

Statistical Mechanics

E0415

Fall 2020, lecture 8
Quantum phase transitions

... take home...

- "I have chosen *Brain Entropy Mapping Using fMRI*, for I am working in a Finnish medical imaging company (although mostly on CT) so the topic generally fits my interest."
- "This was a tough choice, I thought both of them were super interesting, but I ended up choosing the Brain entropy article. I have always been intrigued by brain research and how our brains work in general, so finding out that our brains have their own entropy and just examining brains from the point of view of statistical mechanics settled my choice."

.... On the papers

"In the study, they mapped the brain entropy of 1049 subjects and computed the entropy for their brains based on the fMRI. To reduce the noise in the imaging, they also computed the entropy for a water phantom to serve as a base line. In the study they identified eight clusters in the brain, where one was assumed to be a peripheral boundary. These clusters corresponded to the prior knowledge of the brain's regions. Furthermore, the study suggests that the brain entropy could serve as a well-quantifiable measure of the brain activity and help to detect abnormalities in the brain. The living-organisms are presumed to have lower entropy in comparison to the non-living matter, which could be used as a tool in the search of extra-terrestrial life. "

"The paper is about computing the different entropy contributions, vibrational and configurational entropies, of two metallic glasses. The authors do this computationally with a molecular dynamics simulation, and the results show that most of the entropy of the glass is vibrational, corresponding to the regular dynamical degrees of freedom of the glass, while some of it is configurational, related to the different (non-crystal) configurations the glass could assume when quickly cooled from the liquid phase. The authors find that their results match experiments pretty closely. Furthermore, the configurational entropy of one of the glasses, one with aluminum added to copper and zirconium, is significantly higher than the one without aluminum. They attribute this as one of the reasons why this alloy has a higher glass-forming ability, as there are more possible configurations for the glass to set to near the transition point."

Outline of lecture

- 1) Idea of a QPT
- 2) Quantum Transverse Ising model
- 3) Phase diagrams
- 4) Scaling hypothesis: classical vs. quantum
- 5) Classical-quantum mapping
- 6) Quantum annealing
- 7) Kibble-Zurek mechanism

Quantum Ising

transverse-field quantum Ising model:

$\langle ij \rangle$: nearest neighbours

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - Jg \sum_i \hat{\sigma}_i^x$$

- each site i has spin- $\frac{1}{2}$ d.o.f.
- $\hat{\sigma}_i^\mu$: operators obeying $[\hat{\sigma}_i^\mu, \hat{\sigma}_j^\nu] = -2i\epsilon_{\mu\nu\rho} \hat{\sigma}_i^\rho \delta_{ij}$ $s, s' \in \{+1, -1\}$
- in $\hat{\sigma}^z$ basis, $|\uparrow\rangle_i, |\downarrow\rangle_i$, $\hat{\sigma}_i^\mu |s\rangle_i = (\boldsymbol{\sigma}^\mu)_{ss'} |s'\rangle_i$ $\boldsymbol{\sigma}^\mu$: Pauli matrix

$$\begin{aligned} \hat{\sigma}_i^z |\uparrow\rangle_i &= +|\uparrow\rangle_i & \hat{\sigma}_i^z |\downarrow\rangle_i &= -|\downarrow\rangle_i \\ \hat{\sigma}_i^x |\uparrow\rangle_i &= |\downarrow\rangle_i & \hat{\sigma}_i^x |\downarrow\rangle_i &= |\uparrow\rangle_i \end{aligned}$$

Quantum Ising model has symmetry under spin-flip operator $U = \prod_i \hat{\sigma}_i^x$

i.e., $[\mathcal{H}, U] = 0$

$$\hat{\sigma}_i^z \xrightarrow{U} U \hat{\sigma}_i^z U^{-1} = -\hat{\sigma}_i^z$$

$$\hat{\sigma}_i^z \hat{\sigma}_j^z \xrightarrow{U} \hat{\sigma}_i^z \hat{\sigma}_j^z$$

$$\hat{\sigma}_i^x \xrightarrow{U} \hat{\sigma}_i^x$$

Paramagnet

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - Jg \sum_i \hat{\sigma}_i^x$$

$$\left. \begin{array}{l} \hat{\sigma}_i^x |\uparrow\rangle_i = |\downarrow\rangle_i \\ \hat{\sigma}_i^x |\downarrow\rangle_i = |\uparrow\rangle_i \end{array} \right\} \hat{\sigma}_i^x |\rightarrow\rangle_i = +|\rightarrow\rangle_i \text{ where } |\rightarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$$

