Title: Classical algorithms, correlation decay, and complex zeros of partition functions of quantum many-body systems

Speakers: Mehdi Soleimanifar

Series: Perimeter Institute Quantum Discussions

Date: May 13, 2020 - 3:30 PM

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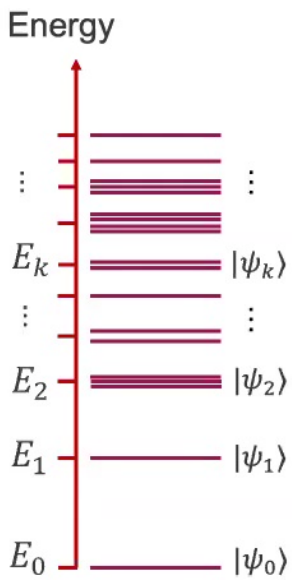
Abstract: Basic statistical properties of quantum many-body systems in thermal equilibrium can be obtained from their partition function. In this talk, I will present a quasi-polynomial time classical algorithm that estimates the partition function of quantum many-body systems at temperatures above the thermal phase transition point. It is known that in the worst case, the same problem is NP-hard below this temperature. This shows that the transition in the phase of a quantum system is also accompanied by a transition in the computational hardness of estimating its statistical properties. The key to this result is a characterization of the phase transition and the critical behavior of the system in terms of the complex zeros of the partition function. I will also discuss the relation between these complex zeros and another signature of the thermal phase transition, namely, the exponential decay of correlations. I will show that in a system of n particles above the phase transition point, where the complex zeros are far from the real axis, the correlation between two observables whose distance is at least log(n) decays exponentially. This is based on joint work with Aram Harrow and Saeed Mehraban.

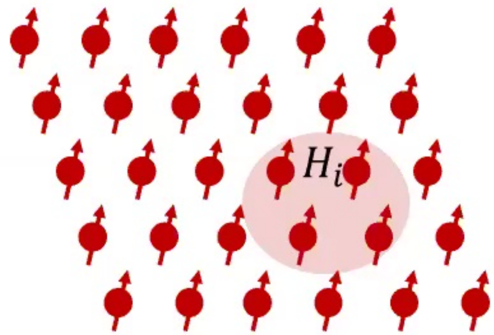
Classical algorithms, correlation decay, and complex zeros of quantum partition functions

Mehdi Soleimanifar (MIT)

Joint work with
Aram Harrow and Saeed Mehraban

arXiv:1910.09071, STOC’20

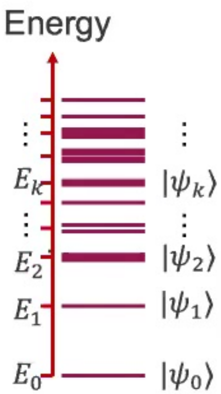


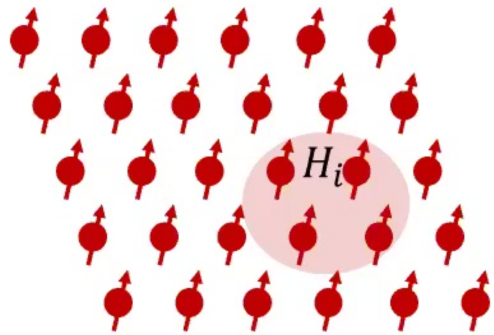


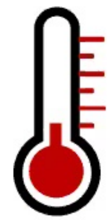
n qudits (or spins) on a lattice

Interactions described by $H = \sum_i H_i$

H_i acting on a spatially-local region





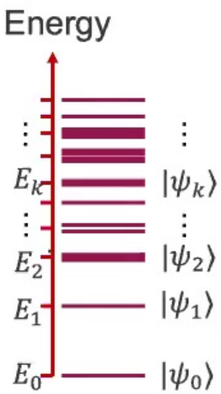


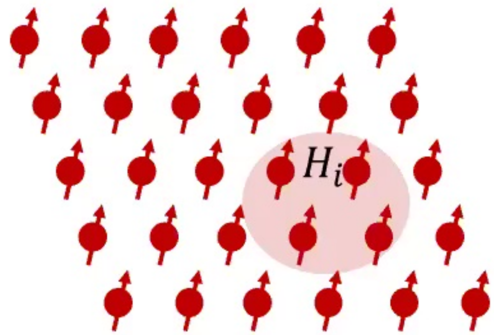
How hard is it to approximate E_0 in the worst case?

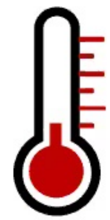
It is QMA-complete [K'02, KKR'05, …]

Efficient algorithms in special cases [ALVV'16, BH'13, …]

1D Lattice
H gapped







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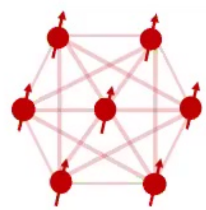
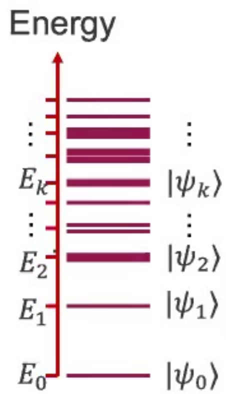
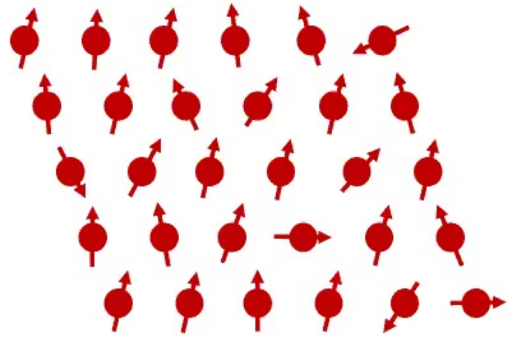
Dense Lattice







At non-zero temperature $T = 1/\beta$, system in state

Gibbs state $\rho = \frac{1}{Z}\sum_k e^{-\beta E_k} |\psi_k\rangle\langle\psi_k|$

Partition function $Z(\beta) = \sum_k e^{-\beta E_k} = \mathrm{Tr}[e^{-\beta H}]$

$\beta \to \infty, \rho \to |\psi_0\rangle\langle\psi_0|$

$\beta \to 0, \rho \to I/d^n$

Free energy $F(\beta) = -\frac{1}{\beta}\log Z = \mathrm{Tr}[H\rho] - \frac{1}{\beta}S(\rho)$

$\beta \to \infty, F \to E_0$

Finding $Z(\beta)$ exactly is #P-hard [Val'79]

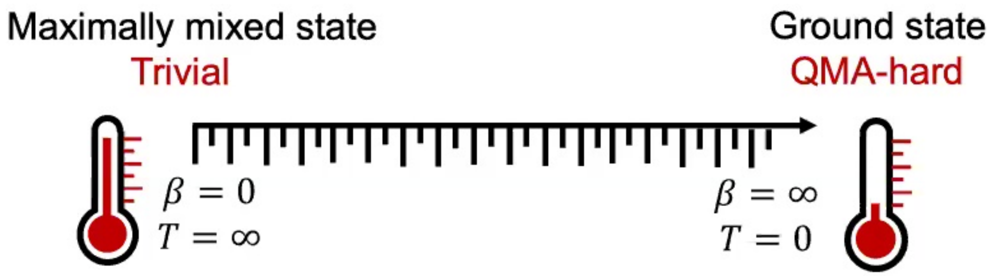
Goal: design an approximation algorithm that

