Statistical Mechanics
E0415

Fall 2023, lecture 8
Quantum phase transitions

… take home…

“I chose the article “Brain entropy mapping using fMRI” since I am in general interested in brain and neuro related concepts. I have not heard of brain entropy (BEN) before, so this is a new topic for me.

The article presents how functional MRI (fMRI) can be analyzed with the help of brain entropy to view brain activity. The fMRI data are time-dependent voxels, hundreds of thousands of which need to be analyzed. For one voxel and so-called embedded vectors are used to compute the sample entropy with a logarithmic function, where the inputs are sums of all the voxel values. The data describes regional changes in cerebral blood flow and metabolism. The article does not really specify the meaning behind using entropy, except that the brain aims to keep orderly, so “fighting” against entropy is necessary. The point of the analysis seems to be to see if entropy is a good way to view how much activity there is in a region in the brain. Abnormal changes also would be seen from the entropy measurements. The article concludes with disc”ussion of the successful results: the results agreed with previous theoretical estimations. The description of why this entropy was a useful metric was quite faint from a physics point of view. “

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 $[\hat{\sigma}_i^\mu, \hat{\sigma}_j^\nu] = -2\mathrm{i}\epsilon_{\mu\nu\rho}\hat{\sigma}_i^\rho \delta_{ij}$
- in $\hat{\sigma}^z$ basis, $|\uparrow\rangle_i$, $|\downarrow\rangle_i$, $\hat{\sigma}_i^\mu \, |s\rangle_i = (\boldsymbol{\sigma}^\mu)_{ss'} \, |s'\rangle_i$

$s, s' \in \{+1, -1\}$

$\boldsymbol{\sigma}^\mu$: Pauli matrix

$$\hat{\sigma}_i^z |\uparrow\rangle_i = +|\uparrow\rangle_i \qquad \hat{\sigma}_i^z |\downarrow\rangle_i = -|\downarrow\rangle_i$$
$$\hat{\sigma}_i^x |\uparrow\rangle_i = |\downarrow\rangle_i \qquad \hat{\sigma}_i^x |\downarrow\rangle_i = |\uparrow\rangle_i$$

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

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

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

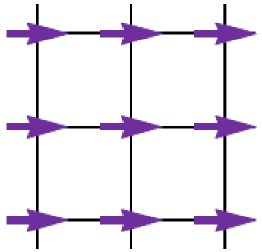
For $g \to +\infty$, $|\text{g.s.}\rangle = \prod_i |\rightarrow\rangle_i$

spins align with applied field: "quantum paramagnet"

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

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

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, $|\text{g.s.}\rangle = \prod_i |\rightarrow\rangle_i$ + 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 $\xi \to 0$ for $g \to \infty$

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

("kinetic"/"potential" depends on choice of basis)

Ferromagnet

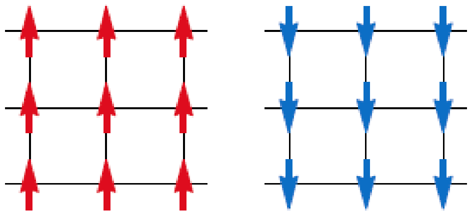
$$\mathcal{H} = -J\sum_{\langle ij\rangle}\hat{\sigma}_i^z\hat{\sigma}_j^z - Jg\sum_i \hat{\sigma}_i^x$$

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 ($U|\Uparrow\rangle = |\Downarrow\rangle$)

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



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 $\to 0$ as $N \to \infty$

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

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

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

"potential energy (i.e., diagonal term) wins"

Partititon function

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

$$Z = \operatorname{Tr} e^{-\beta\mathcal{H}}$$
$$= \sum_s \langle s|e^{-\beta\mathcal{H}}|s\rangle \qquad \text{for any (orthonormal) basis } \{|s\rangle\}$$

