Quantum Phase Transitions - The Quantum-Classical Mapping

Daniel Lechner

University of Vienna

13.6.2014

1. General Aspects

Quantum Fluctuations and Quantum Critical Point

- Quantum phase transition: non-analyticity in the ground state energy
- QPTs not driven by thermal fluctuations
- Quantum fluctuations = Heisenberg uncertainity fluctuations
- For $T \neq 0$: Quantum fluctuations always overpowered by thermal fluctuations (close to critical point)

Consequence

Quantum phase transitions can only take place at T = 0!

Quantum Critical Point

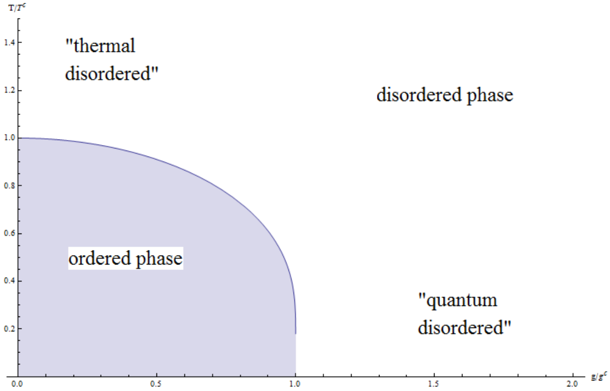
- Hamiltonian often of the form:

$$\hat{H} = \hat{H}_0 + g\hat{H}_1$$

- Tuning of g across a critical value g^c at $T = 0$ induces a quantum phase transition
- Quantum critical point:

$$g = g_c \quad \text{at} \quad T_c = 0$$

A Quantum Phase Diagram



Quantum-Classical Mapping

- Exact spectrum $\hat{H}(g)\left|\psi\right\rangle = \epsilon(g)\left|\psi\right\rangle$ almost never accessible
- Especially powerful for investigating QPTs: QC-Mapping
- D-dim. quantum model usually maps onto (D+1)-dim. classical model
- (imaginary) time $\rightarrow$ additional spatial direction

Strategy of QC-Mapping

1. Map to classical model
2. Solve classical model
3. Find the classical critical point(s)
4. Identify quantum critical point(s) (QCP) via map

2. Quantum Ising Chain in a Transverse Field

Hamiltonian

Quantum Ising chain in a transverse field

$$\hat{H} = -J \sum_{i=1}^{N} \hat{\sigma}^z_{i+1} \hat{\sigma}^z_i - h \sum_{i=1}^{N} \hat{\sigma}^x_i$$

- Note: $\mathcal{H}_N = \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_1 = \bigotimes_{i=1}^{N} \mathcal{H}_1$
- Ferromagnetic part:

$$\hat{H}_0 = -J \sum_{i=1}^{N} \hat{\sigma}^z_{i+1} \hat{\sigma}^z_i$$

- Paramagnetic part:

$$\hat{H}_1 = -h \sum_{i=1}^{N} \hat{\sigma}^x_i$$

Limiting Cases - $h = 0$

- $h = 0 \rightarrow$ ferromagnetic part

$$\hat{H} \rightarrow \hat{H}_0 = -J \sum_{i=1}^{N} \hat{\sigma}^z_{i+1} \hat{\sigma}^z_i$$

- Ground state:

$$|\{S^z_0\}\rangle \equiv \prod_{i=1}^{N} |\uparrow\rangle_i \quad \textbf{or} \quad |\{S^z_0\}\rangle \equiv \prod_{i=1}^{N} |\downarrow\rangle_i$$

- Hamiltonian:

$$H \equiv \langle \{S^z\}| \hat{H} |\{S^z\}\rangle = -J \sum_{i=1}^{N} S^z_{i+1} S^z_i$$

- Partition function:

$$Z \to \sum_{\{S^z_i\}} e^{\beta J \sum_{i=1}^{N} S^z_{i+1} S^z_i} =$$

$$= (2\cosh(\beta J))^N + (2\sinh(\beta J))^N$$

Limiting Cases - $J = 0$

- $J = 0 \rightarrow$ paramagnetic part

$$\hat{H} \rightarrow \hat{H}_1 = -h \sum_{i=1}^{N} \hat{\sigma}_i^x$$

- Ground state:

$$|\{S_0^x\}\rangle \equiv \prod_{i=1}^{N} |\rightarrow\rangle_i \quad \text{where} \quad |\rightarrow\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle + |\downarrow\rangle\right)$$

