

6 Quantum phase transitions: Primes

6.1 Classical and quantum fluctuations

Partition function (canonical ensemble).

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

Classical systems:

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

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

• $Z = \underbrace{\text{Tr} [e^{-\beta T}]}_{\text{analytic}} \text{Tr} [e^{-\beta V}]$ factorizes

• any nonanalyticity can only arise from $\text{Tr} [e^{-\beta V}]$

Conclusion (classical systems):

- Statics and dynamics decouple
- Exponents $\alpha, \beta, \nu, \delta, \nu, \gamma$ (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:

$$\xi \rightarrow \infty \text{ and } \tau_c \rightarrow \infty \text{ at criticality}$$

Energy scale for order-parameter fluctuations:

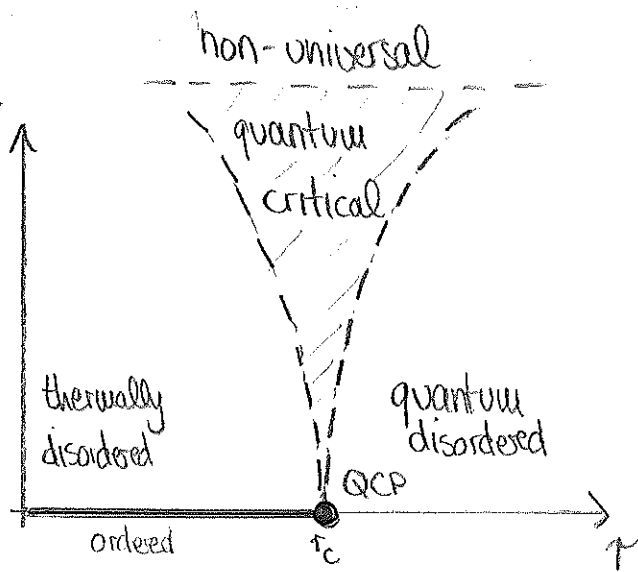
$$\hbar \omega_c \sim \frac{1}{\tau_c} \rightarrow 0 \text{ at criticality}$$

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

Conclusion:

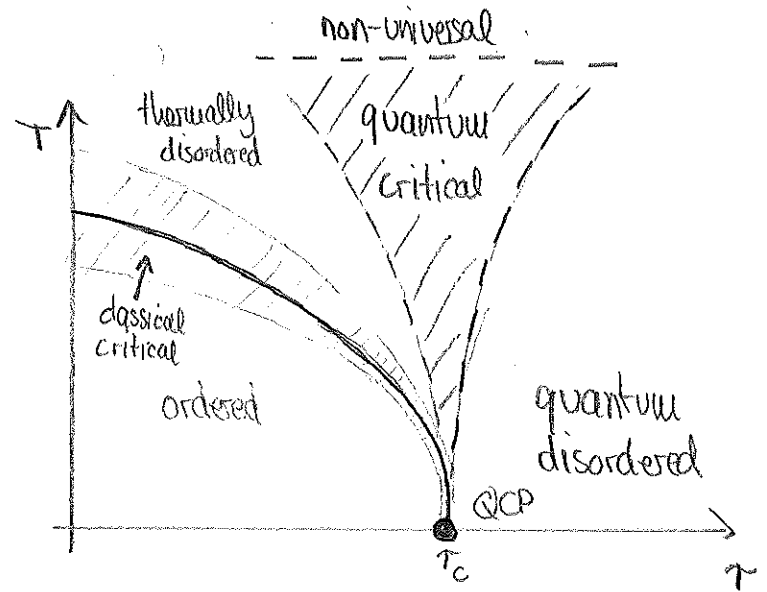
- Any critical point with $T_c > 0$ is (asymptotically) classical, in the sense that long-distance fluctuations are governed by classical statistical mechanics
[N.B.: not a statement about the physics underlying the different phases, e.g., superconductivity]
- Any critical point at $T = 0$ is "quantum",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

Systems w/o thermal transition



Examples: 1D Ising, 2D Heisenberg

System w/ thermal transition



Examples: 2D Ising, 3D Heisenberg

Different regimes:

(a) Quantum disordered ($\tau > \tau_c, T \text{ small}$)

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

(b) Ordered ($\tau < \tau_c, T < T_c(\tau)$)

- 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 ($\tau < \tau_c, T \approx T_c(\tau)$)

