6 General aspects of quantum phase transitions

6.1 Classical and quantum fluctuations

Partition function (canonical ensemble):

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

Classical systems:

$$Z = \mathrm{Tr}\left[e^{-\beta T} e^{-\beta V}\right] \quad \text{with } H = T + V \ , \ [T,V]=0$$

Example: $T = \sum_i \frac{p_i^2}{2m}$ and $V = V(x_i)$

- $Z = \underbrace{\mathrm{Tr}\left[e^{-\beta T}\right]}_{\text{analytic}} \mathrm{Tr}\left[e^{-\beta V}\right]$ factorizes
- any nonanalyticity can only arise from $\mathrm{Tr}\left[e^{-\beta V}\right]$

Conclusion (classical systems):

- Statics and dynamics decouple
- Exponenents $\alpha, \beta, \gamma, \delta, \nu, \eta$ (but not z) determined by static (p-independent) piece of H ("static universality class")
- z is an independent exponent

Quantum systems:

- $[\hat{T}, \hat{V}] \neq 0 \Rightarrow e^{-\beta \hat{H}} \neq e^{-\beta \hat{T}} e^{-\beta \hat{V}}$

- Statics and dynamics coupled

- Dynamical exponent z integral part of universality class

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Quantum versus classical transitions

Correlation length and correlation time:

$$\xi \to \infty \quad \text{and} \quad \tau_c \to \infty \quad \text{at criticality}$$

Energy scale for order-parameter fluctuations:

$$\hbar \omega_c \simeq \frac{\hbar}{\tau_c} \to 0 \quad \text{at criticality}$$

Classical transition: $k_B T_c \gg \hbar \omega_c$

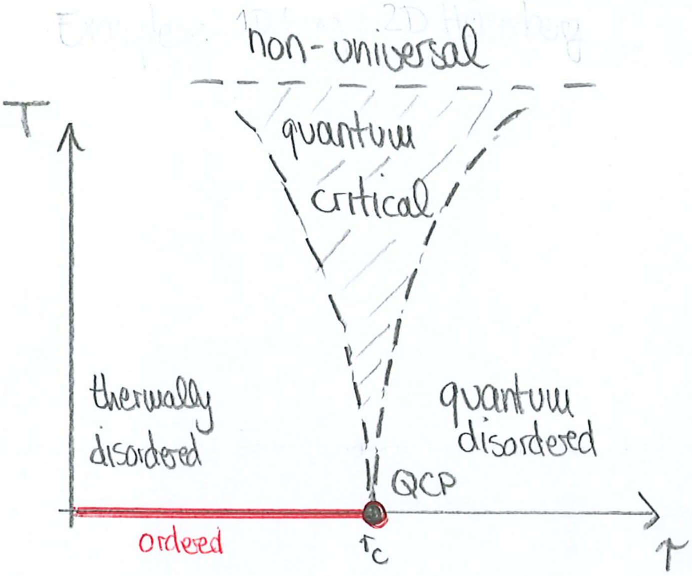
Conclusion:

- Any critical point with $T_c > 0$ is (asymptotically) classical, in the sense that long-distance fluctuations are governed by classical statistical mechanics
  [N.B.: not a statement about the physics underlying the different phases, e.g., superconductivity]

- Any critical point at $T = 0$ is "quantum", in the sense that quantum statistics is needed to describe order-parameter fluctuations
  (often QCP is an endpoint of a line of thermal critical points)

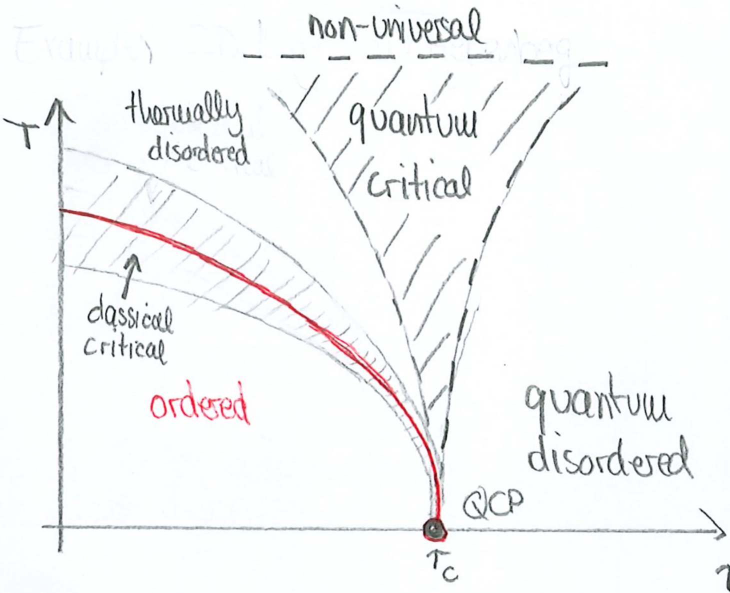
6.2 Phenomenology: Phase diagrams and crossovers

