

5 Theoretical models for quantum phase transition

5.1 Quantum Ising model

Hamiltonian (transverse-field Ising model):

$$H_I = -J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - Jg \sum_i \sigma_i^x$$

↑ coupling constant
↑ sum over nearest neighbors
↑ Pauli matrices
↑ "transverse field"

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 $[S_i^x, S_i^y] = i S_i^z$, 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) $g \rightarrow 0$:
- 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

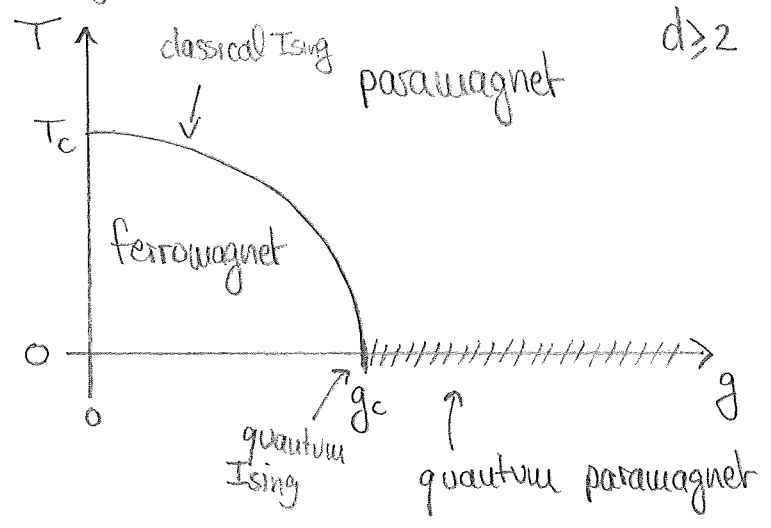
(b) $g \rightarrow \infty$: • ground state $|0\rangle = \text{polarized state } \prod_i |1\rangle_i$,

$$\sigma_i^x |1\rangle_i = + |1\rangle_i$$

- no spontaneous symmetry breaking
- large finite g will allow admixture of $|1\rangle_i$ spins, but system remains disordered

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

Phase diagram:



Experimental examples:

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

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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:

$$[n_\alpha, p_\beta] = i \delta_{\alpha\beta} \quad \alpha, \beta = 1, \dots, N$$

\uparrow
 conjugate
 momenta

Rotor angular momentum:

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

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

Example ($N=3$):

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

Kinetic energy:

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

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

Eigenvalues:

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

Hamiltonian (lattice of rotors):

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

Symmetry:

$$O(N): \vec{n}_i \mapsto \overset{\substack{\text{rotation matrix} \\ \downarrow}}{R} \vec{n}_i$$

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

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

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")

$$[\vec{L}_i = \vec{S}_{i1} + \vec{S}_{i2}, \vec{n}_i \propto \vec{S}_{1i} - \vec{S}_{2i}]$$

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5.3 Coupled-dimers model

Hamiltonian:

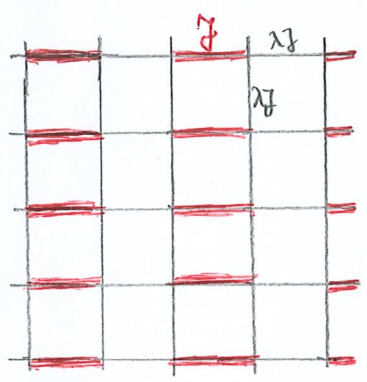
$$H_{\text{CD}} = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

with $J_{ij} > 0$ antiferromagnetic

$$J_{ij} = \begin{cases} J & \text{intradimer bonds} \\ \lambda J & \text{inter-dimer bonds} \end{cases}$$

and $J > 0$ antiferromagnetic

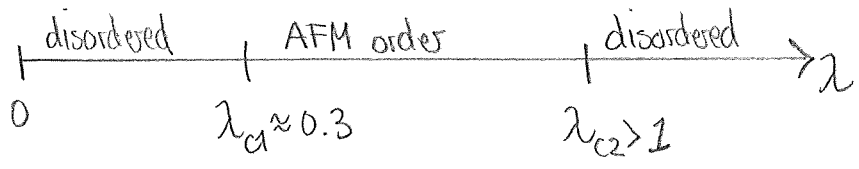
Example:



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:

- TlCuCl3 [3D coupled-dimers system with $\lambda \propto p$]
- BaCuSi2O6 [2D layers of dimers]