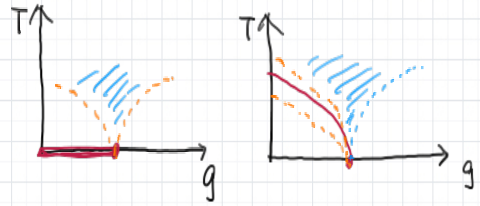
$Z = \int \mathcal{D}\phi\, e^{-S_E[\phi]}$

- the dynamic critical exponent z: $x' = x e^{-l}$, $t' = t e^{-zl}$, $\phi' = \phi e^{\dim[\phi] l}$

keeping the Lagrangian scale invariant.
(∵ critical point)

- Caveats:
  - mapping holds for thermodynamics only
  - resulting classical system can be unusual and anisotropic ($z \neq 1$)
  - extra complication w/ no classical counterpart may arise
    e.g. Berry phases, sign problem

2)



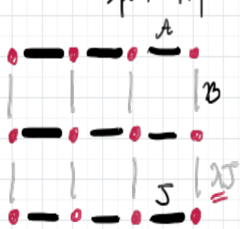
- T_c? matter of whether classical transition (long range order) is permitted in the thermodynamic limit ← lower critical dimension
- How do the curves bend? dimension of g.
- What determines the crossovers? correlation functions.
- Real life?

II. Coupled dimer model : pressure driven QPT in $TlCuCl_3$

field-driven QPT in $TlCuCl_3$ & $BaCuSi_2O_6$ (Han purple)

Refs: $TlCuCl_3$: Matsumoto et al PRB 69, 54423 (04)
$BaCuSi_2O_6$: Sebastian et al Nature 441, 617 (06)
Bond op. rep: Sachdev & Bhatt. PRB 41, 9313 (1990)
HW: Sachdev cond-mat 0401041.

o The model
- quantum spin $S = 1/2$ on sites
- Spatially anisotropic exchange



$$H = J \sum_{\langle ij \rangle \in A} \vec{S}_i \cdot \vec{S}_j + \lambda J \sum_{\langle ij \rangle \in B} \vec{S}_i \cdot \vec{S}_j - \sum_j \vec{B} \cdot \vec{S}_j$$

o Consider $B=0$ first.

① $\lambda = 0$ limit : indep. dimers (J)

We know how to solve!

spin gap $\Delta = J$
$|S=1, S_z=1\rangle, |1,0\rangle, |1,-1\rangle$ triplet
$|S=0\rangle$ singlet $\equiv \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$ (J)

② $\lambda = 1$ limit : Heisenberg AF
Neel order.

Schematic PD

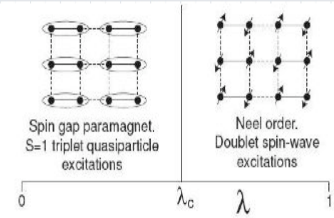
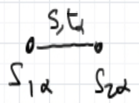


Fig. 4. Ground states of H_d as a function of λ The quantum critical point is at [28] $\lambda_c = 0.52337(3)$. The compound $TlCuCl_3$ undergoes a similar quantum phase transition under applied pressure [8].

o From QPM (small λ) Side, (refer to the HW for typed Eq's)

- Use bond operator formalism, represent spins with singlons & triplons, (s, t_x, t_y, t_z)



$$S_{1\alpha} = \frac{1}{2}\left(s^\dagger t_\alpha + t_\alpha^\dagger s - i\epsilon_{\alpha\beta\gamma} t_\beta^\dagger t_\gamma\right)$$

$$S_{2\alpha} = \frac{1}{2}\left(-s^\dagger t_\alpha - t_\alpha^\dagger s - i\epsilon_{\alpha\beta\gamma} t_\beta^\dagger t_\gamma\right)$$

where
$$|s\rangle \equiv s^\dagger|0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle); \quad |t_x\rangle \equiv t_x^\dagger|0\rangle = -\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)$$
$$|t_y\rangle \equiv t_y^\dagger|0\rangle = -\frac{i}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle); \quad |t_z\rangle \equiv t_z^\dagger|0\rangle = -\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle).$$

under the constraint $s^\dagger s + t_\alpha^\dagger t_\alpha = 1$ (two spins have to be in one of these four states.)

You can check the above rep. satisfies spin 1/2 SU(2) algebra.