- Hamiltonian:

$$H \equiv \langle \{S^x\}| \hat{H} |\{S^x\}\rangle = -h \sum_{i=1}^{N} S_i^x$$

- Partition function:

$$Z \rightarrow \sum_{\{S_i^x\}} e^{\beta h \sum_{i=1}^{N} S_i^x} = (2\cosh(\beta h))^N$$

Quantum-to-Classical Mapping

- General situation: $J \neq 0, h \neq 0$
- Goal: Partition function

$$Z = Tr\left[e^{-\beta \hat{H}}\right] = Tr\left[e^{-\beta \hat{H}_0 - \beta \hat{H}_1}\right]$$

- i.e.

$$Z = \sum_{\{S^z\}} \langle \{S^z\}| \, e^{\beta J \sum_{i=1}^{N} \hat{\sigma}^z_{i+1} \hat{\sigma}^z_i + \beta h \sum_{i=1}^{N} \hat{\sigma}^x_i} \, |\{S^z\}\rangle$$

- Problem:

$$[\hat{H}_0, \hat{H}_1] \neq 0$$

Trotter Decomposition

Trotter´s theorem

$$e^{-\beta(A+B)} = s - \lim_{L\to\infty} \left(e^{-\frac{\beta}{L}A} e^{-\frac{\beta}{L}B}\right)^L$$

for bounded-from-below, self adjoint operators A,B.

- Exponential inside the trace:

$$e^{-\beta\hat{H}_0 - \beta\hat{H}_1} \approx \left(e^{-\frac{\beta}{L}\hat{H}_0} e^{-\frac{\beta}{L}\hat{H}_1}\right)^L \equiv \left(e^{-\delta\tau\hat{H}_0} e^{-\delta\tau\hat{H}_1}\right)^L$$

$$\delta\tau = \frac{\beta}{L}$$

- Note: $\approx$ becomes $=$ in the limit $L \to \infty$

- Applying Trotters formula to the partition function:

$$Z = \sum_{\{S^z\}} \langle \{S^z\}| \, e^{-\beta \hat{H}_1 - \beta \hat{H}_0} \, |\{S^z\}\rangle =$$

$$= \sum_{\{S^z\}} \langle \{S^z\}| \prod_{l=1}^{L} \left(e^{-\delta\tau \hat{H}_1} e^{-\delta\tau \hat{H}_0} \right) |\{S^z\}\rangle$$

- Insert complete sets

$$1 = \prod_{i=1}^{N} \left[\sum_{S_i^z = \pm 1} |S_i^z\rangle \langle S_i^z| \right] \equiv \sum_{\{S^z\}} |\{S^z\}\rangle \langle \{S^z\}|$$

- Hence:

$$Z = \sum_{\{S^z_{i,l}\}} \prod_{l=1}^{L} \left\langle \{S^z_{l+1}\} \right| e^{-\delta\tau \hat{H}_0} e^{-\delta\tau \hat{H}_1} \left| \{S^z_l\} \right\rangle$$

- $\hat{H}_0$ acts on eigenstates:

$$\left\langle \{S^z_{l+1}\} \right| e^{-\delta\tau \hat{H}_1} e^{-\delta\tau \hat{H}_0} \left| \{S^z_l\} \right\rangle =$$

$$= e^{\delta\tau J \sum_{i=1}^{N} S^z_{i+1,l} S^z_{i,l}} \left\langle \{S^z_{l+1}\} \right| e^{-\delta\tau \hat{H}_1} \left| \{S^z_l\} \right\rangle$$

- The remaining matrix element is:

$$\left\langle \{S^z_{l+1}\} \right| e^{-\delta\tau \hat{H}_1} \left| \{S^z_l\} \right\rangle = \prod_{i=1}^{N} \left\langle S^z_{i,l+1} \right| e^{\delta\tau h \hat{\sigma}^x_i} \left| S^z_{i,l} \right\rangle$$