Systems w/o thermal transition



Examples: 1D Ising, 2D Heisenberg

System w/ thermal transition



Examples: 2D Ising, 3D Heisenberg

Different regimes:

(a) Quantum disordered ($r > r_c$, T small)

- well-defined quasiparticles with gap $\Delta > 0$
- density of excited quasiparticles $n \sim e^{-\frac{\Delta}{k_B T}}$

(b) Ordered ($r < r_c$, $T < T_c(r)$)

- well-defined quasiparticles
- gap $\Delta = 0$ if continuous symmetry spontaneously broken (Goldstone), but Δ can be finite if only discrete symmetry broken

(c) Classical critical ($r < r_c$, $T \approx T_c(r)$)

- classical critical power laws, fully described within classical statistics
- width vanishes for $r \nearrow r_c$ $(T \searrow 0)$

(d) thermally disordered ($r < r_c$, $T > T_c(r)$)

- thermal fluctuations destroy long-range order

(e) quantum critical ($r \approx r_c$, T small)

- no quasiparticle description possible
- gapless continuum of excitations
- unconventional thermodynamic and transport properties
- crossover scale : $k_B T_{QC} \sim \Delta \sim \frac{\hbar}{\tau_c} \sim \left(\frac{1}{\xi}\right)^z \sim |r - r_c|^{\nu z}$

(f) non-universal (T large)

- microscopic details become important
- crossover scale $k_B T_{mic} \sim J$ (relevant microscopic energy scale, can be large!)

6.3 Quantum ϕ^4 theory

Partition function:

$$Z = \int \mathcal{D}\varphi(\vec{x},\tau)\, e^{-S[\varphi]}$$

Action:

$$S = \int d^d x \int_0^\beta d\tau \left[\frac{1}{2} (\partial_\tau \varphi)^2 + \underbrace{\frac{c^2}{2}}_{\text{"velocity"}} (\partial_i \varphi)^2 + \frac{r}{2} \varphi^2 + \frac{u}{4!} \varphi^4 \right]$$

with $(\partial_i)_{i=1,..,d} = \vec{\nabla}$.

Remarks:

- The form of S follows from $\mathbb{Z}_2$ symmetry: $\varphi \to -\varphi$ and time-reversal invariance: $\tau \to -\tau$
- Higher-order terms $\propto \varphi^6$ or $\partial^2\varphi^4$, etc. are irrelevant in $d>2$.
- Dynamical exponent z: $\tau_c \propto \xi^z$ with $z=1$ due to space-time ("Lorentz") symmetry
- $T=0$ $(\beta\to\infty)$: τ enters as $z=1$ additional space dimension
- Quantum-to-classical mapping: quantum critical point in d dimensions $\hat{=}$ classical critical point in $d+z$ dimensions
- In general: z can take any value
- $T>0$ $(\beta<\infty)$: Fluctuations frozen for $\tau_c \gtrsim \beta$ $\Rightarrow \varphi(\vec{x},\tau) \simeq \varphi(\vec{x})$ and $\int_0^\beta d\tau (..) \simeq \beta (...)$ $\Rightarrow$ classical
- Quantum critical regime: $\tau_c \sim \beta$ $\Rightarrow$ thermal and quantum fluctuations equally important

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6.4 Quantum scaling hypothesis

Classical scaling hypothesis (reprise):

$$f_s(t,h) = b^{-d} f_s(t b^{y_t}, h b^{y_h}) \qquad \text{for } d < d_c^+$$

with tuning parameter t ("reduced temperature"), external source h ("magnetic field"), and rescaling factor $b > 1$.

