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)


: STM inhomogeneity

\( \equiv \) QPT in the presence of disorder?

Lect 3. What if there is no order parameter?

: Topological QPT.

Lecture 1. The Standard Lore.

1. Introduction: Quantum Phase Transitions (Continuous)

0 Continuous PT (2nd order)

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

--- Equilibrium state has lower symmetry than the effective Hamiltonian.

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1) \( H = -J \sum_i \sigma_i \sigma_{i+1} \) symmetry \( \sigma_i \rightarrow -\sigma_i \) \( \Rightarrow H \rightarrow -H \) (def. of spinon)

But an ordered state to the other ordered state

with \( \frac{1}{N} \sum_i \sigma_i = m \) \( \Rightarrow \frac{1}{N} \sum_i \sigma_i = -m \)

- divergence/regularities in thermodynamic quantities \( C, \chi \)

- diverging correlation lengths \( \xi \) \( \Rightarrow \) absence of momentum scale \( \Rightarrow \) scale invariance

- LG free energy functional

\[
AF[\psi] = \frac{1}{2} \left( \psi^* \partial_x \psi \right)^2 + \frac{1}{2} m^2 + \frac{1}{4} \mu^4 + \ldots \quad \text{t.e. } \frac{T - T_c}{T_c} \text{ tunes the distance to the CP.}
\]

\[
AF[\psi] = \left| \partial_x \right|^2 \hat{\psi}^* \hat{\psi} + \frac{1}{2} m^2 + \mu^4 \hat{\psi}^* \hat{\psi} + \ldots \quad \text{for complex CP field} \ \hat{\psi}(x)
\]

Reading suggestion: EMD 69, 315 (1997)

Sondhi, Girvin, Carini, Schultz
Quantum Phase Transition

- Transition between distinct ground states

- In a quantum Hamiltonian, there are terms that do not commute.

- Quantum, in the sense that the tunnelling parameter has to fight against the system's tendency to order in the absence of anisotropic effect, via the uncertainty principle. Quantum fluctuations:

  \[ \langle \text{interaction vs quantum fluctuation} \rangle \propto \langle \text{quantum dynamics} \rangle \]

- All finite temperature PTs are classical even when QM is necessary for the order parameter.

  \[ \langle \text{quantum fluctuations are unimportant at long distances sufficiently close to } T_c \rangle \]

  \[ k_B T \lesssim \frac{\pi}{2} \]

- Some effective Hamiltonians are classical by design, e.g., \( H = -J \sum \sigma_i \sigma_j \)

- For some Hamiltonians we ignore quantum fluctuation and classical limit.

\[ \text{If } T \ll T_c, \text{ then quantum fluctuations are ignored in the large } S \text{ limit.} \]

The Standard Lorentzian

\[ d \rightarrow d + \varepsilon \]

1) \[ d \rightarrow d + \varepsilon \]

\[ \hat{H} = \hat{K} + \hat{U} \text{ in } d\text{-dim space} \]

\[ \text{do not commute.} \]

\[ \text{with } \hat{Q}^T \]

\[ \langle 0 | \phi \rangle = e^{-\hat{Q}^T} \]

\[ \langle \phi | = e^{\hat{Q}^T} \]

\[ \hat{[Q]} = [dt \hat{S}[d \hat{L}[\phi]]] \]

\[ \hat{L}[\phi(d)] = T \hat{d} \hat{\phi} - \hat{V} \]

\[ \varepsilon \hat{[Q]} \]

\[ \varepsilon \]

\[ \text{with quantum statistical mechanics} \]

\[ Z = Tr \hat{\rho} = Tr e^{-\beta \hat{H}} \]

\[ \text{choose your basis} \]

\[ Z = \left[ \begin{array}{c} e^{-\beta \hat{A}} \end{array} \right] \]

\[ \text{Deal with } e^{-\beta \hat{A}} \] by slicing up.

\[ \beta = \text{Not, } N \rightarrow \infty \]

\[ Z = \left[ e^{-\beta E} \right] \]
- the dynamic critical exponent $\gamma'$: $\gamma' = \frac{\phi}{\phi} = e^{-\frac{1}{\phi}}$