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

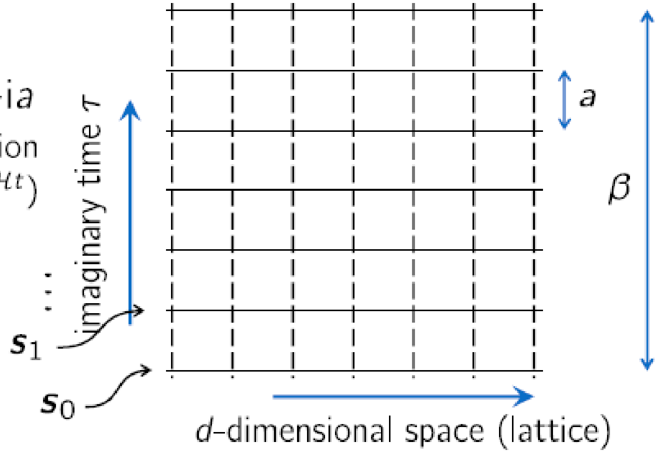
$$Z = \sum_{s_0} \langle s_0|\underbrace{e^{-a\mathcal{H}}e^{-a\mathcal{H}}\cdots e^{-a\mathcal{H}}}_{M}|s_0\rangle \qquad \sum_s |s\rangle\langle s| = 1$$
$$= \sum_{s_0,s_1,\dots,s_{M-1}} \langle s_0|e^{-a\mathcal{H}}|s_1\rangle\langle s_1|e^{-a\mathcal{H}}|s_2\rangle\langle s_2|\cdots|s_{M-1}\rangle\langle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

$e^{-a\mathcal{H}}$: evolution by "imaginary time" $t = -ia$

(real-time evolution operator $e^{-i\mathcal{H}t}$)

$\sum_{s_0,s_1,\dots,s_{M-1}}$: sum over trajectories

"path integral" representation of Z



Quantum model to classical mapping

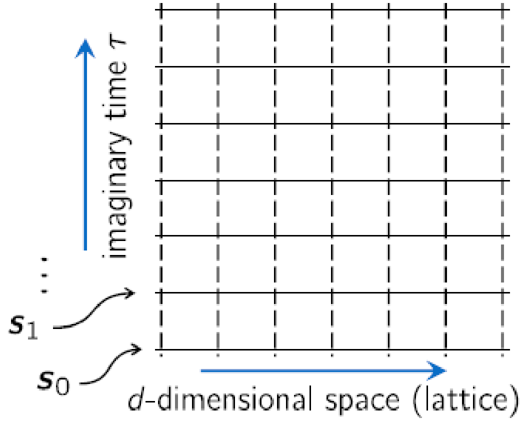
$$Z = \sum_{s_0, s_1, \ldots, s_{M-1}} \langle s_0 | e^{-a\mathcal{H}} | s_1 \rangle \langle s_1 | e^{-a\mathcal{H}} | s_2 \rangle \langle s_2 | \cdots | s_{M-1} \rangle \langle s_{M-1} | e^{-a\mathcal{H}} | s_0 \rangle$$

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

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

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

where $\boldsymbol{s}_M \equiv \boldsymbol{s}_0$ (periodicity in τ)



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

$$E_{\text{cl}} = \sum_i [E_1(\boldsymbol{s}_i) + E_2(\boldsymbol{s}_i, \boldsymbol{s}_{i+1})]$$

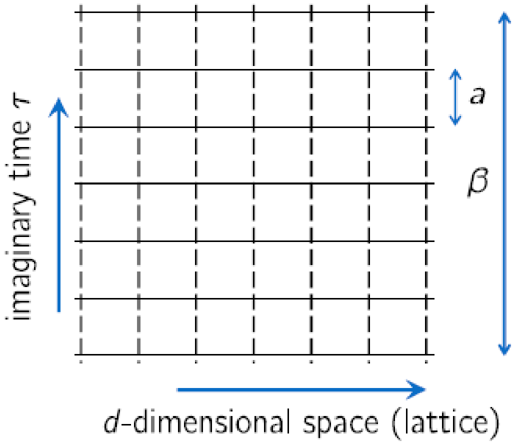
E_1: layer configuration energy
E_2: interaction between adjacent layers