For $g \rightarrow +\infty$, $|\text{g.s.}\rangle = \prod_i |\rightarrow\rangle_i$

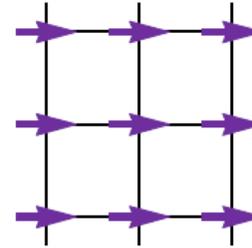
spins align with applied field: “quantum paramagnet”

g.s. is symmetric under spin flip: $U|\text{g.s.}\rangle = |\text{g.s.}\rangle$

$$\langle \text{g.s.} | \hat{\sigma}_i^z | \text{g.s.} \rangle = 0$$

$$U = \prod_i \hat{\sigma}_i^x$$

product state, so no correlations: $\langle \text{g.s.} | \hat{\sigma}_i^z \hat{\sigma}_j^z | \text{g.s.} \rangle = \delta_{ij}$



For large finite g , $|\text{g.s.}\rangle = \prod_i |\rightarrow\rangle_i + \text{perturbative corrections in } 1/g$

correlations $\langle \text{g.s.} | \hat{\sigma}_i^z \hat{\sigma}_j^z | \text{g.s.} \rangle \sim e^{-|x_i - x_j|/\xi}$ with $\xi \rightarrow 0$ for $g \rightarrow \infty$

“kinetic energy (i.e., off-diagonal term) wins”

(“kinetic” / “potential” depends on choice of basis)

Ferromagnet

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - Jg \sum_i \hat{\sigma}_i^x$$

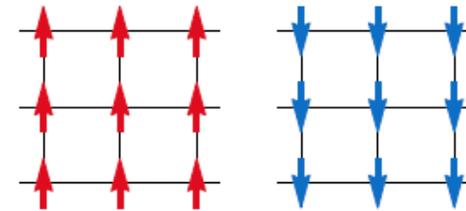
For $g = 0$, two degenerate ground states: $|\uparrow\rangle = \prod_i |\uparrow\rangle_i$ and $|\downarrow\rangle = \prod_i |\downarrow\rangle_i$

spins align with each other: ferromagnet

both states break spin-flip symmetry ($U|\uparrow\rangle = |\downarrow\rangle$)

$$\langle \text{g.s.} | \hat{\sigma}_i^z | \text{g.s.} \rangle = 1$$

$$\text{product state: } \langle \text{g.s.} | \hat{\sigma}_i^z \hat{\sigma}_j^z | \text{g.s.} \rangle = \langle \text{g.s.} | \hat{\sigma}_i^z | \text{g.s.} \rangle \langle \text{g.s.} | \hat{\sigma}_j^z | \text{g.s.} \rangle = 1$$



For $g = 0^+$, superpositions $|\uparrow\rangle \pm |\downarrow\rangle$ are e'states, but splitting $\rightarrow 0$ as $N \rightarrow \infty$

$N = \infty$: macroscopic superpos'ns unstable; take $|\uparrow\rangle$, $|\downarrow\rangle$ as degenerate g.s.

for small g and $N = \infty$, $|\text{g.s.}_+\rangle = \prod_i |\uparrow\rangle_i + \text{perturbative corrections in } g$

$|\text{g.s.}_-\rangle = \prod_i |\downarrow\rangle_i + \text{perturbative corrections in } g$

“potential energy (i.e., diagonal term) wins”

Partititon function

at temperature $T = 1/\beta$, partition function

$$\begin{aligned}
 Z &= \text{Tr} e^{-\beta\mathcal{H}} \\
 &= \sum_{\mathbf{s}} \langle \mathbf{s} | e^{-\beta\mathcal{H}} | \mathbf{s} \rangle
 \end{aligned}$$

