5 Theoretical models for quantum phase transition

5.1 Quantum Ising model

Hamiltonian (transverse-field Ising model):

$$H_I = -\underbrace{J}_{\text{coupling constant}} \underbrace{\sum_{\langle ij\rangle}}_{\text{sum over nearest neighbors}} \underbrace{\sigma_i^z \sigma_j^z}_{\text{Pauli matrices}} - J\underbrace{g}_{\text{"transverse field"}} \sum_i \sigma_i^x$$

defined on a regular d-dimensional lattice.

H_I describes quantum spins $\frac{1}{2}$, $\vec{S}_i = \frac{1}{2}\vec{\sigma}_i$ with $[S_i^x, S_i^y] = i S^z$, in an external magnetic field $\vec{H} \parallel \vec{e}_x$.

$\mathbb{Z}_2$ symmetry:

$$\sigma_i^z \mapsto -\sigma_i^z$$

Limiting cases:

(a) $g \to 0$:
- ground state $|0\rangle$ = ferromagnet $|\Uparrow\rangle \equiv \prod_{i=1}^{M} |\uparrow\rangle_i$ or $|\Downarrow\rangle \equiv \prod_{i=1}^{M} |\downarrow\rangle_i$
- $\mathbb{Z}_2$ symmetry spontaneously broken
- long-range order with order parameter $\langle 0|\sigma_i^z|0\rangle = \pm N_0$
- small finite g will reduce N_0, but system remains ordered

(b) $g \to \infty$: • ground state $|0\rangle$ = polarized state $\prod_i |\rightarrow\rangle_i$,

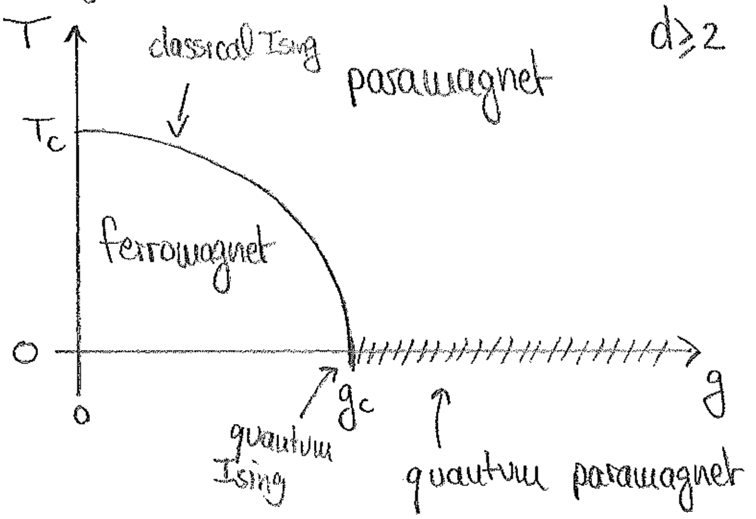
$\sigma_i^x |\rightarrow\rangle_i = + |\rightarrow\rangle_i$

• no spontaneous symmetry breaking

• large finite g will allow admixture of $|\leftarrow\rangle_i$ spins, but systems remains disordered

Conclusion : There must be a QPT at some critical $g = g_c$
(later: universality class = cl. Ising in d+1 dimensions)

Phase diagram :



Experimental examples :

- $LiHoF_4$ (3D Ising + long-range dipolar interaction)
- $CoNb_2O_6$ (1D Ising)

4.6.18

5.2 Quantum rotor model

Quantum rotor : particle on unit sphere in N dimensions ($N \geq 2$), orientation $\vec{n}$ with constraint $\vec{n}^2 = 1$.

Commutation relation:

$$[n_\alpha, \underset{\substack{\uparrow \\ \text{conjugate} \\ \text{momentum}}}{p_\beta}] = i\,\delta_{\alpha\beta} \qquad \alpha, \beta = 1, \dots, N$$

Rotor angular momentum:

$$L_{\alpha\beta} := n_\alpha p_\beta - n_\beta p_\alpha \qquad \text{with } \frac{N(N-1)}{2} \text{ components}$$

$L_{\alpha\beta}$ are the <u>generators</u> of the O(N) rotations of $\vec{n}$ on the unit sphere