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

if $\mathcal{E}(\boldsymbol{s}, \boldsymbol{s}')$ 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 $\mathrm{e}^{-a\mathcal{H}}$	Boltzmann weight (transfer matrix) $\mathrm{e}^{-\mathcal{E}(s,s')} = \langle \boldsymbol{s} \vert \mathrm{e}^{-a\mathcal{H}} \vert \boldsymbol{s}' \rangle$
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 $\mathcal{E}(\boldsymbol{s},\boldsymbol{s}') = -\log\langle\boldsymbol{s}|\mathrm{e}^{-a\mathcal{H}}|\boldsymbol{s}'\rangle$

use $\hat\sigma_i^z$ basis, $|\!\uparrow\rangle_i\,, |\!\downarrow\rangle_i$:

$$|\boldsymbol{s}\rangle = |\{s_1, s_2, \ldots s_N\}\rangle = \prod_i^N |s_i\rangle_i,$$

$$Z = \sum_{\boldsymbol{s}_0,\boldsymbol{s}_1,\ldots,\boldsymbol{s}_{M-1}} \mathrm{e}^{-\sum_{i=0}^{M-1}\mathcal{E}(\boldsymbol{s}_i,\boldsymbol{s}_{i+1})}$$

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

$$\begin{aligned}\langle\boldsymbol{s}|\,\mathrm{e}^{-a\mathcal{H}}\,|\boldsymbol{s}'\rangle &\approx \langle\boldsymbol{s}|\,\mathrm{e}^{aJg\sum_i\hat\sigma_i^x}\mathrm{e}^{aJ\sum_{\langle ij\rangle}\hat\sigma_i^z\hat\sigma_j^z}\,|\boldsymbol{s}'\rangle \\ &= \langle\boldsymbol{s}|\,\mathrm{e}^{aJg\sum_i\hat\sigma_i^x}\,|\boldsymbol{s}'\rangle\,\mathrm{e}^{aJ\sum_{\langle ij\rangle}s_i's_j'} \\ &= \mathrm{e}^{aJ\sum_{\langle ij\rangle}s_i's_j'}\prod_i\langle s_i|\,\mathrm{e}^{aJg\hat\sigma^x}\,|s_i'\rangle \\ &= [A(aJg)]^N\mathrm{e}^{aJ\sum_{\langle ij\rangle}s_i's_j' + B(aJg)\sum_i s_is_i'}\end{aligned}$$

$$\langle s|\mathrm{e}^{\alpha\hat\sigma^x}|s'\rangle = A(\alpha)\mathrm{e}^{B(\alpha)ss'}$$

$$B(\alpha) = -\tfrac{1}{2}\log\tanh\alpha$$

$$\mathcal{E}(\boldsymbol{s},\boldsymbol{s}') = -aJ\sum_{\langle ii\rangle}s_i's_j' - B(aJg)\sum_i s_is_i' + \text{const}$$

Ising II

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

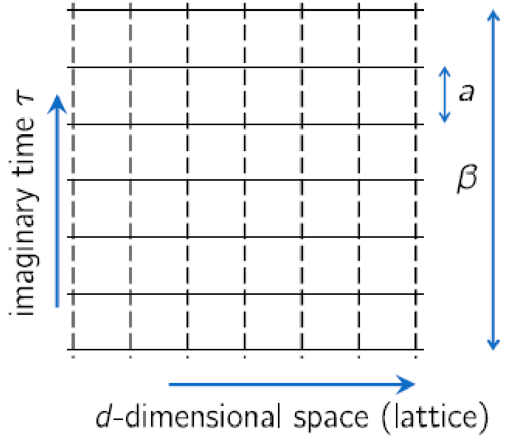
$$Z = \sum_{\mathbf{s}_0,\mathbf{s}_1,\ldots,\mathbf{s}_{M-1}} \mathrm{e}^{-\sum_{i=0}^{M-1} \mathcal{E}(\mathbf{s}_i,\mathbf{s}_{i+1})}$$