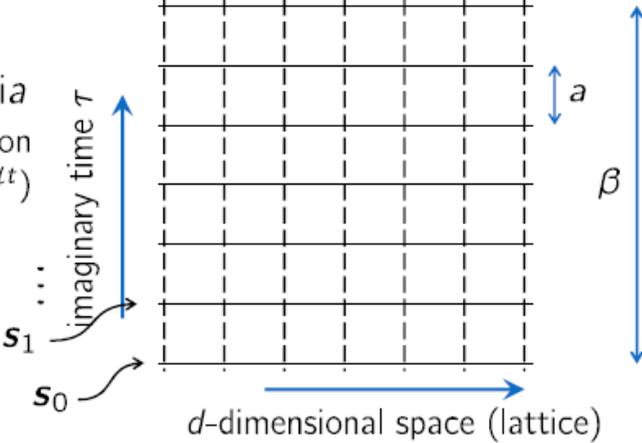
for any (orthonormal) basis $\{|\mathbf{s}\rangle\}$

split operator $e^{-\beta\mathcal{H}}$ into M pieces $e^{-a\mathcal{H}}$ with $Ma = \beta$:

$$\begin{aligned}
 Z &= \sum_{\mathbf{s}_0} \langle \mathbf{s}_0 | \underbrace{e^{-a\mathcal{H}} e^{-a\mathcal{H}} \dots e^{-a\mathcal{H}}}_M | \mathbf{s}_0 \rangle && \sum_{\mathbf{s}} |\mathbf{s}\rangle \langle \mathbf{s}| = 1 \\
 &= \sum_{\mathbf{s}_0, \mathbf{s}_1, \dots, \mathbf{s}_{M-1}} \langle \mathbf{s}_0 | e^{-a\mathcal{H}} | \mathbf{s}_1 \rangle \langle \mathbf{s}_1 | e^{-a\mathcal{H}} | \mathbf{s}_2 \rangle \dots \langle \mathbf{s}_{M-1} | e^{-a\mathcal{H}} | \mathbf{s}_0 \rangle
 \end{aligned}$$

$e^{-a\mathcal{H}}$: evolution by "imaginary time" $t = -ia$
 (real-time evolution operator $e^{-i\mathcal{H}t}$)

$\sum_{\mathbf{s}_0, \mathbf{s}_1, \dots, \mathbf{s}_{M-1}}$: sum over trajectories
 "path integral" representation of Z



Quantum model to classical mapping

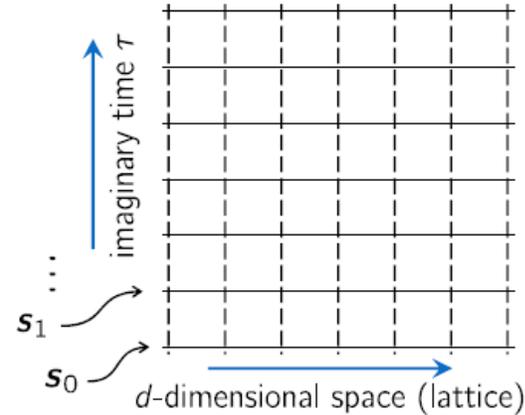
$$Z = \sum_{s_0, s_1, \dots, s_{M-1}} \langle s_0 | e^{-a\mathcal{H}} | s_1 \rangle \langle s_1 | e^{-a\mathcal{H}} | s_2 \rangle \langle s_2 | \dots | s_{M-1} \rangle \langle s_{M-1} | e^{-a\mathcal{H}} | s_0 \rangle$$

choose basis states $|s\rangle$ corresponding to classical configurations \mathbf{s}

define $\mathcal{E}(\mathbf{s}, \mathbf{s}') = -\log \langle \mathbf{s} | e^{-a\mathcal{H}} | \mathbf{s}' \rangle = [\mathcal{E}(\mathbf{s}', \mathbf{s})]^*$

$$Z = \sum_{s_0, s_1, \dots, s_{M-1}} e^{-\sum_{i=0}^{M-1} \mathcal{E}(s_i, s_{i+1})}$$

where $s_M \equiv s_0$ (periodicity in τ)



cf. classical statistical system with reduced Hamiltonian E_{cl} on $(d+1)$ -dimensional lattice (with p.b.c.)