- The Hamiltonian has interaction terms for bond operators.

$$H = H_0 + H_1 + H_2 + H_3,$$
$$H_0 = J\sum_l \left(-\frac{3}{4}s_l^\dagger s_l + \frac{1}{4}t_{l,\alpha}^\dagger t_{l,\alpha}\right) - \sum_l \mu_l (s_l^\dagger s_l + t_{l,\alpha}^\dagger t_{l,\alpha} - 1) +$$
$$H_1 = \sum_{lm} a(l,m)(t_{l\alpha}^\dagger t_{m\alpha} s_m^\dagger s_l + t_{l\alpha}^\dagger t_{m\alpha}^\dagger s_m s_l + h.c.)$$
$$H_2 = \sum_{lm} b(l,m) i\epsilon_{\alpha\beta\gamma}(t_{m\alpha}^\dagger t_{l\beta}^\dagger t_{l\gamma} s_m + t_{l\alpha}^\dagger t_{m\beta}^\dagger t_{m\gamma} s_l + h.c.)$$
$$H_3 = \sum_{lm} c(l,m)(t_{l\alpha}^\dagger t_{m\alpha}^\dagger t_{m\beta} t_{l\beta} - t_{l\alpha}^\dagger t_{m\beta}^\dagger t_{m\alpha} t_{l\beta}), \tag{8}$$

- Solving the constraint in small λ approximation (HW prob 1.)

$$H_{HP} = J\sum_l t_{l,\alpha}^\dagger t_{l,\alpha} + \sum_{l,\hat\delta} a(l, l+\hat\delta)(t_{l,\alpha}^\dagger t_{l+\hat\delta,\alpha} + t_{l,\alpha}^\dagger t_{l+\hat\delta,\alpha}^\dagger + h.c.). \tag{12}$$

- F.T. and find the gap is minimum at $\vec{k} = (0, \pi)$ (trying to be an AFM)

- Gradient expansion around $(0,\pi)$

$$t_{l\alpha} = \tilde{t}_\alpha(\vec{r}_l)\, e^{i(0,\pi)\cdot\vec{r}_l}$$

$$S = \int d^2r d\tau \left[\tilde{t}_\alpha^\dagger \frac{\partial \tilde{t}_\alpha}{\partial\tau} + C\tilde{t}_\alpha^\dagger \tilde{t}_\alpha - \frac{D}{2}(\tilde{t}_\alpha \tilde{t}_\alpha + H.c.) + K_{1x}|\partial_x \tilde{t}_\alpha|^2 + K_{1y}|\partial_y \tilde{t}_\alpha|^2 \right.$$
$$\left. + \frac{1}{2}(K_{2x}(\partial_x \tilde{t}_\alpha)^2 + K_{2y}(\partial_y \tilde{t}_\alpha)^2 + H.c.) + \cdots \right] \tag{13}$$

- Decompose the complex field $\tilde{t}_\alpha$ into real and imaginary parts

$$\tilde{t}_\alpha = \varphi_\alpha + i\pi_\alpha$$ → remains massive ⇒ integrate out.

- The field theory for the QPM − AFM QCP.

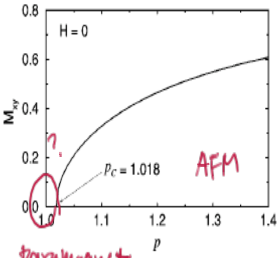
$$\boxed{S_\varphi = \int d^2r d\tau \left[\frac{1}{2}(\partial_\tau\varphi_\alpha)^2 + c_x^2(\partial_x\varphi_\alpha)^2 + c_y^2(\partial_y\varphi_\alpha)^2 + \Delta^2\varphi_\alpha^2 + \frac{u}{24}(\varphi_\alpha^2)^2\right], \quad (15)}$$

O(3) model

- TlCuCl$_3$

: use pressure to tune λ

Staggered moment.



paramagnet

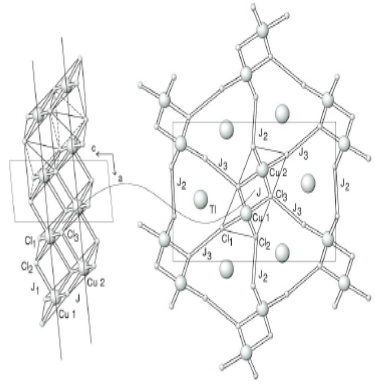


FIG. 1. Structure of TlCuCl$_3$: small circles represent Cl$^-$ ions, medium-sized circles Cu^{2+} ions, and large circles Tl$^+$ ions.

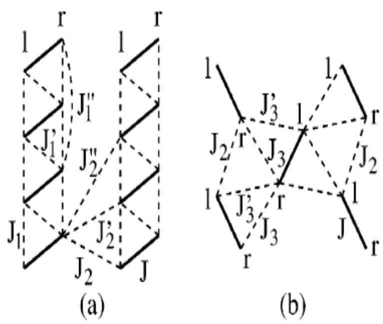
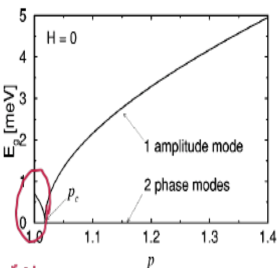


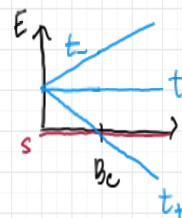
FIG. 2. Schematic representation of relevant interdimer couplings in XCuCl$_3$: (a) a-c plane and (b) b-c plane.



with spin gap : Quantum paramagnet.