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

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

layer configuration energy

interaction between adjacent layers



- Transverse-field Ising model in d dimensions maps to highly anisotropic ($a \to 0$) 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:

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

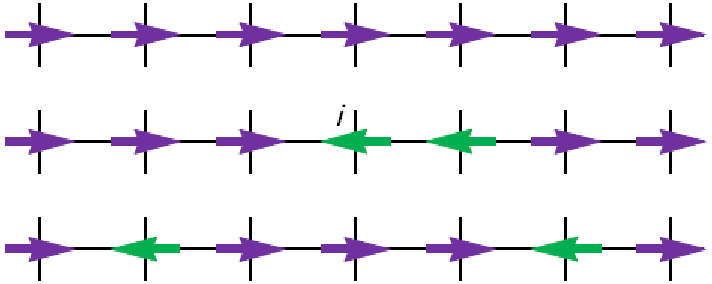
(related to 2D classical Ising model, so ordering transition at g_c)

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



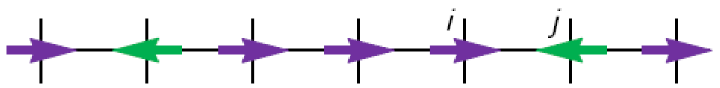
$$|\rightarrow\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle + |\downarrow\rangle \right) \qquad \hat{\sigma}^z |\rightarrow\rangle = |\leftarrow\rangle$$

$$|\leftarrow\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle - |\downarrow\rangle \right) \qquad \hat{\sigma}^z |\leftarrow\rangle = |\rightarrow\rangle$$

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

$$\hat{\sigma}_i^x = 1 - 2n_i \qquad n_i = 0$$

$$\hat{\sigma}_i^z = b_i + b_i^\dagger \qquad n_j = 1$$

- as fermions—double occupation automatically forbidden, *but* fermion operators anticommute on different sites:

$$\{c_i, c_j^\dagger\} = \delta_{ij}$$

$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = \delta_{ij}$$

$$[\hat{\sigma}_i^\mu, \hat{\sigma}_j^\nu] = -2\mathrm{i}\epsilon_{\mu\nu\rho}\hat{\sigma}_i^\rho\delta_{ij}$$

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

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

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

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

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

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

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

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

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

result: quadratic Hamiltonian in terms of fermion operators

$$\mathcal{H} = -J\sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}^\dagger + c_{i+1}c_i - 2gc_i^\dagger c_i + g\right)$$

(see practice problems)

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

$$\mathcal{H} = \sum_k \varepsilon_k(\gamma_k^\dagger\gamma_k - \tfrac{1}{2})$$

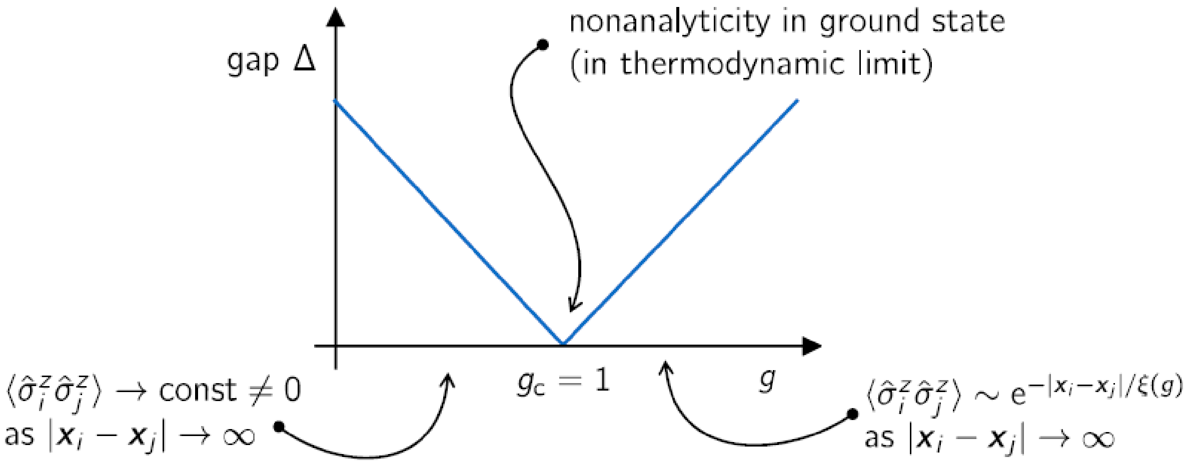
ground state $|\text{g.s.}\rangle$: $\gamma_k|\text{g.s.}\rangle = 0$ (all k)