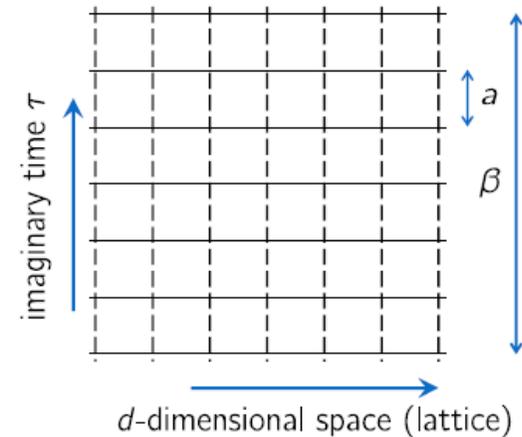
$$E_{cl} = \sum_i [E_1(\mathbf{s}_i) + E_2(\mathbf{s}_i, \mathbf{s}_{i+1})] \quad \begin{array}{l} E_1: \text{layer configuration energy} \\ E_2: \text{interaction between adjacent layers} \end{array}$$

$$= \sum_i \left\{ \frac{1}{2} [E_1(\mathbf{s}_i) + E_1(\mathbf{s}_{i+1})] + E_2(\mathbf{s}_i, \mathbf{s}_{i+1}) \right\} = \sum_{i=0}^{M-1} E(\mathbf{s}_i, \mathbf{s}_{i+1})$$

if $\mathcal{E}(\mathbf{s}, \mathbf{s}')$ is real, interpret Z as partition f'n for classical $(d+1)$ -dimensional system

Summary

quantum	classical
imaginary time τ	extra spatial dimension τ
inverse temperature $\beta = \frac{1}{T}$	system size L_τ in τ direction
imaginary-time evolution $e^{-a\mathcal{H}}$	Boltzmann weight (transfer matrix) $e^{-\mathcal{E}(s,s')} = \langle s e^{-a\mathcal{H}} s' \rangle$
sum over trajectories ("path integral")	sum over configurations (canonical ensemble)
quantum critical phenomena at $T = 0$ in d dimensions	classical critical phenomena in $d + 1$ dimensions



- at zero temperature, $\beta = 1/T = \infty$: imaginary-time direction is infinite
- n.b., distinct from relationship between classical stochastic dynamics (in d dimensions) and quantum mechanics (in d dimensions)

Ising again

transverse-field quantum Ising model: $\mathcal{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - Jg \sum_i \hat{\sigma}_i^x$

define $\mathcal{E}(\mathbf{s}, \mathbf{s}') = -\log \langle \mathbf{s} | e^{-a\mathcal{H}} | \mathbf{s}' \rangle$ use $\hat{\sigma}_i^z$ basis, $|\uparrow\rangle_i, |\downarrow\rangle_i$:
 $Z = \sum_{s_0, s_1, \dots, s_{M-1}} e^{-\sum_{i=0}^{M-1} \mathcal{E}(s_i, s_{i+1})}$ $|\mathbf{s}\rangle = |\{s_1, s_2, \dots, s_N\}\rangle = \prod_i^N |s_i\rangle_i$

for sufficiently small a , use $e^{a(A+B)} = e^{aA}e^{aB}[1 + \mathcal{O}(a)]$

$$\begin{aligned} \langle \mathbf{s} | e^{-a\mathcal{H}} | \mathbf{s}' \rangle &\approx \langle \mathbf{s} | e^{aJg \sum_i \hat{\sigma}_i^x} e^{aJ \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z} | \mathbf{s}' \rangle \\ &= \langle \mathbf{s} | e^{aJg \sum_i \hat{\sigma}_i^x} | \mathbf{s}' \rangle e^{aJ \sum_{\langle ij \rangle} s'_i s'_j} & \langle s | e^{\alpha \hat{\sigma}^x} | s' \rangle &= A(\alpha) e^{B(\alpha) s s'} \\ &= e^{aJ \sum_{\langle ij \rangle} s'_i s'_j} \prod_i \langle s_i | e^{aJg \hat{\sigma}_i^x} | s'_i \rangle & B(\alpha) &= -\frac{1}{2} \log \tanh \alpha \\ &= [A(aJg)]^N e^{aJ \sum_{\langle ij \rangle} s'_i s'_j + B(aJg) \sum_i s_i s'_i} \end{aligned}$$

$$\mathcal{E}(\mathbf{s}, \mathbf{s}') = -aJ \sum_{\langle ij \rangle} s'_i s'_j - B(aJg) \sum_i s_i s'_i + \text{const}$$

Ising II

transverse-field quantum Ising model: $\mathcal{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - Jg \sum_i \hat{\sigma}_i^x$