∘ Consider the effect of $\vec{B}$

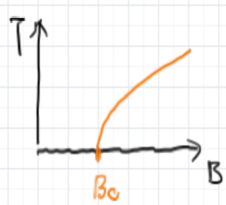
- For $\lambda=0$, $\vec{B}$ splits the triplet, closes the spin gap for $|S=1, S_z=1\rangle$



level crossing : QPT at $B=B_c$ between QPM & Canted order

- For $\lambda \neq 0$: interacting problem

↳ Can use bosonic rep. of triplons, map to BEC of triplons.



⇒ the QCP is of XY universality class.

∵ The component of φ_α along $\vec{B}$ can be integrated out.
due to $(\partial_\tau \varphi_\alpha)^2 \to (\partial_\tau \varphi_\alpha + i\epsilon_{\alpha\beta\gamma} B_\beta \varphi_\gamma)^2$

Say $\vec{B} = B\hat{z}$, integrate out φ_z

⇒ The effective action

$$\boxed{S_\Psi = \int d^d r \int_0^{1/T} d\tau \left[\Psi^* \partial_\tau \Psi + \frac{1}{2m} |\nabla \Psi|^2 - \mu |\Psi|^2 + \frac{\tilde{u}}{2} |\Psi|^4 \right]} \quad (45)$$

BEC of charged (complex) boson.

in terms of *complex field* Ψ defined as

$$\Psi = \frac{\varphi_x + \varphi_y}{\sqrt{B}} \quad (46)$$

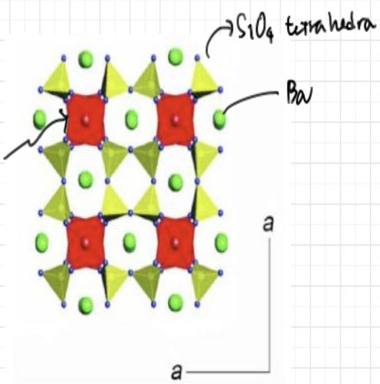
and m and $\tilde{u}$ defined as

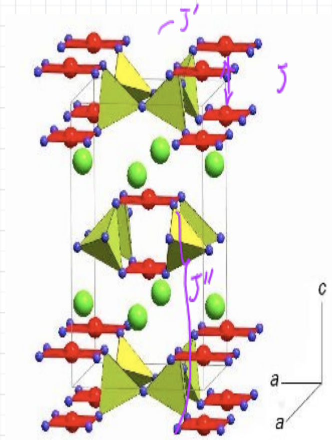
$$m \equiv c^2/2B, \quad \tilde{u} \equiv u/12B. \quad (47)$$

- Han purple pigment $BaCuSi_2O_6$
  ↳ first synthesized by Chinese Han people 2000yrs ago

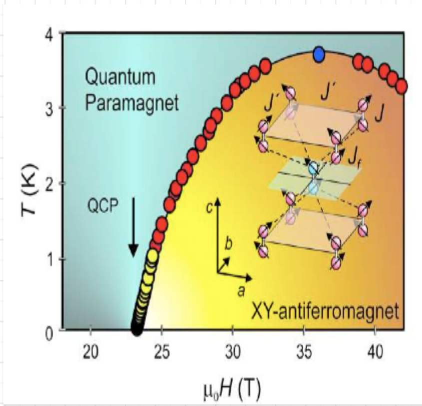
$BaCuSi_2O_6$

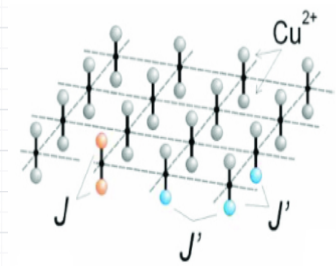
I41/acd spacegroup



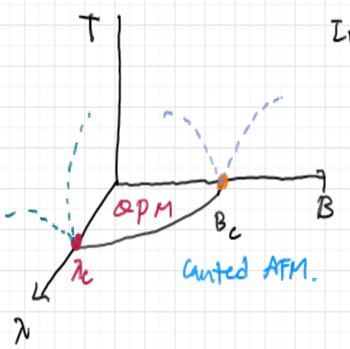


$J'' \ll J' \ll J$





○ Summary of the coupled dimer model.



In $d=2$, $T=0$ $D=4$ XY universality class for the QCP at B_c

$D=3$ $O(3)$ ϕ^4 model: Wilson-Fisher F.P (HW prob 2)

$T\neq 0$. No long range order in $d=2$ for $N \gtrsim 2$

But finite T phase diagram contains crossovers.

In the prob. 2, a large N approach is used to

1) study the correlation function of fluctuations.

2) identify an tuning parameter dep. energy scale Δ that vanishes at the QCP

3) Define the crossover by $\Delta(g)$ vs. T
 ↖ a generic knob

In $d=3$, $T=0$ $D=5 >$ upper critical dim.
→ MFT exponents.
$D=4$ ↗

$T\neq 0$: LRO at finite Tc.

classical critical region vs quantum
↳ Ginzburg criteria ↳ $\Delta(g) \lesssim T$

⇒ (HW prob 3.)