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

gap $\Delta = E_1 - E_{\text{g.s.}} = \varepsilon_0 = 2J|1-g|$

Chain: QPT

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



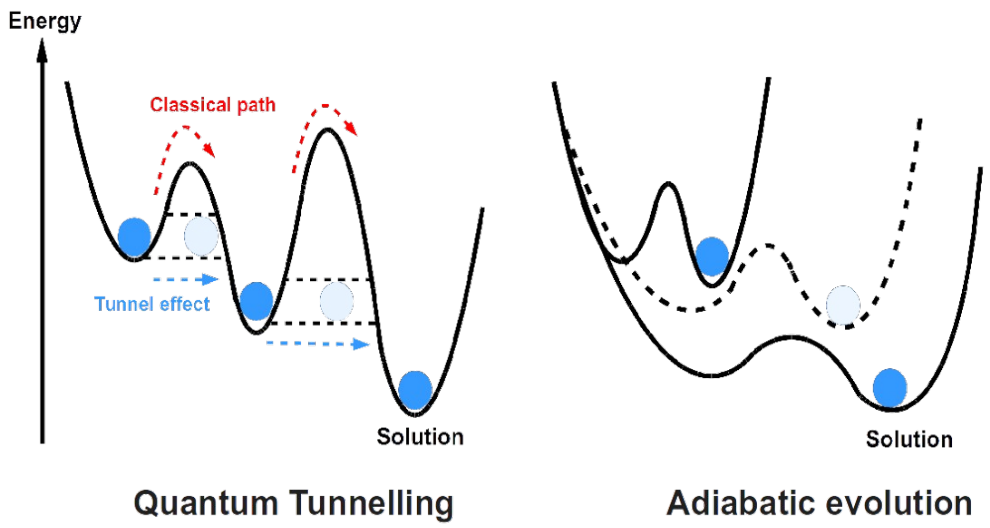
$$\varepsilon_k = 2J\sqrt{1 + g^2 - 2g\cos k}$$