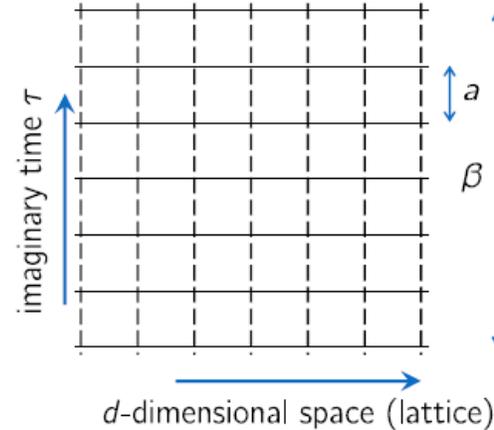
$$Z = \sum_{s_0, s_1, \dots, s_{M-1}} e^{-\sum_{i=0}^{M-1} \mathcal{E}(s_i, s_{i+1})}$$

For $a \rightarrow 0$, $B(\alpha) = -\frac{1}{2} \log \tanh \alpha$

$$\mathcal{E}(s, s') = -aJ \sum_{\langle ij \rangle} s'_i s'_j - B(aJg) \sum_i s_i s'_i$$

layer configuration energy

interaction between adjacent layers



- Transverse-field Ising model in d dimensions maps to highly anisotropic ($a \rightarrow 0$) classical Ising model in $d + 1$ dimensions
- By universality, quantum Ising model has identical critical properties to isotropic classical Ising model in $d + 1$ dimensions

Ising chain

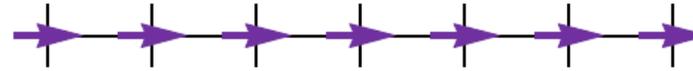
transverse-field quantum Ising model in 1D:

$$\mathcal{H} = -J \sum_i [\hat{\sigma}_i^z \hat{\sigma}_{i+1}^z + g \hat{\sigma}_i^x]$$

(related to 2D classical Ising model, so ordering transition at g_c)

for $g = \infty$, $|\text{g.s.}\rangle = \prod_i |\rightarrow\rangle_i$

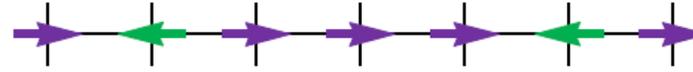
excited states have
flipped spins



for large g , use perturbation
theory, with $\delta\mathcal{H} = \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z$



$\delta\mathcal{H}$ creates flipped spins in pairs &
hops them between sites



$$|\rightarrow\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle)$$

$$\hat{\sigma}^z |\rightarrow\rangle = |\leftarrow\rangle$$

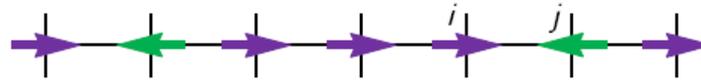
$$|\leftarrow\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle - |\downarrow\rangle)$$

$$\hat{\sigma}^z |\leftarrow\rangle = |\rightarrow\rangle$$

so treat flipped spins as particles

Use a transformation....

Treat flipped spins as particles



either:

- as bosons—but then need interactions to forbid two flipped spins on one site

$\hat{\sigma}_i^x = 1 - 2n_i$	$n_i = 0$
$\hat{\sigma}_i^z = b_i + b_i^\dagger$	$n_j = 1$
- as fermions—double occupation automatically forbidden, *but* fermion operators anticommute on different sites:

$$\begin{aligned} \{c_i, c_j^\dagger\} &= \delta_{ij} & [\hat{\sigma}_i^\mu, \hat{\sigma}_j^\nu] &= -2i\epsilon_{\mu\nu\rho}\hat{\sigma}_i^\rho\delta_{ij} \\ \{c_i, c_j\} &= \{c_i^\dagger, c_j^\dagger\} = \delta_{ij} \end{aligned}$$

Jordan–Wigner transformation (in 1D): add a string of minus signs

$$\begin{aligned} \hat{\sigma}_i^x &= 1 - 2n_i & n_j &= c_j^\dagger c_j \\ \hat{\sigma}_i^z &= -(c_i + c_i^\dagger) \prod_{j<i} (1 - 2n_j) \end{aligned}$$

including this string, $[\hat{\sigma}_i^x, \hat{\sigma}_j^z] = 0$ for $i \neq j$, as required

... diagonalize... exact spectrum.