Input: H, β, ε

Output: estimate $\hat{Z}(\beta)$ such that

$$|\log Z(\beta) - \log \hat{Z}(\beta)| \leq \varepsilon$$

Hardness depends on temperature



Transition in the hardness

but we also know about

Transition in the phase

Maximally mixed state
Trivial

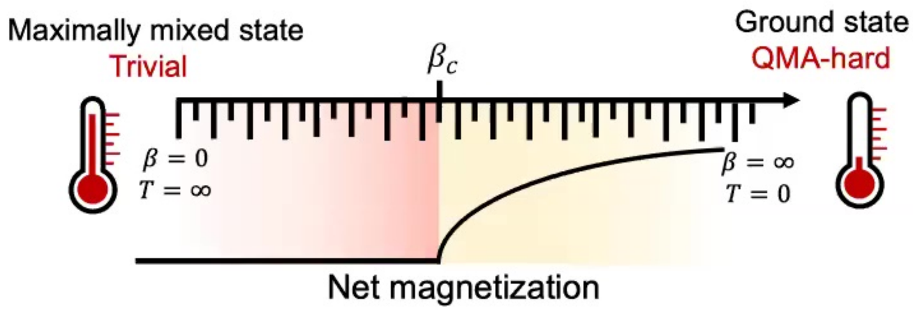
Ground state
QMA-hard

Transition in the hardness

but we also know about

Transition in the phase

Physical properties abruptly change



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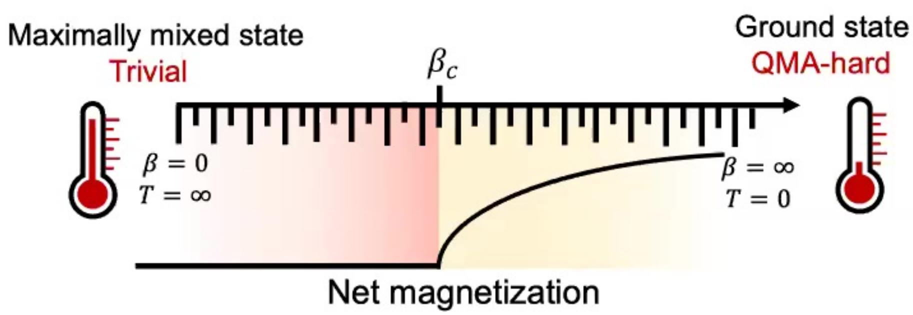


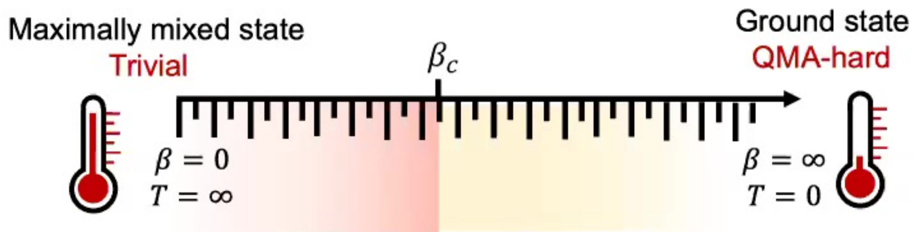
Transition in the hardness

but we also know about

Transition in the phase

Physical properties abruptly change

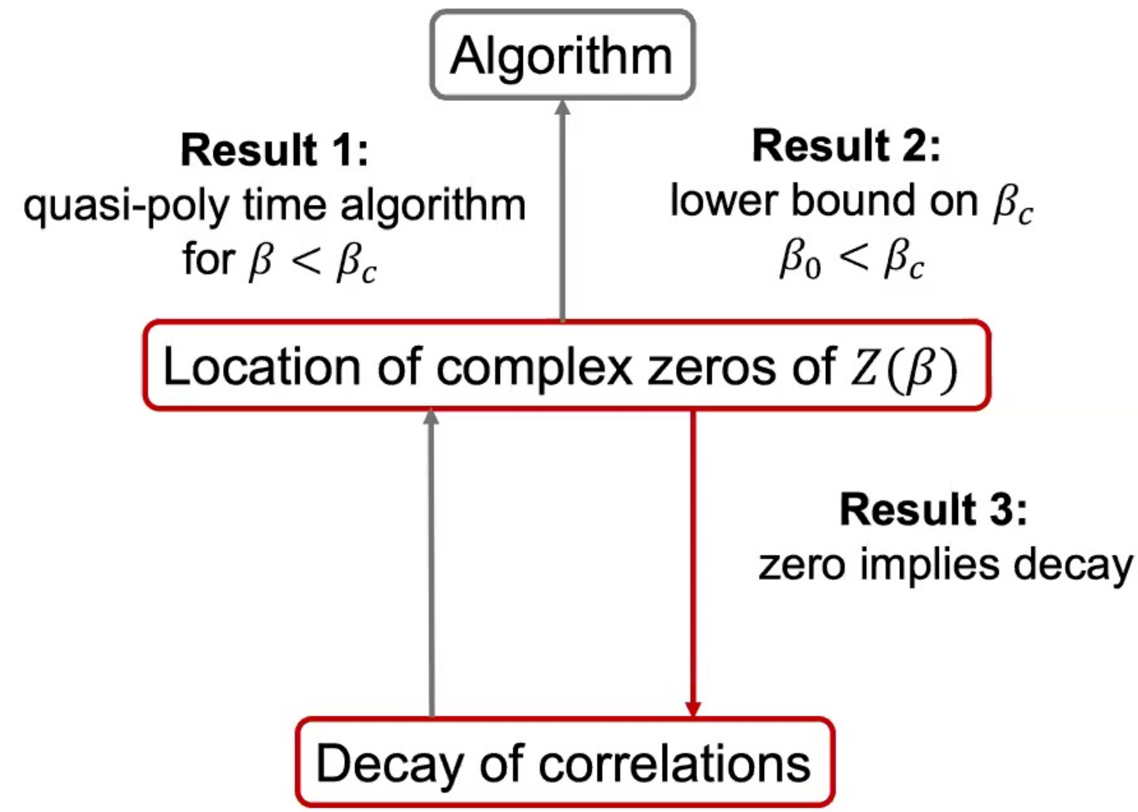
Hardness of approximating $Z(\beta)$
vs
Physical phase transition?



For **classical** Ising model

- Above T_c there is a polynomial time algorithm
- Below T_c no efficient algorithm unless $\mathrm{NP} = \mathrm{RP}$ [Sly'10]

Computational phase transition
matches
Physical phase transition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for $\beta < \beta_c$
Result 2:
lower bound on β_c
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Location of complex zeros of $Z(\beta)$
Result 3:
zero implies decay
Decay of correlations


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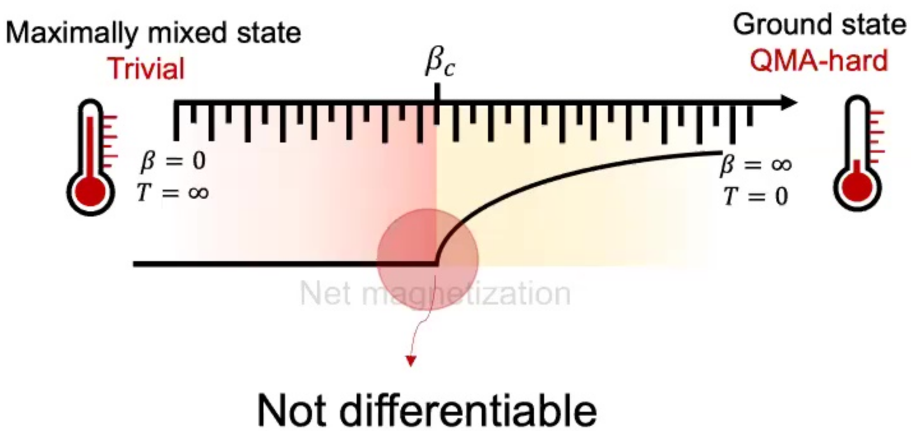
Complex zeros vs phase transition