Quantum scaling hypothesis:

$$f_s(t,h,T) = b^{-(d+z)} f_s(t b^{y_t}, h b^{y_h}, T b^{y_T})$$

where the tuning parameter t ("distance to criticality") is, e.g.,

$t = \frac{r - r_c}{r_c}$ (quantum ϕ^4 theory), $t = \frac{p - p_c}{p_c}$ (pressure-induced QCP), etc.

Scaling transformation:

$$x \longrightarrow x' = \frac{x}{b} \qquad \text{lengths}$$

$$\tau \longrightarrow \tau' = \frac{\tau}{b^z} \qquad \text{times}$$

Correlation-length exponent:

$$\boxed{\nu = \frac{1}{y_t}}$$

Dynamical critical exponent:

$$T \mapsto b^{y_T} T \qquad \text{(scaling hypothesis)}$$

$$T \sim \frac{1}{\tau} \mapsto b^{z} \frac{1}{\tau}$$

$$\Rightarrow \boxed{z = y_T}$$

Scaling relation for $b = |t|^{-\frac{1}{y_t}} = |t|^{-\nu}$:

$$f_s(t,h,T) = |t|^{\nu(d+z)} f_s\left(\pm 1, \frac{h}{|t|^{\nu y_h}}, \frac{T}{|t|^{\nu z}}\right)$$

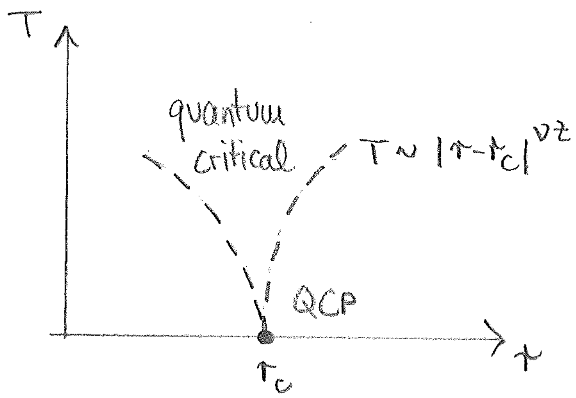
$$f_s(t,h,T) = |t|^{\nu(d+z)} F_\pm\left(\frac{h}{|t|^{\nu y_h}}, \frac{T}{|t|^{\nu z}}\right)$$

with scaling function $F_\pm(\cdot,\cdot)$.

Finite-temperature behavior:

$$\frac{T}{|t|^{\nu z}} \begin{cases} \gg 1 & \text{quantum critical regime} \\ \ll 1 & \text{stable-phase regime} \end{cases}$$

Crossover lines: $T \sim |t|^{\nu z}$



Scaling relation for $h=0$:

$$f_s(t,T) = |t|^{\nu(d+z)} F_\pm\left(0, \frac{T}{|t|^{\nu z}}\right)$$

$$= T^{\frac{d+z}{z}} \tilde{F}_\pm\left(\frac{T}{|t|^{\nu z}}\right)$$

with $\tilde{F}_\pm(x) \equiv x^{-\frac{d+z}{z}} F_\pm(0,x)$.

Quantum critical regime $\left(\frac{T}{|t|^{\nu z}} \to \infty\right)$:

$$f_s(0,T) = T^{\frac{d+z}{z}} \text{ const.}$$

Quantum critical scaling of specific heat:

$$\boxed{C_{t=0} = VT \frac{\partial^2 f_s}{\partial T^2} \propto T^{d/z}} \quad \text{for } d < d_c^+$$

Grüneisen parameter:

$$\Gamma := \frac{B}{C} \quad \text{with} \quad B := \frac{\partial S}{\partial t}$$

Example (pressure-induced QCP):

$$t = \frac{p-p_c}{p_c} \quad \text{and} \quad B = \frac{\partial S}{\partial t} \propto \left(\frac{\partial S}{\partial p}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_p \propto \alpha$$

"thermal expansion coefficient"

$$\Rightarrow \Gamma \propto \frac{\alpha}{C_p}$$

Quantum critical scaling of Γ:

- thermal expansion:

$$B \propto \frac{\partial^2 f_s}{\partial t\, \partial T} = |t|^{\nu d - 1} F_\pm^{(B)}\left(\frac{T}{|t|^{\nu z}}\right) = T^{\frac{d}{z} - \frac{1}{\nu z}} \tilde{F}_\pm^{(B)}\left(\frac{T}{|t|^{\nu z}}\right)$$

- specific heat:

$$C \propto T \frac{\partial^2 f_s}{\partial T^2} = |t|^{\nu d} F_\pm^{(C)}\left(\frac{T}{|t|^{\nu z}}\right) = T^{d/z} \tilde{F}_\pm^{(C)}\left(\frac{T}{|t|^{\nu z}}\right)$$

- Grüneisen parameter:

$$\Gamma = \frac{B}{C} = \begin{cases} G_t\, |t|^{-1} & \text{for } T=0,\ t \to 0 \\ G_T\, T^{-1/(\nu z)} & \text{for } t=0,\ T \to 0 \end{cases}$$

Conclusion:

Γ diverges at a QCP, but not at a thermal critical point (with only one tuning parameter t)

$\Rightarrow$ unique signature of quantum criticality

6.5 Quantum-to-classical mapping

Classical Ising chain

Hamiltonian:

$$H = -K \sum_{i=1}^{M} \sigma_i \sigma_{i+1} - h \sum_{i=1}^{M} \sigma_i \qquad \text{with } \sigma_i = \pm 1 , \quad \sigma_{M+1} \equiv \sigma_1 ,$$

and the dimensionless parameters $K = \frac{J}{k_B T}$ and $h = \frac{H_0}{k_B T}$.

Transfer matrix method:

$$Z = \sum_{\{\sigma_i\}} e^{-H}$$

$$= \sum_{\{\sigma_i\}} \prod_{i=1}^{M} T(\sigma_i , \sigma_{i+1})$$

with

$$T(\sigma_i , \sigma_j) = e^{K\sigma_i\sigma_j + \frac{h}{2}(\sigma_i + \sigma_j)}$$

Matrix notation:

$$T(\sigma_i , \sigma_j) \equiv \langle \sigma_i | T | \sigma_j \rangle$$

with $T = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix}$ and $|\sigma_i\rangle = |\pm\rangle \in \left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$

"transfer matrix"

Partition sum:

$$Z = \sum_{\{\sigma_i\}} \prod_{i=1}^{M} \langle \sigma_i | T | \sigma_j \rangle$$

$$= \sum_{\{\sigma_i\}} \langle \sigma_1 | T | \sigma_2 \rangle \langle \sigma_2 | T | \sigma_3 \rangle \ \dots \ \langle \sigma_M | T | \sigma_1 \rangle$$

$$= \mathrm{Tr}\left[T^M \right]$$

Diagonalization of T:

$$T = O D O^T \quad \text{with } O^T O = \mathbb{1} \text{ and } D = \begin{pmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_2 \end{pmatrix}$$

Eigenvalues:

$$\varepsilon_{1,2} = e^{K} \cosh h \pm \sqrt{e^{2K} \sinh^2 h + e^{-2K}}$$

Partition sum: $\boxed{Z = \varepsilon_1^M + \varepsilon_2^M}$

Correlation function ($h=0$):

$$\langle \sigma_i \sigma_j \rangle = \frac{1}{Z} \sum_{\{\sigma_i\}} \sigma_i \sigma_j \, e^{-H}$$

$$= \frac{1}{Z} \mathrm{Tr}\left[T^{i-1} S \, T^{j-i} S \, T^{M-j+1} \right] \quad \text{with } S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\langle \sigma_i | S | \sigma_j \rangle = \sigma_i \, \delta_{\sigma_i \sigma_j}$$

$$= \frac{\varepsilon_1^{M-j+i} \varepsilon_2^{j-i} + \varepsilon_2^{M-j+i} \varepsilon_1^{j-i}}{\varepsilon_1^M + \varepsilon_2^M}$$

Thermodynamic limit ($M \to \infty$):

$$\langle \sigma_i \sigma_j \rangle \to \left(\frac{\varepsilon_2}{\varepsilon_1}\right)^{j-i} = (\tanh K)^{j-i} \qquad (\varepsilon_1 > \varepsilon_2)$$