transverse-field quantum Ising model in 1D: $\mathcal{H} = -J \sum_i [\hat{\sigma}_i^z \hat{\sigma}_{i+1}^z + g \hat{\sigma}_i^x]$

JW transformation: $\hat{\sigma}_i^x = 1 - 2n_i$ $n_j = c_j^\dagger c_j$

$$\hat{\sigma}_i^z = -(c_i + c_i^\dagger) \prod_{j < i} (1 - 2n_j)$$

$$\hat{\sigma}_i^z \hat{\sigma}_{i+1}^z = (c_i + c_i^\dagger)(c_{i+1} + c_{i+1}^\dagger) \prod_{j < i} (1 - 2n_j) \prod_{j < i+1} (1 - 2n_{j'})$$

$$= (c_i + c_i^\dagger)(c_{i+1} + c_{i+1}^\dagger)(1 - 2n_i) \quad \{c_i, c_j^\dagger\} = \delta_{ij}$$

$$= (-c_i + c_i^\dagger)(c_{i+1} + c_{i+1}^\dagger) \quad \{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = \delta_{ij}$$

result: quadratic Hamiltonian in terms of fermion operators

$$\mathcal{H} = -J \sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}^\dagger + c_{i+1} c_i - 2g c_i^\dagger c_i + g \right) \quad (\text{see practice problems})$$

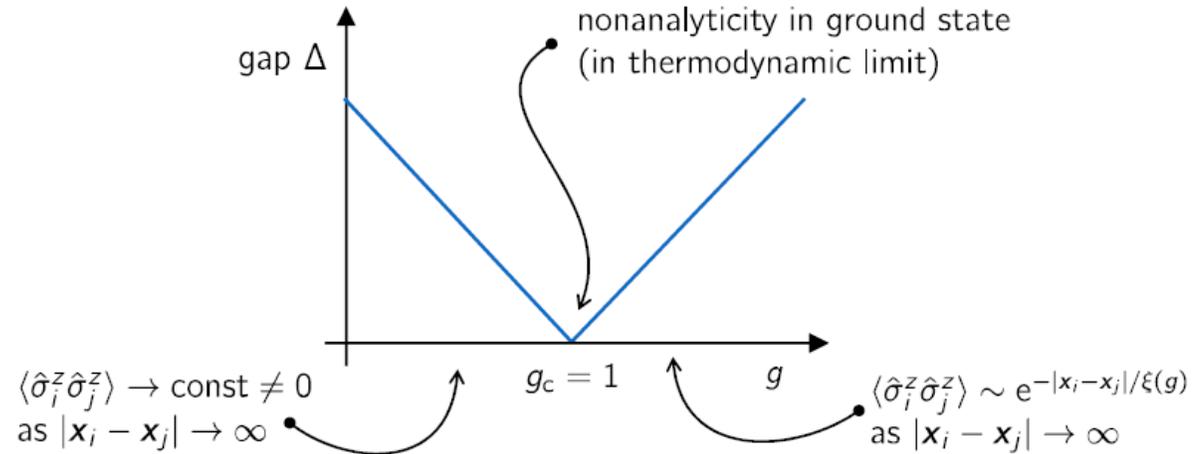
diagonalize with FT and unitary transformation: $c_k = u_k \gamma_k + i v_k \gamma_{-k}^\dagger$ $\{\gamma_k, \gamma_{k'}^\dagger\} = \delta_{k,k'}$

$$\mathcal{H} = \sum_k \varepsilon_k (\gamma_k^\dagger \gamma_k - \frac{1}{2}) \quad \text{ground state |g.s.}: \gamma_k |g.s.\rangle = 0 \quad (\text{all } k)$$

$$\varepsilon_k = 2J \sqrt{1 + g^2 - 2g \cos k} \quad \text{gap } \Delta = E_1 - E_{g.s.} = \varepsilon_0 = 2J|1 - g|$$

Chain: QPT

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - Jg \sum_i \hat{\sigma}_i^x = \sum_k \epsilon_k (\gamma_k^\dagger \gamma_k - \frac{1}{2})$$