Example ($N=3$):

$$L_\alpha := \frac{1}{2} \underset{\substack{\downarrow \\ \text{antisymmetric tensor}}}{\varepsilon_{\alpha\beta\gamma}} L_{\beta\gamma} \quad \Rightarrow \quad \begin{aligned} [L_\alpha, L_\beta] &= i\,\varepsilon_{\alpha\beta\gamma} L_\gamma \\ [L_\alpha, n_\beta] &= i\,\varepsilon_{\alpha\beta\gamma} n_\gamma \end{aligned}$$

Kinetic energy:

$$H_K = \frac{Jg}{2} \underbrace{L_{\alpha\beta}^2}_{\equiv \mathbb{L}^2} \propto \begin{cases} L_z^2 & \text{for } N=2 \\ \vec{L}^2 & \text{for } N=3 \end{cases}$$

with moment of inertia $I = \frac{1}{Jg}$.

Eigenvalues:

$$\varepsilon_K = \begin{cases} \frac{Jg}{2} \ell^2, & \ell = 0,1,2,\dots \text{ (two-fold degenerate for } \ell \neq 0\text{), for } N=2 \\ \frac{Jg}{2} \ell(\ell+1), & \ell = 0,1,2,\dots \text{ (}2(\ell+1)\text{ degenerate), for } N=3 \end{cases}$$

Hamiltonian (lattice of rotors):

$$H_R = -J \sum_{\langle ij \rangle} \vec{n}_i \cdot \vec{n}_j + \frac{Jg}{2} \sum_i \mathbb{L}_i^2$$

Symmetry:

$$O(N): \quad \vec{n}_i \mapsto \underset{\text{rotation matrix}}{R}\, \vec{n}_i$$

Limiting cases ($d \geq 2$):

(a) $g \ll 1$:
- $O(N)$ spontaneously broken
- long-range order $|\langle 0|\vec{n}_i|0\rangle| = N_0$ and

$$\lim_{|\vec{r}_i - \vec{r}_j| \to \infty} \langle 0|\vec{n}_i \cdot \vec{n}_j|0\rangle = N_0^2$$

(b) $g \gg 1$:
- ground state symmetric
- no long-range order, $\langle 0|\vec{n}_i \cdot \vec{n}_j|0\rangle \sim e^{-|\vec{r}_i - \vec{r}_j|/\xi}$

Conclusion: QPT at finite $g = g_c$
Universality class: $O(N)$ in $d+1$ dimensions

Examples:
- $N=2$: lattice of superconducting islands
- $N=3$: lattice of spin pairs ("coupled dimers")

5.3 Coupled-dimer model

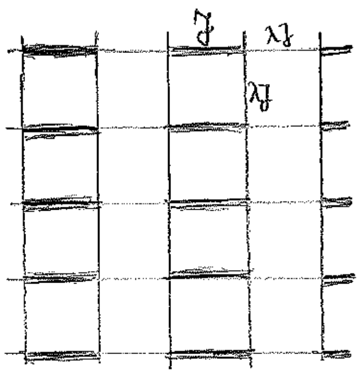
Hamiltonian:

$$H_{CD} = \sum_{\langle ij \rangle} J_{ij} \, \vec{S}_i \cdot \vec{S}_j$$

with

$$J_{ij} = \begin{cases} J & \text{intradimer bonds} \\ \lambda J & \text{interdimer bonds} \end{cases} \qquad \text{and } J>0 \text{ antiferromagnetic}$$

Example:



Limiting cases (square lattice):

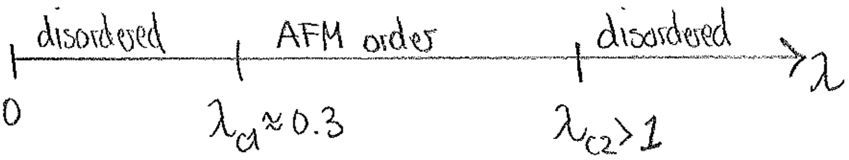
(a) $\lambda = 0$: disconnected spin singlets with $S=0$, triplets with $S=1$ gapped with $\Delta = J$

(b) $\lambda \ll 1$: weakly-coupled dimers, disordered

(c) $\lambda \sim 1$: strongly-coupled dimers, antiferromagnetic long-range order, SU(2) spontaneously broken

(d) $\lambda \gg 1$: decoupled spin ladders, disordered

Phase diagram:



Universality class: O(3) Heisenberg in d+1 dimension

Experimental examples:

- $TlCuCl_3$ [3D coupled-dimer system with $\lambda \propto p$]
- $BaCuSi_2O_6$ [2D layers of dimers]