- Now use the identity

$$\left\langle S^z_{i,l+1} \right| e^{\delta\tau h \hat{\sigma}^x_i} \left| S^z_{i,l} \right\rangle = \Lambda e^{\gamma S^z_{i,l+1} S^z_{i,l}}$$

- where:

$$\gamma = -\tfrac{1}{2} \ln\left[\tanh\left(\delta\tau h\right)\right], \qquad \Lambda^2 = \sinh\left(\delta\tau h\right) \cosh\left(\delta\tau h\right)$$

- Matrix element:

$$\left\langle \{S^z_{l+1}\} \right| e^{-\delta\tau \hat{H}_1} e^{-\delta\tau \hat{H}_0} \left| \{S^z_l\} \right\rangle =$$
$$= \Lambda^N e^{\delta\tau J \sum_{i=1}^{N} S^z_{i+1,l} S^z_{i,l} + \gamma \sum_{i=1}^{N} S^z_{i,l} S^z_{i,l+1}}$$

- Substituting leads to the

Partition function of the QIC

$$Z = \Lambda^{NL} \sum_{\{S^z_{i,l}\}} e^{\delta\tau J \sum_{i=1}^{N} \sum_{l=1}^{L} S^z_{i+1,l} S^z_{i,l} + \gamma \sum_{i=1}^{N} \sum_{l=1}^{L} S^z_{i,l} S^z_{i,l+1}}$$

Comparison with Classical 2D Model

Partition function of the QIC

$$Z = \Lambda^{NL} \sum_{\{S^z_{i,l}\}} e^{\delta\tau J \sum_{i=1}^{N} \sum_{l=1}^{L} S^z_{i+1,l} S^z_{i,l} + \gamma \sum_{i=1}^{N} \sum_{l=1}^{L} S^z_{i,l} S^z_{i,l+1}}$$

Partition function of the classical 2D Ising model

$$Z = \sum_{\{S_{i,j}\}} e^{\beta^{cl} J^x \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} S_{i+1,j} S_{i,j} + \beta^{cl} J^y \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} S_{i,j} S_{i,j+1}}$$

- Identify:

$$\delta\tau J = \beta^{cl} J^x \qquad N = N_x$$
$$\gamma = \beta^{cl} J^y \qquad L = N_y$$

Comparison with Classical 2D Model

- Classical model shows PT in the thermodynamic limit $(N_x \to \infty, N_y \to \infty)$
- Kramers-Wannier duality:

$$\sinh\left(2J^x\beta_c^{cl}\right)\sinh\left(2J^y\beta_c^{cl}\right) = 1$$

- Quantum case:

$$\sinh\left(2\delta\tau J_c\right)\sinh\left(2\gamma_c\right) = 1$$

- Remember: $\delta\tau = \frac{\beta}{L}$

$$L \stackrel{!}{\to} \infty \quad \Longrightarrow \quad \beta \to \infty = \beta_c$$

Quantum Critical Point

- Criticality condition:

$$\frac{\sinh(2\delta\tau J_c)}{\sinh(2\delta\tau h_c)} = 1$$

i.e.

$$h_c = J_c$$

- It is more conventional to set $h = gJ$ and keep J fixed:

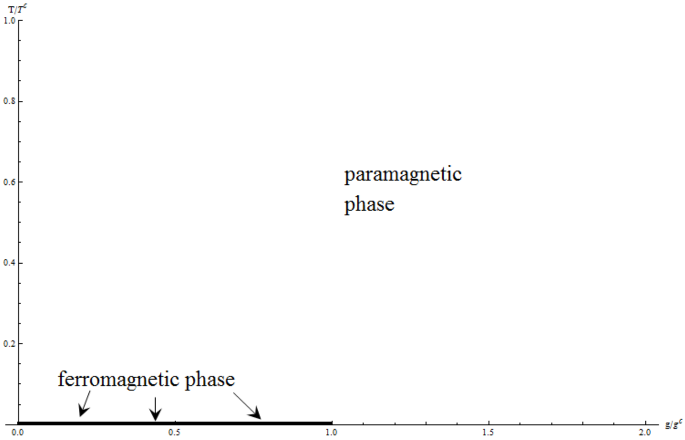
Critical point of the QIC

$$g_c = 1 \quad \text{at} \quad T_c = \frac{1}{\beta_c} = 0$$

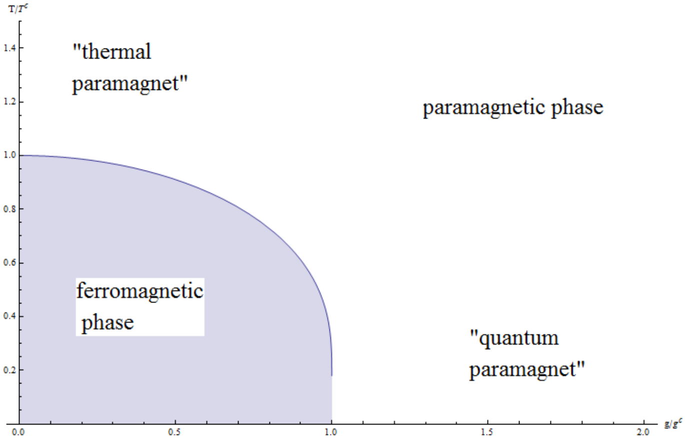
Summarizing

- Starting point: Hamiltonian with non-commuting parts $\hat{H}_0$ and $\hat{H}_1$
- Trace evaluated in product states $|\{S^z\}\rangle$
- Trotter decompositon of the density matrix
- Evaluation of the matrix elements (trivial part with $\hat{\sigma}^z$, non-trivial part with $\hat{\sigma}^x$)
- Result: partition fct. of 2D classical Ising model
- Kramers-Wannier duality $\rightarrow$ critical point
- Map $\rightarrow$ quantum critcal point

Phase Diagram of QIC



Schematic Phase Diagram of 2D Quantum Ising Model



References

- Sachdev, Subir (1999) *Quantum Phase Transitions*. Cambrigde University Press
- Batrouni C.G.. and Scalettar, R.T.. *Quantum Phase Transitions*. Oxford University Press
- Vojta, M. (2002) *Physik Journal*, 1, Nr. 3

3. Backup Slides

Operator Convergence $A_n \to A$

- Norm convergence: $A = \lim_{n\to\infty} A_n$

$$\Leftrightarrow \lim_{n\to\infty} \|A_n - A\| = 0, \quad \text{where} \quad \|A\| = \sup_{\psi\in\mathcal{D}(A)} \frac{\|A\psi\|}{\|\psi\|}$$

- Strong convergence: $A = s - \lim_{n\to\infty} A_n$

$$\Leftrightarrow \lim_{n\to\infty} \|(A_n - A)\psi\| = 0 \quad \forall\psi \in \mathcal{D}(A) \subseteq \mathcal{H}$$

Dual Operator Set

- Pauli matrices obey:

$$\left[\hat{\sigma}_i^x, \hat{\sigma}_j^y\right] = \left[\hat{\sigma}_i^y, \hat{\sigma}_j^z\right] = \left[\hat{\sigma}_i^z, \hat{\sigma}_j^x\right] = 0 \quad (i \neq j)$$

$$\{\hat{\sigma}_i^x, \hat{\sigma}_i^y\} = \{\hat{\sigma}_i^y, \hat{\sigma}_i^z\} = \{\hat{\sigma}_i^z, \hat{\sigma}_i^x\} = 0 \quad (i = j)$$

$$(\hat{\sigma}_i^x)^2 = (\hat{\sigma}_i^y)^2 = (\hat{\sigma}_i^z)^2 = 1$$

- New set of operators that obey the same algebra:

$$\hat{\tau}_i^x = \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z, \qquad \hat{\tau}_i^z = \prod_{k \leq i} \hat{\sigma}_k^x$$

- Subsitution $(\hat{\sigma}_i^x, \hat{\sigma}_i^z) \to (\hat{\tau}_i^z, \hat{\tau}_i^x)$:

$$-J \sum_{i=1}^{N} \hat{\sigma}_{i+1}^z \hat{\sigma}_i^z - h \sum_{i=1}^{N} \hat{\sigma}_i^x \to -h \sum_{i=1}^{N} \hat{\tau}_{i+1}^z \hat{\tau}_i^z - J \sum_{i=1}^{N} \hat{\tau}_i^x$$