Scaling limit ($K \to \infty$):

$$\langle \sigma(\tau)\sigma(0) \rangle = e^{-|\tau|/\xi} \qquad \text{with } \tau = j\underset{\text{lattice spacing}}{a}, \; \sigma(\tau) \equiv \sigma_j$$

with the correlation length $\xi = \dfrac{a}{\ln \coth K} \simeq \dfrac{a}{2} e^{2K} \gg 1$

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Scaling limit and universality

Length scales:

- Large: correlation length ξ, observation scale τ, system size $L_\tau = Ma$
- Small: lattice constant a

Scaling limit: "large" length scale $\gg$ "small" length scale
("continuum limit")

Example: $a \to 0$ with ξ, τ, L_τ finite

Free energy density:

$$f = \frac{-\ln Z}{Ma} = -\frac{\ln(\varepsilon_1^M + \varepsilon_2^M)}{Ma}$$

Transfer-matrix eigenvalues:

$$\varepsilon_{1,2} \simeq \sqrt{\frac{2\xi}{a}}\left(1 \pm \frac{a}{2\xi}\sqrt{1 + 4\check{h}^2 \xi^2}\right) \quad \text{for } \frac{2\xi}{a} \simeq e^{2K} \gg 1 \text{ and } \check{h} = \frac{h}{a} \ll 1$$

Free-energy density for $a \to 0$: [use: $(1+\frac{x}{M})^M \xrightarrow{M\to\infty} e^x$] 68

$$f = \varepsilon_0 - \frac{1}{L_\tau} \ln\left[2\cosh\left(L_\tau \sqrt{\frac{1}{(4\xi)^2} + \tilde{h}^2}\right)\right]$$

with $\varepsilon_0 = -\frac{K}{a}$ the ground-state energy for $T \to 0$ and $\tilde{h} = 0$

Correlation function ($\tilde{h}=0$):

$$\langle \sigma(\tau)\sigma(0)\rangle = \frac{e^{-|\tau|/\xi} + e^{-(L_\tau - |\tau|)/\xi}}{1 + e^{-L_\tau/\xi}}$$

Thermodynamic limit ($L_\tau \gg \xi$):

$$\langle \sigma(\tau)\sigma(0)\rangle = e^{-|\tau|/\xi} \quad \text{as before}$$

Universality (free-energy density):

$$f = \varepsilon_0 + \frac{1}{L_\tau} \Phi_f\left(\frac{L_\tau}{\xi}, \tilde{h} L_\tau\right)$$

with <u>universal</u> scaling function

$$\Phi_f(x,y) = -\ln\left[2\cosh\left(\sqrt{\left(\frac{x}{2}\right)^2 + y^2}\right)\right]$$

valid for all 1D systems with Z_2 symmetry in the scaling limit!

Similarly:

$$\langle \sigma(\tau)\sigma(0)\rangle = \Phi_\sigma\left(\frac{\tau}{L_\tau}, \frac{L_\tau}{\xi}, \tilde{h} L_\tau\right)$$

Mapping to a quantum spin

Scaling limit (transfer matrix):

$$T = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix}$$

$$= e^{K+h}\left(\frac{\mathbb{1}+\sigma^z}{2}\right) + e^{K-h}\left(\frac{\mathbb{1}-\sigma^z}{2}\right) + e^{-K}\sigma^x \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},\ \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= e^{K}\Big(\mathbb{1}_2 + \underbrace{h}_{=a\tilde{h}}\sigma^z + \underbrace{e^{-2K}}_{\simeq \frac{a}{2\xi}}\sigma^x\Big) + O(h^2) \qquad \text{for } a\to 0$$

$$= e^{\overset{-\varepsilon_0 a}{\downarrow}{K}} \cdot e^{a\tilde{h}\sigma^z + \frac{a}{2\xi}\sigma^x} + O(h^2, a^2)$$

$$= e^{-a\left(+\varepsilon_0 - \frac{1}{2\xi}\sigma^x - \tilde{h}\sigma^z\right)} + O(h^2, a^2)$$

$$\equiv e^{-a\hat{H}_Q}$$

with "Hamilton operator":

$$\hat{H}_Q = \varepsilon_0 - \frac{\Delta}{2}\sigma^x - \tilde{h}\sigma^z \quad \text{and} \quad \Delta = \frac{1}{\xi}$$

Partition function:

$$Z = \mathrm{Tr}\left[T^M\right] = \mathrm{Tr}\left[e^{-\hat{H}_Q/T}\right] \quad \text{with } T = \frac{1}{L_\tau} = \frac{1}{Ma}.$$

Z represents the partition function of a single quantum spin $\frac{1}{2}$ in two perpendicular fields $\tilde{h}$, $\frac{\Delta}{2}$ at a "quantum temperature" $T = 1/L_\tau$.