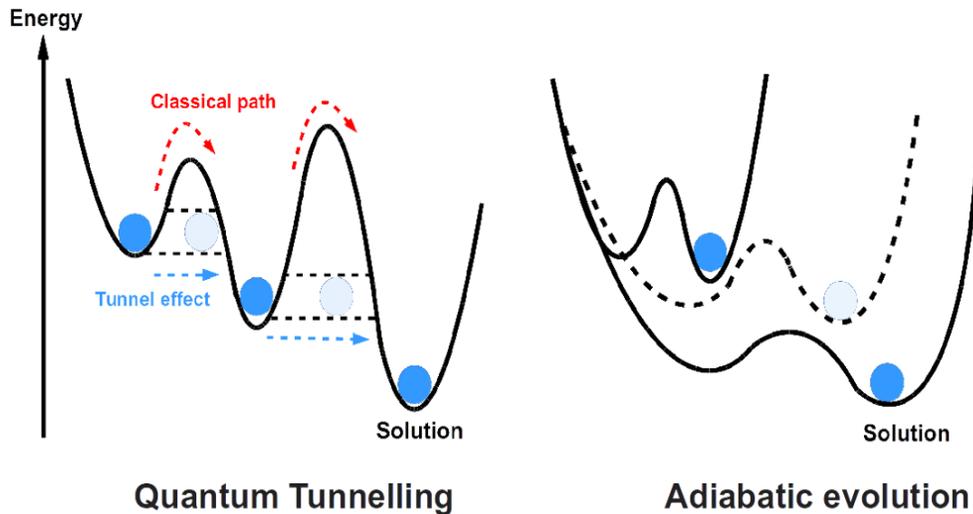
$$\epsilon_k = 2J\sqrt{1 + g^2 - 2g \cos k}$$

$$\Delta = 2J|1 - g| \sim |g - g_c|^{z\nu}$$

critical exponent $z\nu = 1$

Sachdev (1999/2011)

Quantum annealing



Idea: take a classical Hamiltonian (energy function). Instead of doing things at finite T and lowering it (Simulated Annealing)... Glauber dynamics with a decreasing T .

Do the quantum version with decreasing quantum effects.

Tunneling through barriers.

Kibble-Zurek

Approach a 2nd order phase transition at a (fixed) finite rate. Eg. The Ising transition.

At some point, the correlation time / relaxation timescale becomes so large, that the system no longer relaxes (“adiabatically”) or is able to follow the change.

Consequence: topological defects are created. The density depends on the correlation scale (length) and dimension (“coherent volumes”).

Lots of applications...

Physics depends on the rate of approach (velocity).