- Self-duality for $J_c = h_c \quad (h = gJ \Rightarrow g_c = 1)$

Correlation Function

- Dynamic Correlation Function:

$$S\left(\vec{x},\vec{y},t\right)=\left\langle 0\right|\mathcal{O}^{\dagger}\left(\vec{x},0\right)\mathcal{O}\left(\vec{y},t\right)\left|0\right\rangle =$$

- Using: $\mathcal{O}\left(\vec{x},t\right)=e^{-i\hat{H}t}\mathcal{O}\left(\vec{x},0\right)e^{i\hat{H}t}$, $\sum_{m}\left|m\right\rangle\left\langle m\right|$, Fourier transforming and going to imaginary time: $t\rightarrow -i\tau$

$$S(\vec{k},\tau)=\sum_{m}e^{-(E_m-E_0)\tau}\left|\left\langle 0\right|\mathcal{O}(\vec{k},0)\left|0\right\rangle\right|^2\approx$$

$$\approx\left|\left\langle 0\right|\mathcal{O}(\vec{k},0)\left|0\right\rangle\right|^2+e^{-(E_1-E_0)\tau}\left|\left\langle 0\right|\mathcal{O}(\vec{k},0)\left|0\right\rangle\right|^2$$

- Comparison with $e^{-\tau/\xi_\tau}$ shows that time-correlation length ξ_τ diverges for vanishing ground-state energy gap

Exact Spectrum

- It can be shown:

$$H_I = \sum_k \epsilon_k \left(\gamma_k^\dagger \gamma_k - 1/2 \right)$$

$$\epsilon(k) = 2J \left(1 + g^2 - 2g\cos(k)\right)^{1/2}$$

- From this follows:

$$\epsilon(0) = 2J\,|g-1| = 2J\,|g-g_c| \Rightarrow g_c = 1$$

- Correlation length:

$$\xi_\tau \sim |g-g_c|^{-1} \sim \Delta^{-1}$$

Mean Field Analysis

- General d-dimensional Quantum Ising Hamiltonian:

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - gJ \sum_{i=1}^{N} \hat{\sigma}_i^x$$

- $\langle i, j \rangle$ ... sum over nearest neighbours
- Use Mean field approximation

$$\hat{\sigma}_i^z = m_z + \delta\hat{\sigma}_i^z, \quad \text{where} \quad m_z = \langle \hat{\sigma}_i^z \rangle = \frac{Tr\left[\hat{\sigma}_i^z e^{-\beta \hat{H}}\right]}{Tr\left[e^{-\beta \hat{H}}\right]}$$

- Mean field Hamiltonian ($\gamma = 2d$):

$$\hat{H}_{MF} = \gamma J \frac{m_z N}{2} - \gamma J \sum_{i=1}^{N} \left(m_z \hat{\sigma}_i^z + g \hat{\sigma}_i^x \right)$$

- Partition function:

$$Z_{MF} = e^{-\beta N J \gamma m_z^2/2} \left[2\cosh\left(\beta\gamma J \sqrt{m_z^2 + g^2} \right) \right]^N$$

- Landau function $\mathcal{L}_{MF} = -\frac{1}{\beta N} \ln(Z_{MF})$:

$$\mathcal{L}_{MF} = \frac{\gamma J m_z^2}{2} - \frac{1}{\beta} \ln \left[2\cosh\left(\beta\gamma J \sqrt{m_z^2 + g^2} \right) \right]$$

Self-consistency condition

$$\frac{\partial \mathcal{L}_{MF}}{\partial m_z} \overset{!}{=} 0 \quad \Rightarrow \quad \sqrt{m_z^2 + g^2} \overset{!}{=} \tanh\left(\beta\gamma J \sqrt{m_z^2 + g^2} \right)$$

- Important: trivial solution $m_z = 0$ was discarded!
- To obtain the critcal coupling, one now takes the limit $m_z \to 0$:

$$|g_c| = \tanh\left(\beta_c \gamma J \, |g_c|\right)$$

Criticality condition

$$\frac{T_c}{\gamma J} = \frac{|g_c|}{\operatorname{artanh}(|g_c|)}$$

Mean Field Quantum Phase Diagram