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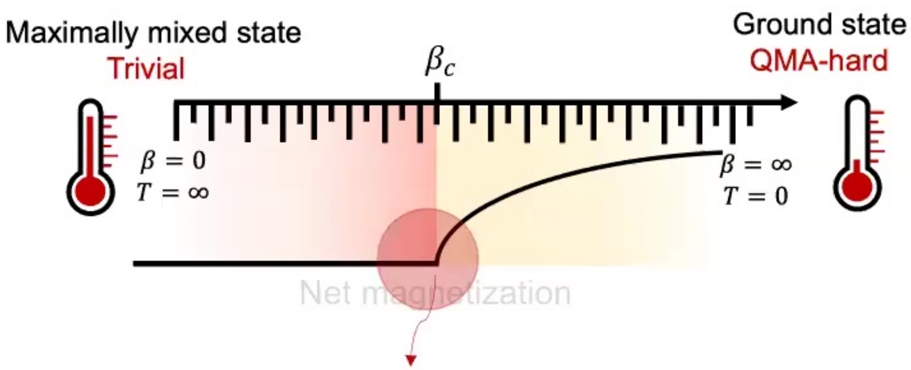
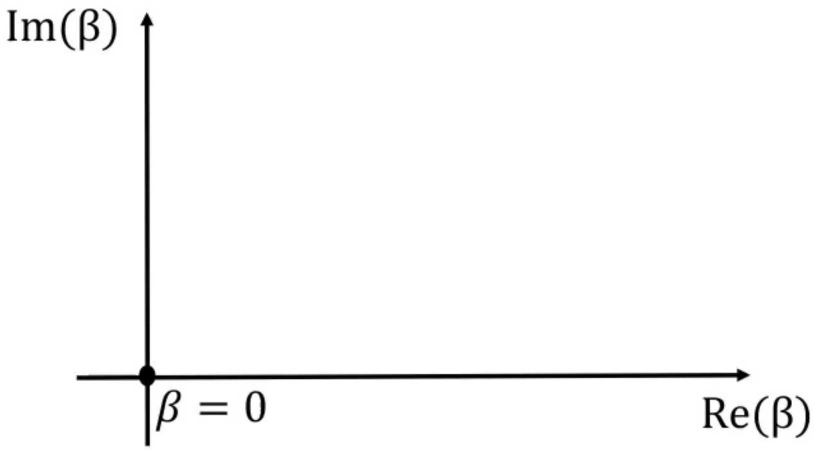


Not differentiable

Singularities at β_c

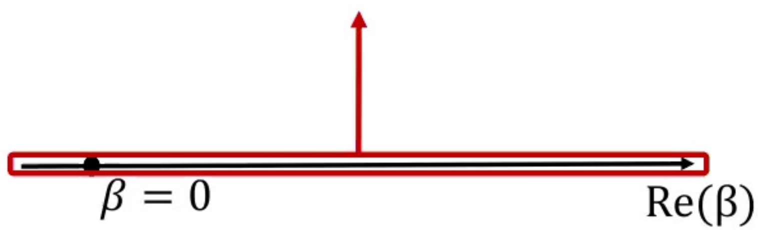
Complex zeros vs phase transition



Complex zeros vs phase transition

$$Z(\beta) = \sum_k e^{-\beta E_k}$$

Sum of strictly positive terms



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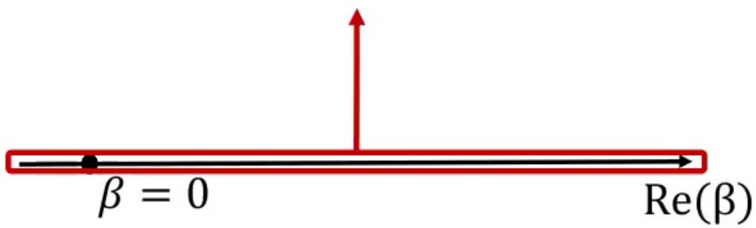
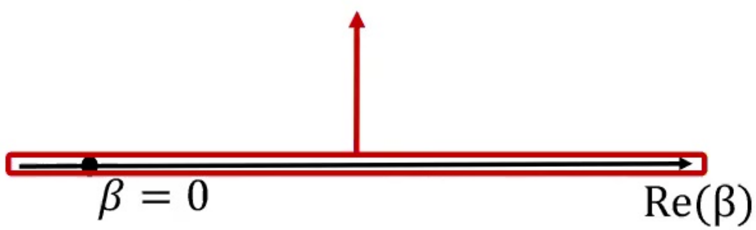


Complex zeros vs phase transition

$$Z(\beta) = \sum_k e^{-\beta E_k}$$

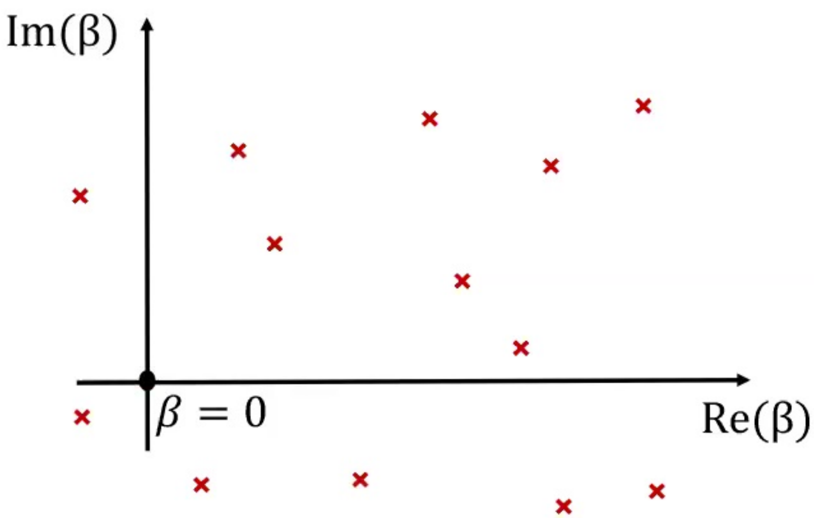
Sum of strictly positive terms

No singularities for free energy



Complex zeros vs phase transition

x : zeros of $Z(\beta) = \sum_k e^{-\beta E_k}$



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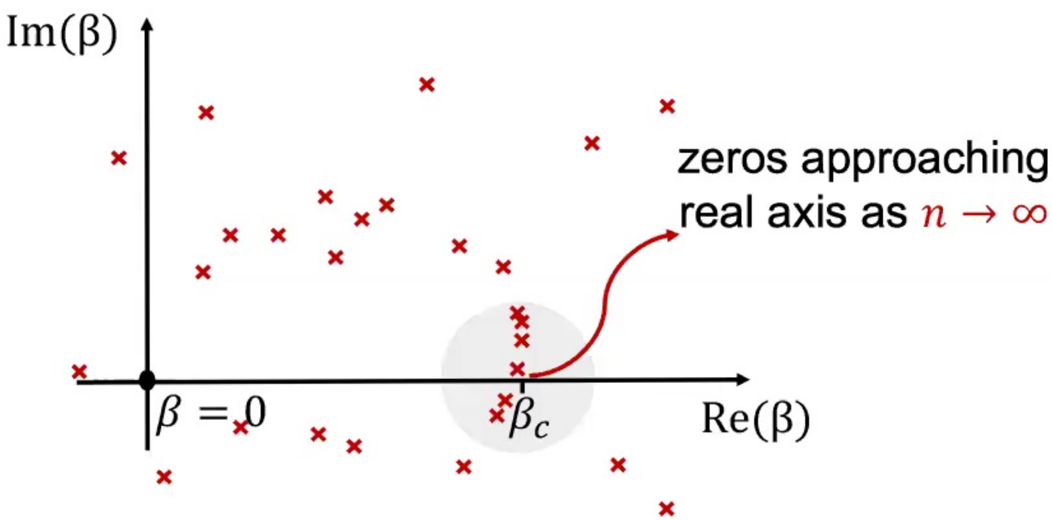