- the Lagrangian scale invariant: $t' = e^{-t}$

- Critical point

- Caveats: mapping holds for thermodynamics only
- resulting classical system can be unusual and anisotropic (2D)
- extra complication w/o classical counterpart may arise:
  - e.g. Berry phases, sign problem

II. Coupled dimer model: pressure driven QPT in TlCuCl$_3$

- The model
  - quantum spin $S=\frac{1}{2}$ on sites
  - spatially anisotropic exchange

- $\mathcal{H} = J \sum_{<ij>} \hat{S}_i \cdot \hat{S}_j + \lambda J \sum_{ij} \hat{S}_i \cdot \hat{S}_j - \sum_j \hat{S}_j$

- Consider $B=0$ first.
  - $\lambda=0$ limit: independent dimer
  - We know how to solve!
  - Spin gap \[\Delta_s = \sqrt{\frac{1}{2} \left( 1, 0 \right)} \] triplet
  - Spin gap $\Delta_1 = \frac{1}{2} \left( 1, 0 \right)$ singlet
  - $\Delta_1 \equiv \frac{1}{\sqrt{2}} (U - \lambda U)$

- $\lambda=1$ limit: Heisenberg AF

Schematic PD

Fig. 4: Ground state of $\mathcal{H}$ as a function of $J$. The maximum critical point is at $\langle J \rangle = 3.8$; $\lambda = 1.2$. $\phi$ increases with increasing pressure; after compression under applied pressure [2].
0 From BPM (Small $\mathcal{N}$) Side, (Refer to the HW for typed Eqs)

- Use bond operator formalism, represent spins with singlets & triplicities, $(S_1, t_2, t_3, t_4)$

\[ S_{2n} = \frac{1}{2}(s_{1a}^+ t_{2a}^+ t_{2a} - i e_{\alpha\beta}^a t_{2a}^+ t_{3a}^+ t_{3a}^+ t_{4a}^+ t_{4a}^+) \]

Where

\[ | s \rangle = \frac{1}{\sqrt{2}} (|11\rangle - |1\rangle |1\rangle), \quad | t_2 \rangle = \frac{1}{\sqrt{2}} (|1\rangle |1\rangle - |1\rangle |1\rangle) \]

Under the constraint \[ S_1 S + t_2 t_4 = 1 \] (two spins have to be in one of these four states).

You can check the above rep satisfies spin $\mathcal{N}/2$ Spin(2) algebra.

- The Hamiltonian has interaction terms for bond operators

\[
H = H_0 + H_1 + H_2 + H_3
\]

\[
H_0 = J \sum_i \left( \frac{3}{4} |s_i\rangle \langle s_i| + \frac{1}{4} t_{2a}^i t_{3a}^i t_{4a}^i - 1 \right) + \sum_i a_i (s_i^a t_{2a}^i + t_{2a}^i s_i^a) + h.c.
\]

\[
H_1 = \sum_{l,m} a(l,m)(t_{2a}^l t_{3a}^m s_{3a}^m s_{3a}^m + t_{2a}^l t_{3a}^m s_{3a}^m s_{3a}^m + h.c.)
\]

\[
H_2 = \sum_{l,m} b(l,m) e_{\alpha\beta}^a t_{2a}^l t_{3a}^m s_{3a}^m + t_{2a}^l t_{3a}^m s_{3a}^m + h.c.
\]

\[
H_3 = \sum_{l,m} c(l,m) (t_{2a}^l t_{3a}^m s_{3a}^m + t_{2a}^l t_{3a}^m s_{3a}^m + h.c.)
\]

(8)

- Solving the constraint in Small \( \mathcal{N} \) approximation

\[
H_{NP} = \sum_i \lambda_{i,a} t_{2a}^i + \sum_{l,m} a(l,m) (t_{2a}^l t_{3a}^m s_{3a}^m s_{3a}^m + t_{2a}^l t_{3a}^m s_{3a}^m s_{3a}^m + h.c.
\]

(12)