Kibble-Zurek II

Kibble-Zurek mechanism in colloidal monolayers

Sven Deutschländer,¹ Patrick Dillmann,¹ Georg Maret,¹ and Peter Keim^{1,*}

PNAS 2015

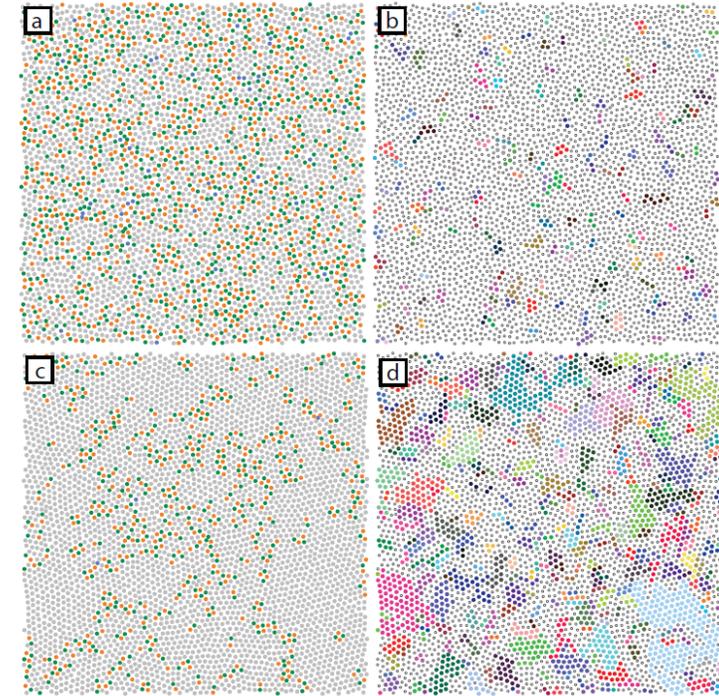
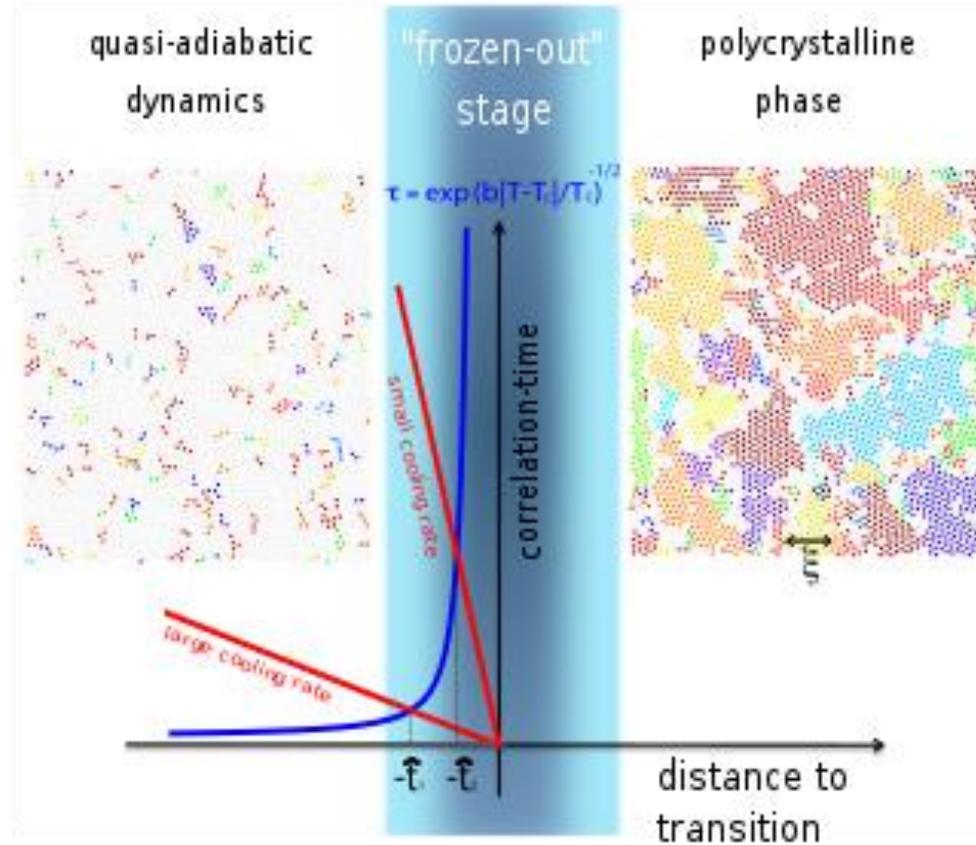


FIG. 5. Snapshot sections of the colloidal ensemble ($992 \times 960 \mu\text{m}^2$, ≈ 4000 particles) illustrating the defect (a,c) and domain configurations (b,d) at the freeze out temperature $\hat{\Gamma}$ for the fastest (a,b: $\hat{\Gamma} = 0.0326 \text{ 1/s}$, $\hat{\Gamma} \approx 30.3$) and slowest cooling rate (c,d: $\hat{\Gamma} = 0.000042 \text{ 1/s}$, $\hat{\Gamma} \approx 66.8$). The defects are marked as follows: Particles with five nearest neighbors are colored red, seven nearest neighbors green and other defects blue. Sixfold coordinated particles are colored grey. Different symmetry broken domains are colored individually and high symmetry particles are displayed by smaller circles.

Quantum take-home

The classic reference for this stuff is by Subir Sachdev (Quantum Phase Transitions) but we utilize here two sets of lecture notes that exploit it. The first set is from Warwick

<https://warwick.ac.uk/fac/sci/physics/mpags/modules/theory/cqpt/lectures9-10.pdf>

And if you want another viewpoint, with partly more detail, check lectures 5 and 6 from Dresden (Lukas Janssen), https://tu-dresden.de/mn/physik/itp/tfp/studium/lehre/ss18/qpt_ss18

For the applications, we have quantum annealing and the Kibble-Zurek mechanism. The take home is now like this: check those notes so that you recall the main points of QPT. Then pick either a topic on quantum annealing (including the D-Wave simulator), in other words

<https://www.nature.com/articles/s41598-019-49172-3>

... or if you want to have more insight on the Kibble-Zurek, you should take

<https://www.nature.com/articles/s41586-019-1070-1>

And your task is like the previous time "2+8" sentences on the selection and main points.