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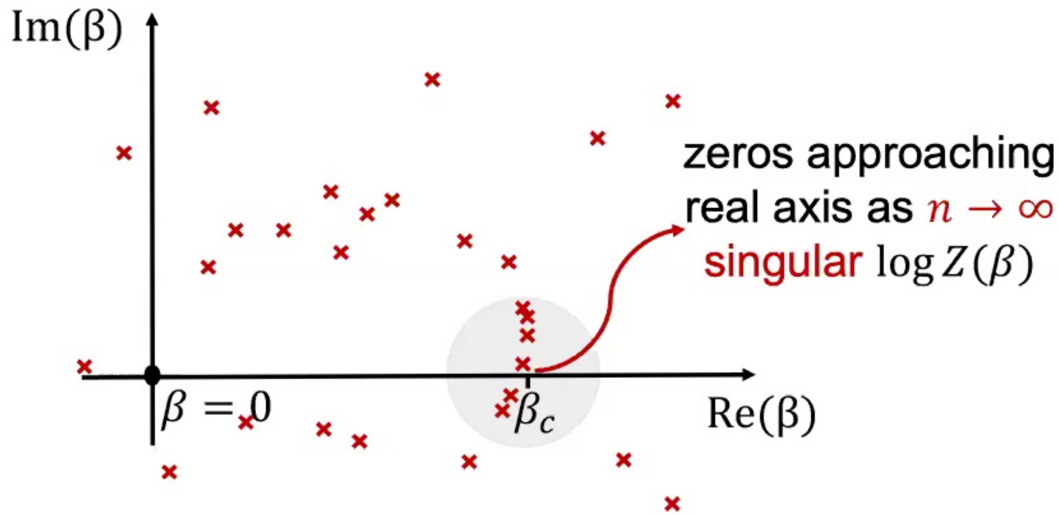
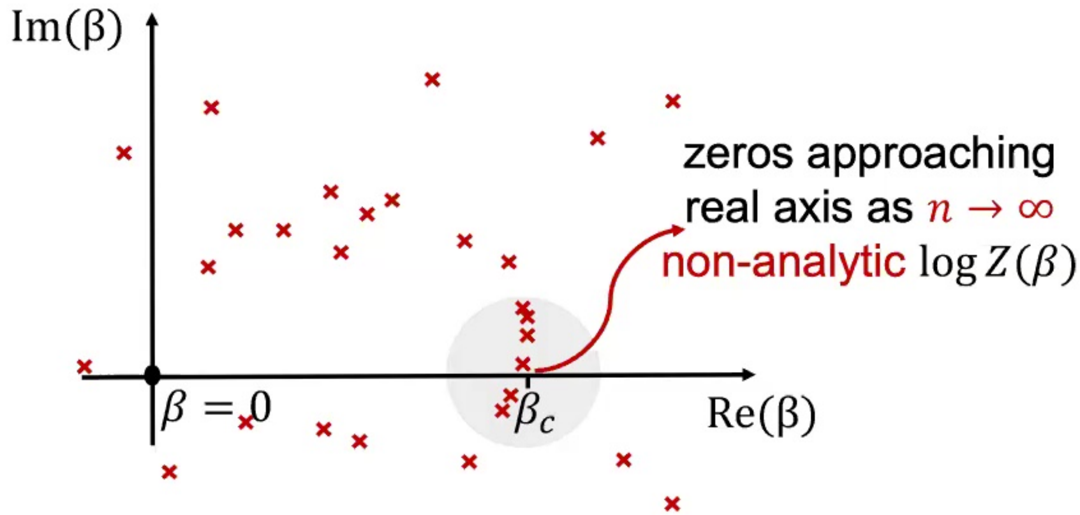


Complex zeros vs phase transition

Location of complex zero of $Z(\beta)$
tells us about
phase transition point

x : zeros of $Z(\beta) = \sum_k e^{-\beta E_k}$



- Studying zeros initiated by Lee and Yang [LY'52]

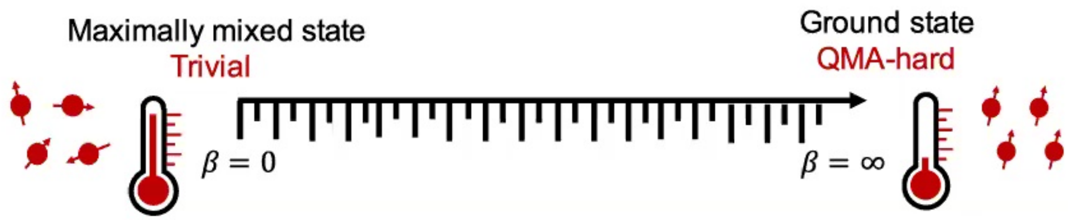
Phase transition in **classical** Ising model by
changing the external magnetic field

- Extended to thermal phase transition by Fisher [F'65]