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

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…

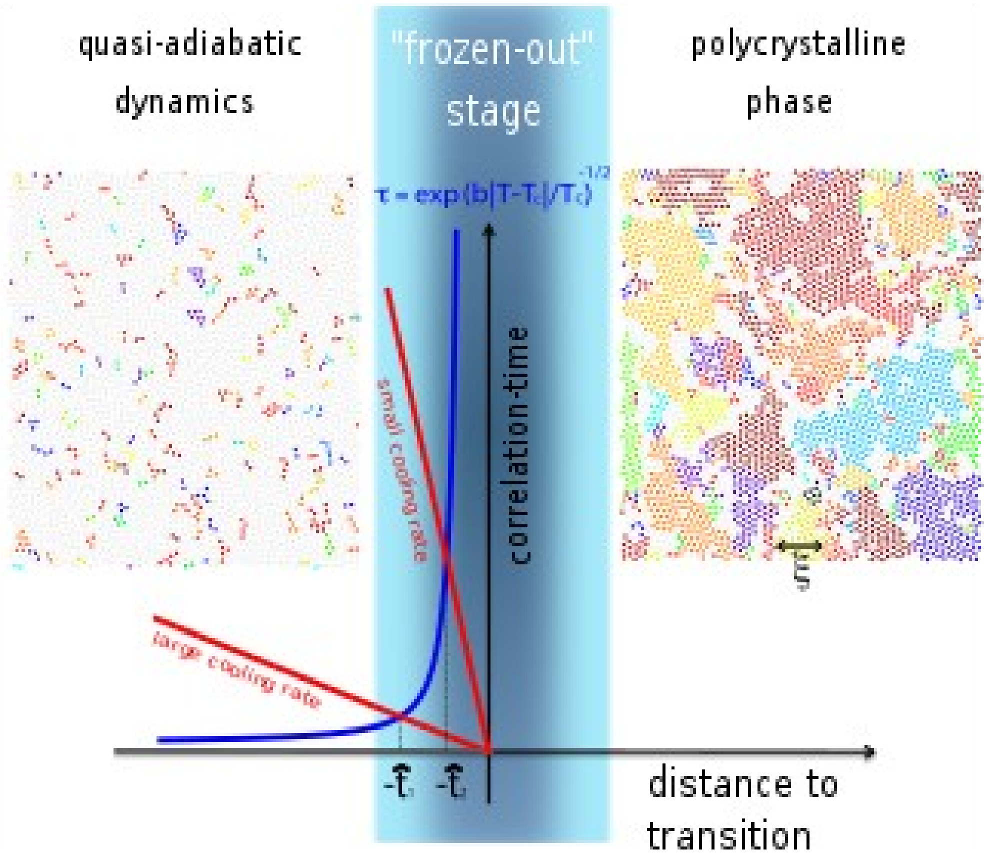
Physics depends on the rate of approach (velocity).

Kibble-Zurek II

Kibble-Zurek mechanism in colloidal monolayers

Sven Deutschländer,[1] Patrick Dillmann,[1] Georg Maret,[1] and Peter Keim[1,*]

PNAS 2015



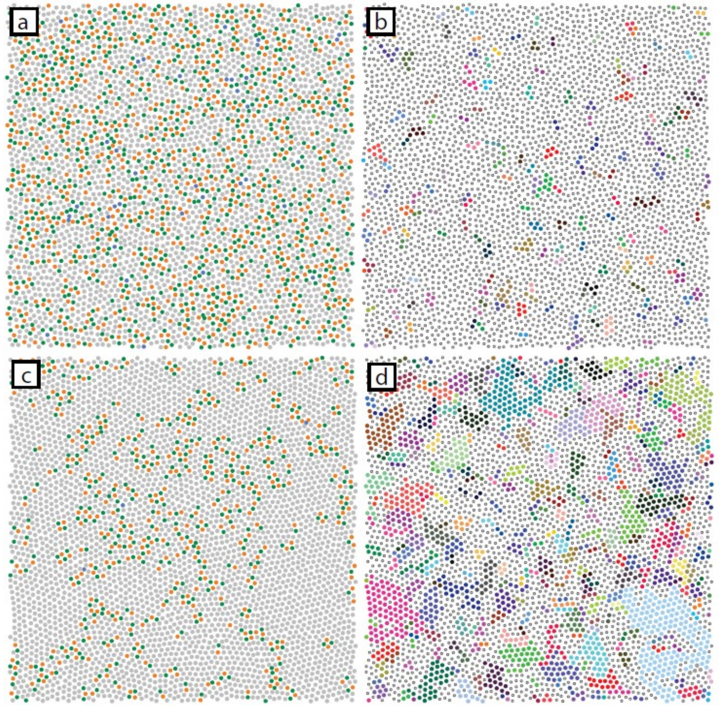


FIG. 5. Snapshot sections of the colloidal ensemble ($992 \times 960\ \mu m^2$, ≈ 4000 particles) illustrating the defect (a,c) and domain configurations (b,d) at the freeze out temperature $\hat{\Gamma}$ for the fastest (a,b: $\dot{\Gamma} = 0.0326$ 1/s, $\hat{\Gamma} \approx 30.3$) and slowest cooling rate (c,d: $\dot{\Gamma} = 0.000042$ 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 Sachdeev (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.