Free energy:

$$F = E_0 - T \ln\left[2\cosh\left(\frac{1}{T}\sqrt{\frac{\Delta^2}{4}+\tilde{h}^2}\right)\right]$$

$\hat{=}$ energy of quantum spin $\frac{1}{2}$ in external field $|\vec{H}_0| = \sqrt{\frac{\Delta^2}{2}+\tilde{h}^2}$.

Conclusion:

Quantum system at temperature T $\hat{=}$ classical system of finite length $L_\tau = \frac{1}{T}$

Quantum-to-classical correspondence:

classical spin chain (1D)	quantum spin (0D)
system size L_τ	inverse temperature $1/T$
correlation length ξ	inverse excitation gap $1/\Delta$

Remark:

Classical: temperature can always be absorbed in rescaling of couplings
Quantum: temperature enters as independent parameter

Mapping: XY chain ⟷ O(2) quantum rotor

Classical XY chain:

$$H_{cl} = -K\sum_{i=1}^{M} \vec{n}_i \cdot \vec{n}_{i+1} - \sum_{i=1}^{M} \vec{h}\cdot\vec{n}_i$$

with $\vec{n}_i = (n_i^x, n_i^y) \in S^1$, i.e., $\vec{n}_i^2 = 1$ for all $i = 1,\dots,M$.

Equivalent quantum system ($\vec{h} \parallel \vec{e}_x$):

$$\hat{H}_Q = -\Delta \frac{\partial^2}{\partial\theta^2} - \tilde{h}\cos\theta \qquad \text{"O(2) quantum rotor"}$$

where $\vec{n}_i \mapsto \vec{n}(\tau) = (\cos\theta(\tau), \sin\theta(\tau))$ with $\tau = ia$, $\tilde{h} = \frac{h}{a}$
and $\Delta = 1/\xi$ ("energy gap") as before.

Mapping: Heisenberg chain ⟷ O(3) quantum rotor

Classical Heisenberg chain:

$$H_{cl} = -K\sum_{i=1}^{M} \vec{n}_i \cdot \vec{n}_{i+1} - \sum_{i=1}^{M} \vec{h}\cdot\vec{n}_i$$

with "classical spins" $\vec{n}_i = (n_i^x, n_i^y, n_i^z) \in S^2$.
Equivalent quantum system:

$$\hat{H}_Q = -\frac{\Delta}{2}\hat{\vec{L}}^2 - \tilde{\vec{h}}\cdot\vec{n}$$

with angular momentum operator $\hat{\vec{L}}$.

Remarks:

- Classical <u>spin</u> maps to O(3) quantum <u>rotor</u>, not to quantum <u>spin</u>
- quantum spins have nontrivial dynamics ("Berry-phase terms") without classical analog

Quantum-to-classical correspondence: Rules and exceptions

General rule:

$$\boxed{\text{QCP in } d \text{ dimensions} \;\hat{=}\; \text{TCP in } d+z \text{ dimension}}$$

Remarks:

- Correspondence applies in scaling limit, i.e., $T \to 0$ for QCP
- Real-time dynamics at $T=0$: $Z = \int D\phi \, e^{iS[\phi]} \leftrightarrow \int D\phi \, e^{-S[\phi]}$

  by "Wick rotation" $\tau \to it$ (analytic continuation)

  $\Rightarrow$ typically not easily obtained

Exceptions to quantum-to-classical correspondence:

- Systems with quenched disorder (disorder frozen in imaginary time)
- Systems with quantum or Berry-phase dynamics, e.g., single quantum particle

$$S = \int d\tau \left[\underbrace{\phi \, \partial_\tau \phi}_{\text{"Berry-phase term"}} - \varepsilon_\alpha \phi^2 \right]$$

- Quantum phase transitions in metallic or semimetallic systems (fermionic low-energy excitations)

- Topological phase transition (no local order parameter)

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