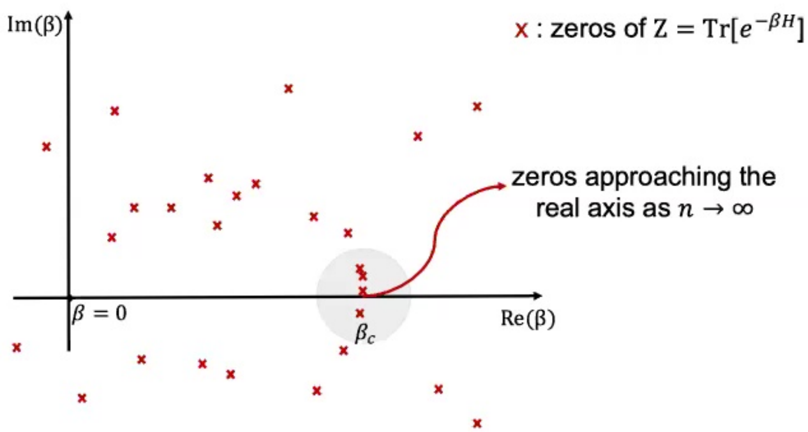
To Recap

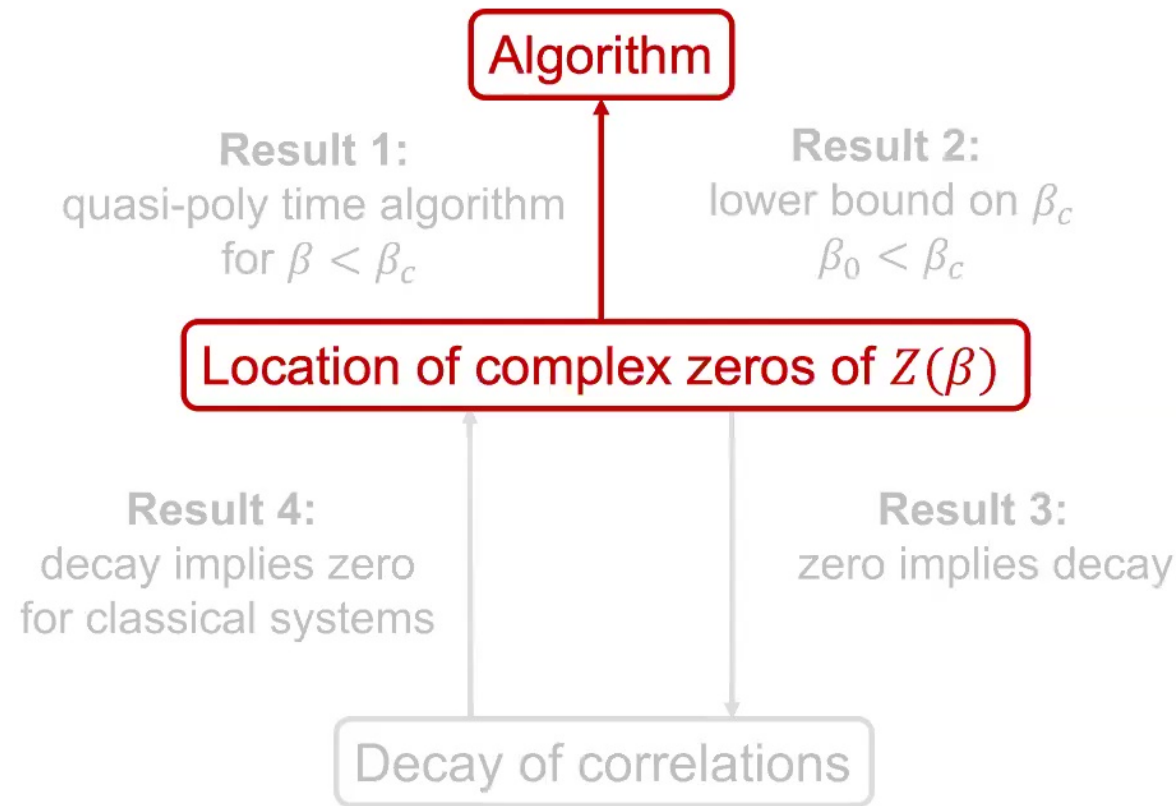
We made two observations

1)



2)

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Result 1:

An approximation algorithm for $Z(\beta)$ with running time $n^{O(\log(n/\varepsilon))}$ that works above the phase transition point

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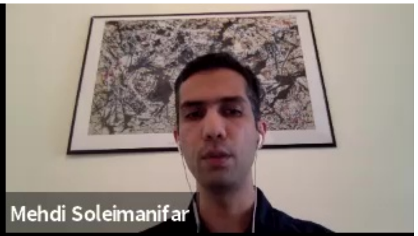
Analysis:

The idea is to

Extrapolate the solution in the easy regime (high T)

to find the solution in the harder regime (lower T)



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Taylor expanding $\log Z(\beta)$

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The idea is to

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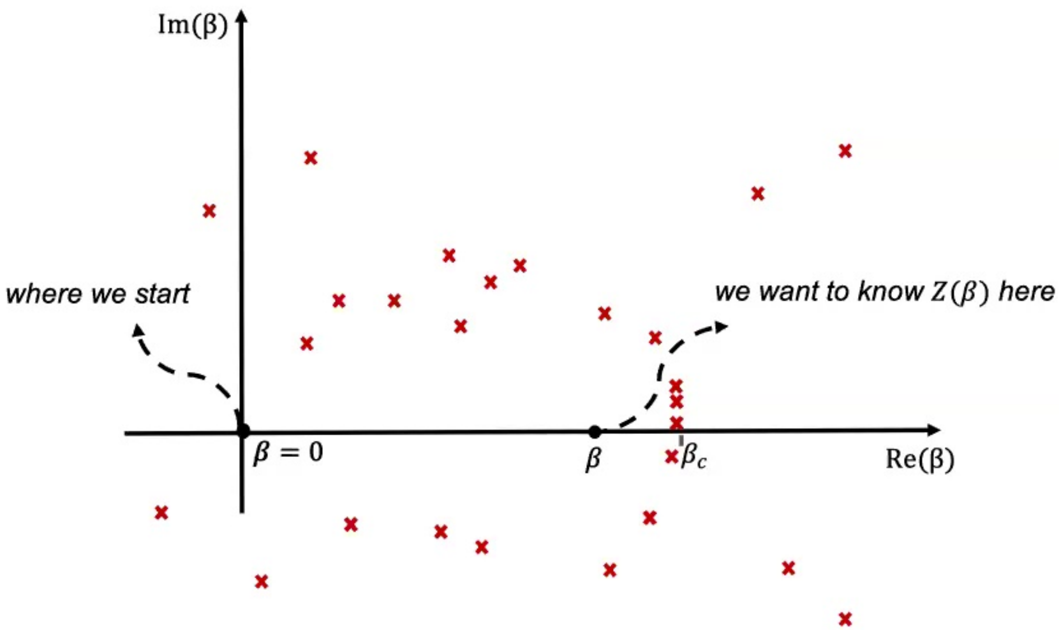
Taylor expanding $\log Z(\beta)$

Need to compute the low order derivatives

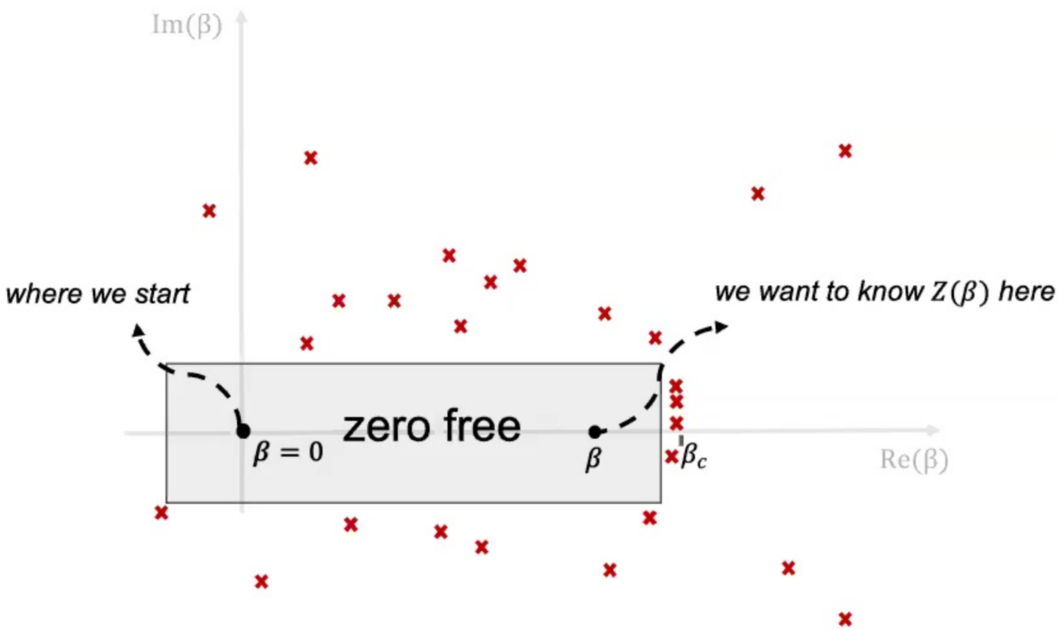
Need to make sure Taylor expansion converges