- F.T. and find the gap is minimum at $\hat{\mathbf{p}} = (0,0)$

- Gradient expansion around $(0,0)$

\[
\hat{t}_{2a} = \mathcal{E}_a(\hat{\mathbf{p}}) + i(\hbar \pi)p \hat{\mathbf{p}}
\]

\[
S = \int d^d\mathbf{r} d\mathbf{r}' \left[ \hat{t}_{2a}^\dagger \hat{t}_{2a} + C\nabla^2 \hat{\mathbf{p}} - \frac{D}{2} (\hat{\mathbf{p}}^2 + H.c.) + K_{12}|\partial_2 \hat{\mathbf{p}}|^2 + K_{13}|\hat{\mathbf{p}}|^2
\]

\[
+ \frac{1}{2} (K_{23} \partial_2^2 \hat{\mathbf{p}}^2 + K_{23} |\partial_2 \hat{\mathbf{p}}|^2 + H.c.) + \cdots \right]
\]

(13)

- Decompose the complex field $\mathcal{E}_a$ into real and imaginary parts

\[
\hat{\mathbf{E}}_a = \hat{\mathbf{E}} + i \hat{\mathbf{P}}_a \quad \rightarrow \text{remaining massive} \quad \hat{\mathbf{E}} \quad \text{integrate out}
\]

- The field theory for the BPM-APM OCP

\[
S_2 = \int d^d\mathbf{r} d\mathbf{r}' \left[ \frac{1}{2} (\partial_2 \hat{\mathbf{r}}_a)^2 + c_2^2 (\partial_2 \hat{\mathbf{r}}_a)^2 + c_3^2 (\partial_2 \hat{\mathbf{r}}_a)^2 + \Delta^2 \hat{\mathbf{r}}_a^2 + \frac{\nabla^2}{24} (\hat{\mathbf{r}}_a^2) \right]
\]

(15) O(5) model
FIG. 1. Structure of TiCuCl₃: small circles represent Cu⁺ ions, medium-sized circles Cu²⁺ ions, and large circles H⁻ ions.

FIG. 2. Schematic representation of relevant interlayer couplings in XCoCl₃. (a) a-c plane and (b) b-c plane.

Consider the effect of $\mathbf{B}$

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

- For $\lambda>0$: interacting problem

$B_0 = B_{\text{c}}$, integrate out $\varphi_B$

$\Rightarrow$ The effective action

\[ S_B = \int d^3x \frac{1}{2m} \left[ \frac{\partial \varphi_B}{\partial x^i} \right]^2 - \frac{1}{2} \left( \frac{\partial \varphi_B}{\partial x^i} - i \frac{\varphi_B}{B_{\text{c}}} \right)^2 + \frac{|\varphi_B|^2}{2} + \frac{\mu}{2} |\varphi_B|^2 + \frac{\varphi_B^* \varphi_B}{2} \]

BEC of charged (complex) boson.

in terms of simpler field $\varphi$ defined as

\[ \varphi = \frac{\varphi_B + \varphi_B^*}{\sqrt{B}} \]

and $m$ and $i$ defined as

\[ m = c^2/2B, \quad i = u/2B. \]
Summary of the coupled dimer model.

In $d=2$, $T=0$ D=4 x$^4$ universality class for the QCP. See 3.

$D=3$ O(3) AF model: Wilson-Fisher F.D. (HW prob 2)

$T=0$. No long range order in $d=2 \text{ or } \mathbb{Z}_2$.

But finite $T$ phase diagram contains crossovers.

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

1) Study the correlation functions of fluctuations.

2) Identify the tuning parameter-dependent energy scale

$\Delta$ that vanishes on the QCP.

3) Define the crossover by $\Delta(g)$ vs $T$

In $d=3$, $T=0$ D=5 $\uparrow$ upper critical dim.

$\Rightarrow$ MFT exponents.

$D=4$

$T=0$, LSQ or finite $T_c$.

Classical critical region vs quantum

$\Rightarrow$ vanishing criticality $\Rightarrow \Delta \leq T$

HW problem 3