- classical critical power laws, fully described within classical statistics
- width vanishes for $\tau \rightarrow \tau_c (T \rightarrow 0)$

d) thermally disordered ($\tau < \tau_c, T > T_c(\tau)$)

- thermal fluctuations destroy long-range order

e) quantum critical ($\tau \approx \tau_c, T \text{ small}$)

- no quasiparticle description possible
- gapless continuum of excitations
- unconventional thermodynamic and transport properties
- crossover scale: $k_B T_{qc} \sim \Delta \sim \frac{\hbar}{\tau_c} \sim \left(\frac{1}{\xi}\right)^2 \sim |\tau - \tau_c|^{Dz}$

f) non-universal ($T \text{ large}$)

- 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:

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

Action:

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

↑
"velocity"

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

Remarks:

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- The form of S follows from \mathbb{Z}_2 symmetry: $\varphi \rightarrow -\varphi$ and time-reversal invariance: $\tau \rightarrow -\tau$
- 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
- $T=0$ ($\beta \rightarrow \infty$): 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 $\tau_c \gtrsim \beta \Rightarrow \varphi(\vec{x}, \tau) \cong \varphi(\vec{x})$
and $\int_0^\beta d\tau (\dots) \cong \beta (\dots) \Rightarrow$ classical
- Quantum critical regime: $\tau_c \sim \beta \Rightarrow$ thermal and quantum fluctuations equally important

6.4 Quantum scaling hypothesis

Classical scaling hypothesis (reprise):

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

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.,

$$t = \frac{T - T_c}{T_c} \quad (\text{quantum } \phi^4 \text{ theory}), \quad t = \frac{P - P_c}{P_c} \quad (\text{pressure-induced QCP}), \text{ etc.}$$

Scaling transformation:

$x \rightarrow b x$	lengths
$\tau \rightarrow b^z \tau$	times
$t \rightarrow b^{y_t} t$	tuning parameter
$h \rightarrow b^{y_h} h$	external source

Correlation-length exponent:

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

Dynamical critical exponent:

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

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

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

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

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

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

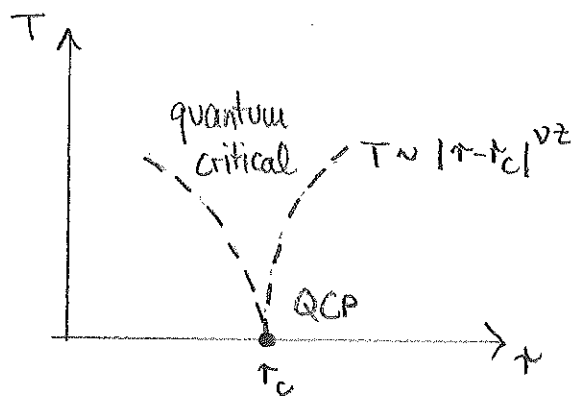
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with scaling function $F_{\pm}(\cdot, \cdot)$.

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 $h=0$:

$$f_S(t, T) = |t|^{v(d+z)} F_{\pm}(0, \frac{T}{|t|^{vz}})$$

$$= T^{\frac{d+z}{z}} \underline{\underline{F_{\pm}(\frac{T}{|t|^{vz}})}}$$

with $\underline{\underline{F_{\pm}(x) = x^{-\frac{d+z}{z}} F_{\pm}(0, x)}}$.

Quantum critical regime ($\frac{T}{|t|^{vz}} \rightarrow \infty$):

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

Quantum critical scaling of specific heat:

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

Grüneisen parameter:

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

Example (pressure-induced QCP):

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

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

"thermal expansion coefficient"

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:

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

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:

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

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:

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

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

"transfer matrix"

Partition sum:

$$\begin{aligned} Z &= \sum_{\{\sigma_i\}} \prod_{i=1}^M \langle \sigma_i | T | \sigma_j \rangle \\ &= \sum_{\{\sigma_i\}} \langle \sigma_1 | T | \sigma_2 \rangle \langle \sigma_2 | T | \sigma_3 \rangle \dots \langle \sigma_M | T | \sigma_1 \rangle \\ &= \text{Tr} [T^M] \end{aligned}$$

Diagonalization of T :

$$T = O D O^T \quad \text{with } O^T O = \mathbb{1} \quad \text{and } D = \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix}$$

Eigenvalues:

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

Partition sum:

$$Z = \epsilon_1^M + \epsilon_2^M$$

Correlation:

Correlation function ($h=0$):

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

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

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

$$= \frac{\epsilon_1^{M-j+i} \epsilon_2^{j-i} + \epsilon_2^{M-j+i} \epsilon_1^{j-i}}{\epsilon_1^M + \epsilon_2^M}$$

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

$$\langle \sigma_i \sigma_j \rangle \rightarrow \left(\frac{\epsilon_2}{\epsilon_1} \right)^{|j-i|} = (\tanh K)^{|j-i|} \quad (\epsilon_1 > \epsilon_2)$$

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

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

$$\text{with the correlation length } \xi = \frac{a}{\ln \coth K} \approx \frac{a}{2} e^{2K} \gg 1$$

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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: $a \rightarrow 0$ with ξ, τ, L_τ finite

Free energy density:

$$f = \frac{-\ln Z}{Ma} = - \frac{\ln(\epsilon_1^M + \epsilon_2^M)}{Ma}$$

Transfer-matrix eigenvalues:

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

Free-energy density for $a \rightarrow 0$:

$$f = \epsilon_0 - \frac{1}{L_\tau} \ln \left[2 \cosh \left(L_\tau \sqrt{\left(\frac{1}{4\xi}\right)^2 + \tilde{h}^2} \right) \right]$$

with $\epsilon_0 = -\frac{k}{a}$ the ground-state energy for $T \rightarrow 0$ 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):

$$f = \epsilon_0 + \frac{1}{L_\tau} \Phi_f \left(\frac{L_\tau}{\xi}, \tilde{h} L_\tau \right)$$

with universal 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):

$$\begin{aligned}
T &= \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix} \\
&= e^{K+h} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + e^{K-h} \begin{pmatrix} 1 & -v^2 \\ 0 & 1 \end{pmatrix} + e^{-K} \sigma^x \\
&= e^K \left(\mathbb{1}_2 + \underbrace{h}_{=a\tilde{h}} v^2 + \underbrace{e^{-2K}}_{\approx \frac{a}{2\tilde{\epsilon}}} \sigma^x \right) + O(h^2) \\
&= e^{-\epsilon_0 a} \cdot e^{a\tilde{h} v^2 + \frac{a}{2\tilde{\epsilon}} \sigma^x} + O(h^2, a^2) \\
&= e^{-a \left(+\epsilon_0 - \frac{1}{2\tilde{\epsilon}} \sigma^x - \tilde{h} v^2 \right)} + O(h^2, a^2) \\
&\equiv e^{-a \hat{H}_Q}
\end{aligned}$$

with "Hamilton operator":

$$\hat{H}_Q = \epsilon_0 - \frac{\Delta}{2} \sigma^x - \tilde{h} v^2 \quad \text{and} \quad \Delta = \frac{1}{\tilde{\epsilon}}$$

Partition function:

$$Z = \text{Tr} [T^M] = \text{Tr} [e^{-\hat{H}_Q / T}] \quad \text{with} \quad T = \frac{1}{L_T} = \frac{1}{M a}.$$

Z represents the partition function of a single (1D) quantum spin $\frac{1}{2}$ in two perpendicular field \vec{h} , $\frac{\Delta}{2}$ at a "quantum temperature" $T = \frac{1}{L_T}$.

Free-energy:

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

$\hat{=}$ energy of quantum spin $\frac{1}{2}$ in external field $|\vec{H}_0| = \sqrt{\frac{\Delta^2}{4} + \vec{h}^2}$.

Conclusion:

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

Quantum-to-classical correspondence:

classical spin chain (1D)	quantum spin (0D)
system size L_T	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:

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

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

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

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

Mapping: Heisenberg chain ↔ O(3) quantum rotor

Classical Heisenberg chain:

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

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

Equivalent quantum system:

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

with angular momentum operator \hat{L} .

Remarks:

- Classical spin maps to $O(3)$ quantum rotor, not to quantum spin
- quantum spins have nontrivial dynamics ("Berry-phase term") 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., $T \rightarrow 0$ for QCP
- Real-time dynamics at $T=0$: $Z = \int \mathcal{D}\phi e^{iS[\phi]} \leftrightarrow \int \mathcal{D}\phi e^{-S[\phi]}$
by "Wick rotation" $\tau \rightarrow i\tau$ (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

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

- Quantum phase transitions in metallic or semimetallic systems (fermionic low-energy excitations)
- Topological phase transition (no local order parameter)

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