Extrapolating $\log Z(\beta)$



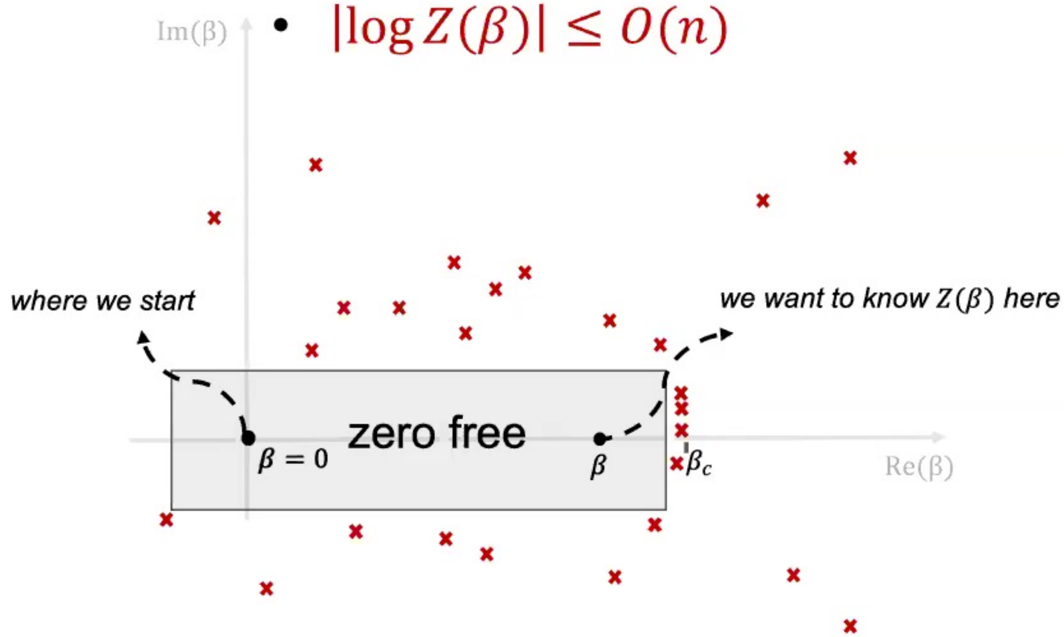
Extrapolating $\log Z(\beta)$

- $\log Z(\beta)$ is analytic in zero free region



Extrapolating $\log Z(\boldsymbol{\beta})$

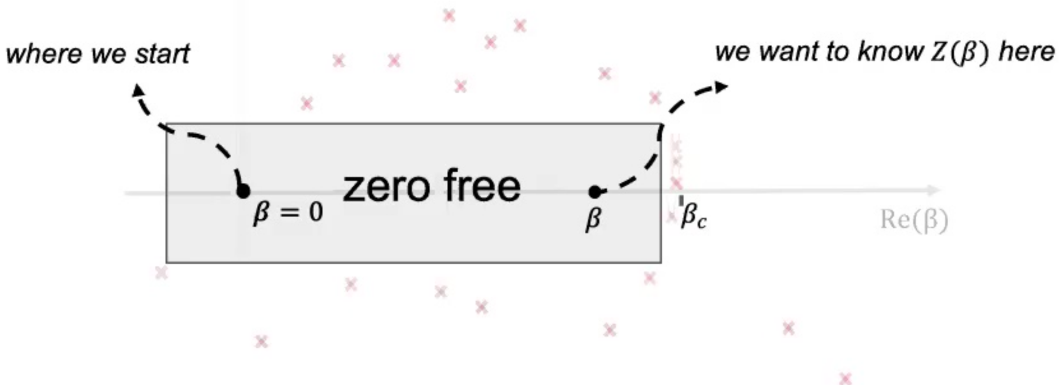
- $\log Z(\beta)$ is analytic in zero free region
- $|\log Z(\beta)| \leq O(n)$



Extrapolating $\log Z(\boldsymbol{\beta})$

- $\log Z(\beta)$ is analytic in zero free region
  - $|\log Z(\beta)| \leq O(n)$

$$\left|\log Z(\beta) - \sum_{\ell=0}^{K} \frac{1}{\ell!} \frac{d^{\ell} \log Z(0)}{d^{\ell}\beta} \beta^{\ell}\right| \leq O(n)\, e^{-\alpha K}$$



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$\downarrow$

$1/\text{poly}(n)$

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$\rightarrow 1/\mathrm{poly}(n)$

$K = O(\log n)$ derivatives needed

How to compute $\mathrm{O}(\log \mathrm{n})$ derivatives of $\log Z(\beta)$?

Sufficient to find $\mathrm{O}(\log \mathrm{n})$ derivative of $Z(\beta)$

$$\frac{d^k Z(0)}{d^k \beta} \propto \mathrm{Tr}[H^k]$$

H is sum of $\mathrm{poly}(n)$ many local terms

$$H = \sum_{i=1}^{\mathrm{poly}(n)} H_i$$

So takes time $n^{O(K)}$ to find $\mathrm{Tr}[H^K]$

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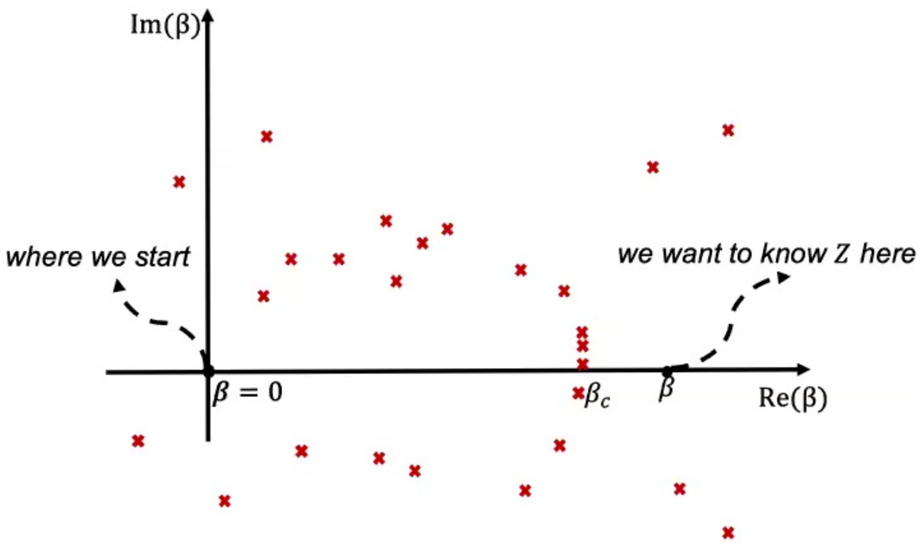
H is sum of $\mathrm{poly}(n)$ many local terms

$$H = \sum_{i=1}^{\mathrm{poly}(n)} H_i$$

So takes time $n^{O(\log n)}$ to find all the derivatives

Why not go beyond the phase transition point?



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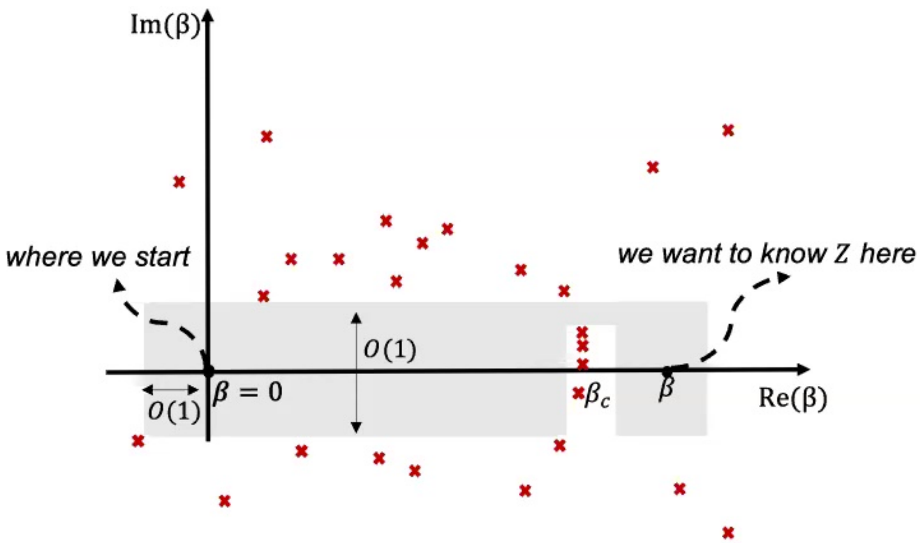

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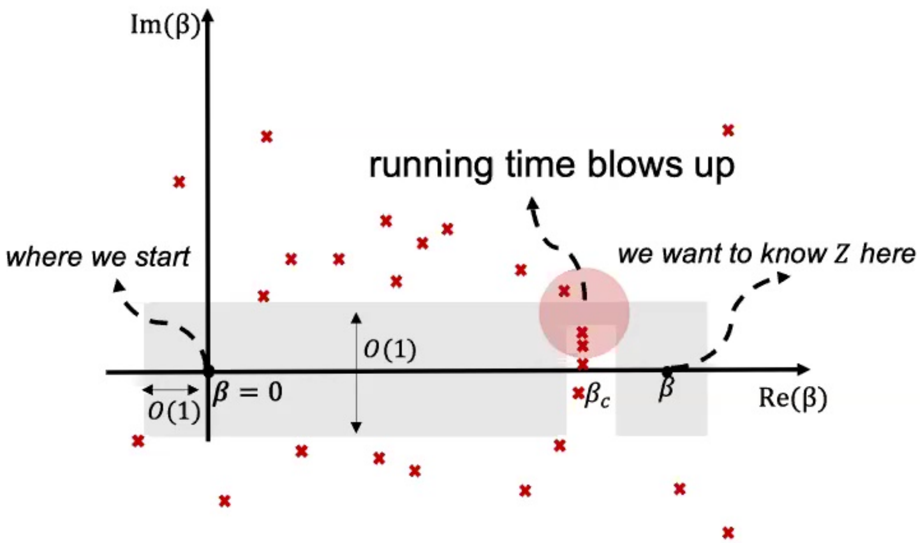

Previous work

- Introduced by Barvinok to compute permanent of matrices [Bar'16]
- Used in many new algorithms for old counting problems [LSS'18, PR'16, EM'18,…]
- Running times are usually quasi-polynomial

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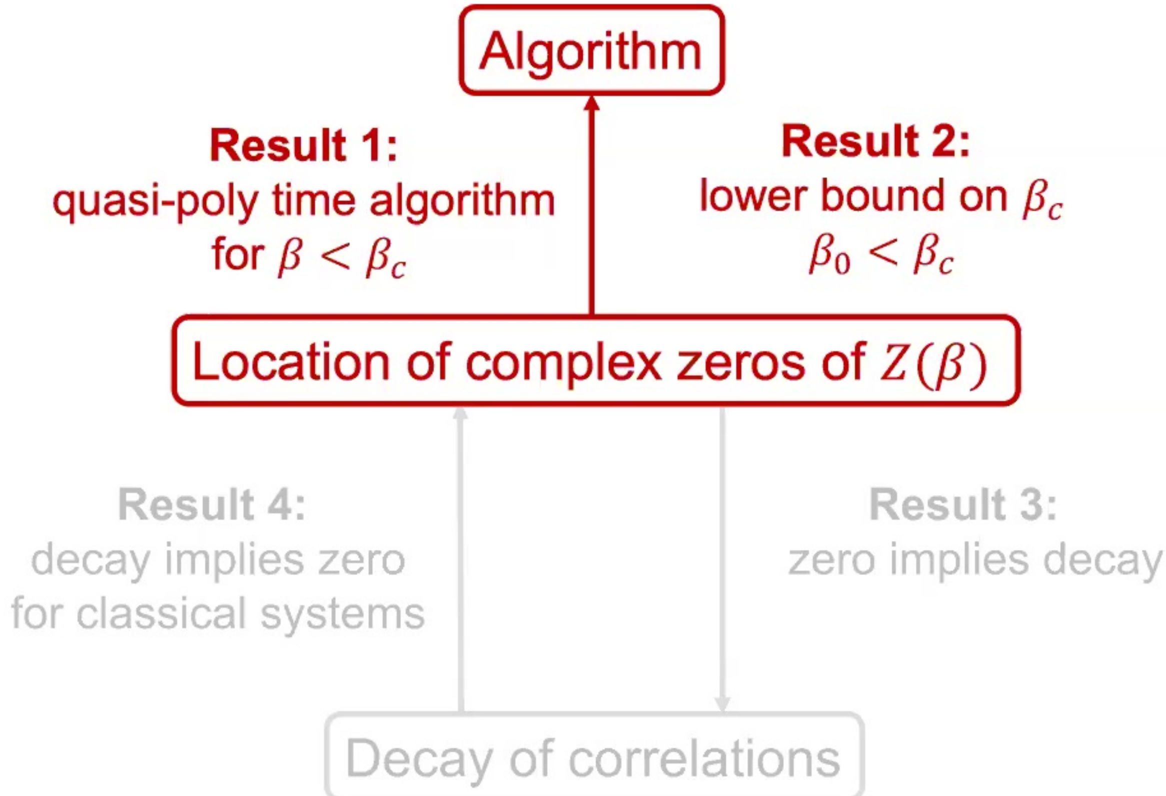
- Running times are usually quasi-polynomial
- More recent results [KKB'19, MH'20] improve our running time to polynomial time at high enough temperatures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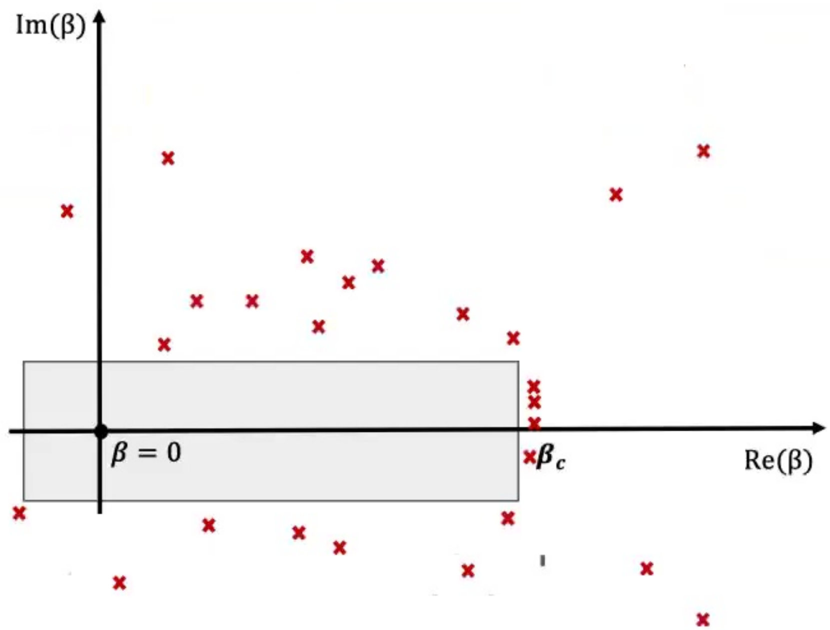
Im(β)
β = 0
β_c
Re(β)


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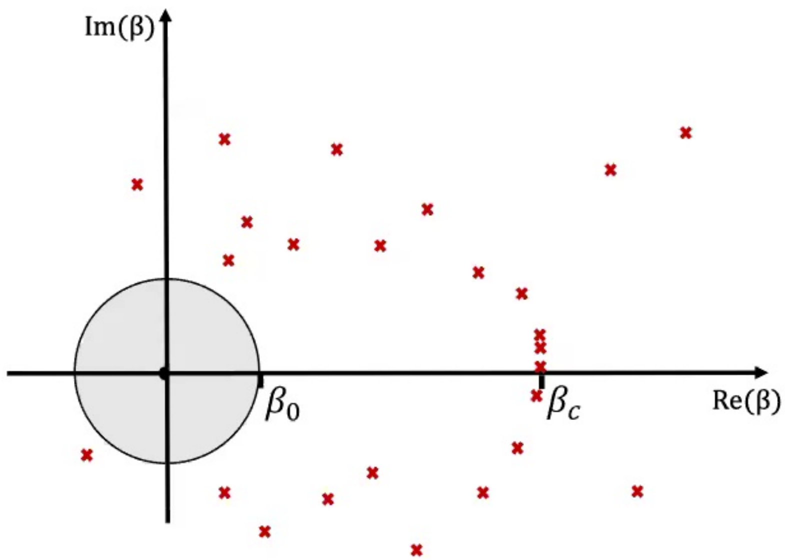
Result 2:

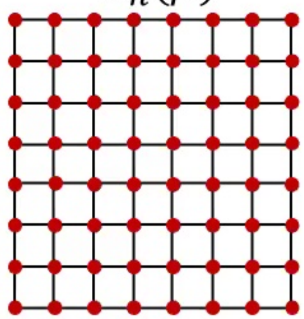
There is a constant β_0 *such that no zeros in disk* $|\beta| \leq \beta_0$



Proof:

We lower bound $Z(\beta)$ recursively
using "cluster expansions" [Hastings'05, KGK+'14]

$Z_n(\beta)$



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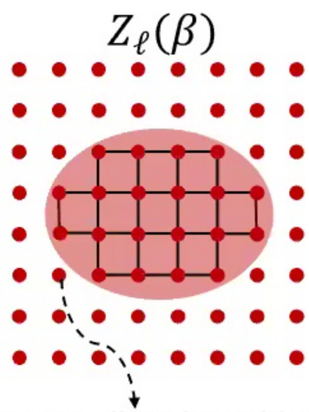
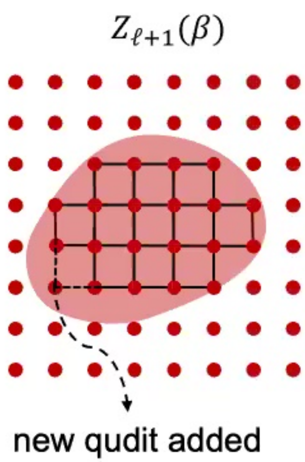
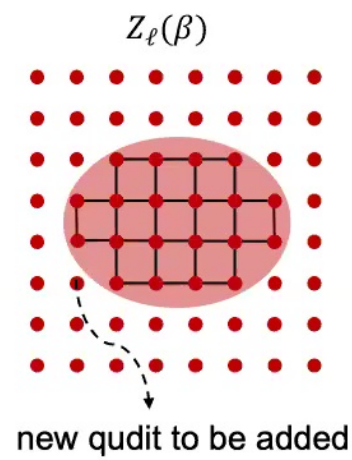


Proof:

First show

$$|Z_{\ell+1}(\beta)| \geq c^{-1}\, |Z_{\ell}(\beta)|$$





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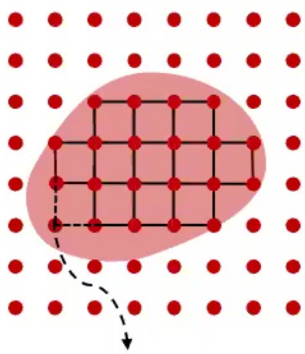
Repeat to get

$$|Z_n(\beta)| \geq c^{-n}|Z_1(\beta)|$$

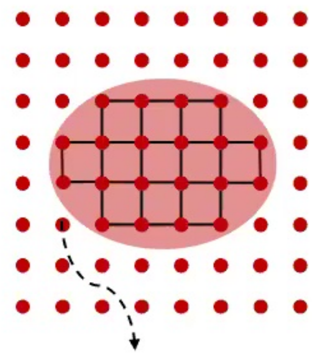
$$|\log Z_n(\beta)| \leq O(n)$$

$Z_{\ell+1}(\beta)$



new qudit added

$Z_\ell(\beta)$



new qudit to be added

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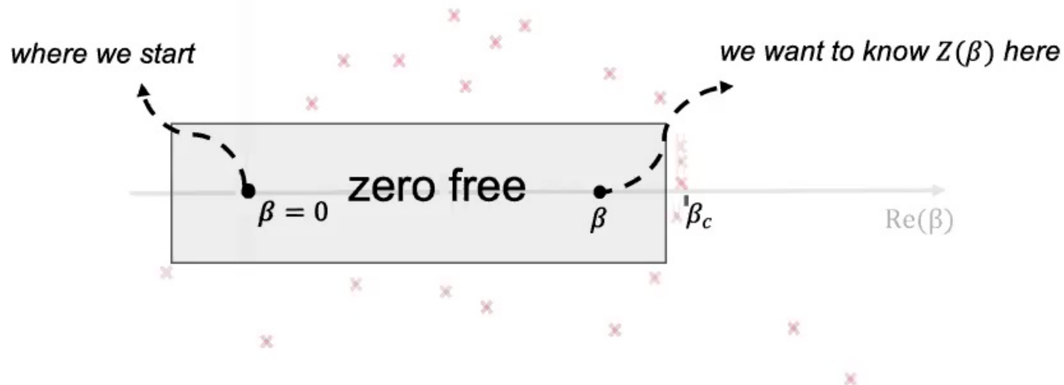
  - $|\log Z(\beta)| \leq O(n)$

$$\left|\log Z(\beta) - \sum_{\ell=0}^{K} \frac{1}{i!} \frac{d^{\ell} \log Z(0)}{d^{\ell}\beta} \beta^{\ell}\right| \leq O(n)\, e^{-\alpha K}$$



Proof:

How to show?

$$|Z_{\ell+1}(\beta)| \geq c^{-1}\,|Z_{\ell}(\beta)|$$

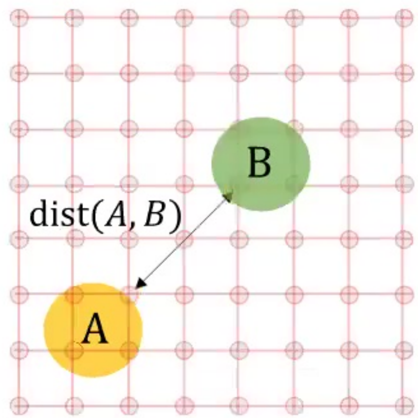
Cluster expansion: for $|\beta| \leq \beta_0$,

$$e^{-\beta H} \approx \sum \text{product of } H_i\text{ 's}$$

$$Z_{\ell+1}(\beta) = Z_{\ell}(\beta) + \text{corrections}$$

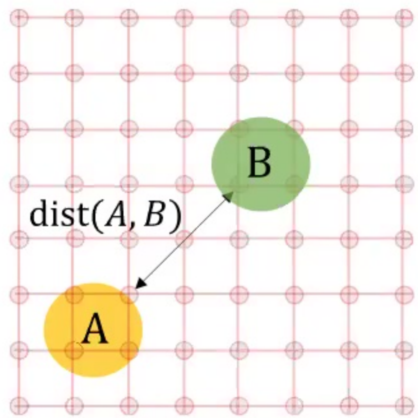
$$|\text{corrections}/Z_{\ell}(\beta)| \leq O(1)$$

Decay of correlations vs phase transition



$$|\operatorname{Tr}[AB\rho] - \operatorname{Tr}[A\rho]\operatorname{Tr}[B\rho]| \leq c\, e^{-\mathrm{dist}(A,B)/\xi}$$

Decay of correlations vs phase transition



$$|\,\mathrm{Tr}[AB\rho] - \mathrm{Tr}[A\rho]\mathrm{Tr}[B\rho]| \leq c\; e^{-\mathrm{dist}(A,B)/\xi}$$

Decay of correlations vs phase transition

Decay of correlations is
a signature of phase transition

- Above T_c exponential decay of correlations
- Below T_c there is long range order

Decay of correlations vs phase transition

Algorithmic implications?

- Classical spin systems [Weitz'99,…]

Mixing in time ← **Mixing in space**

Mixing in time ↓ efficient sampling algorithm

Mixing in space ↓ exponential decay of correlations

Decay of correlations vs phase transition

Algorithmic implications?

- Classical spin systems [Weitz'99,…]

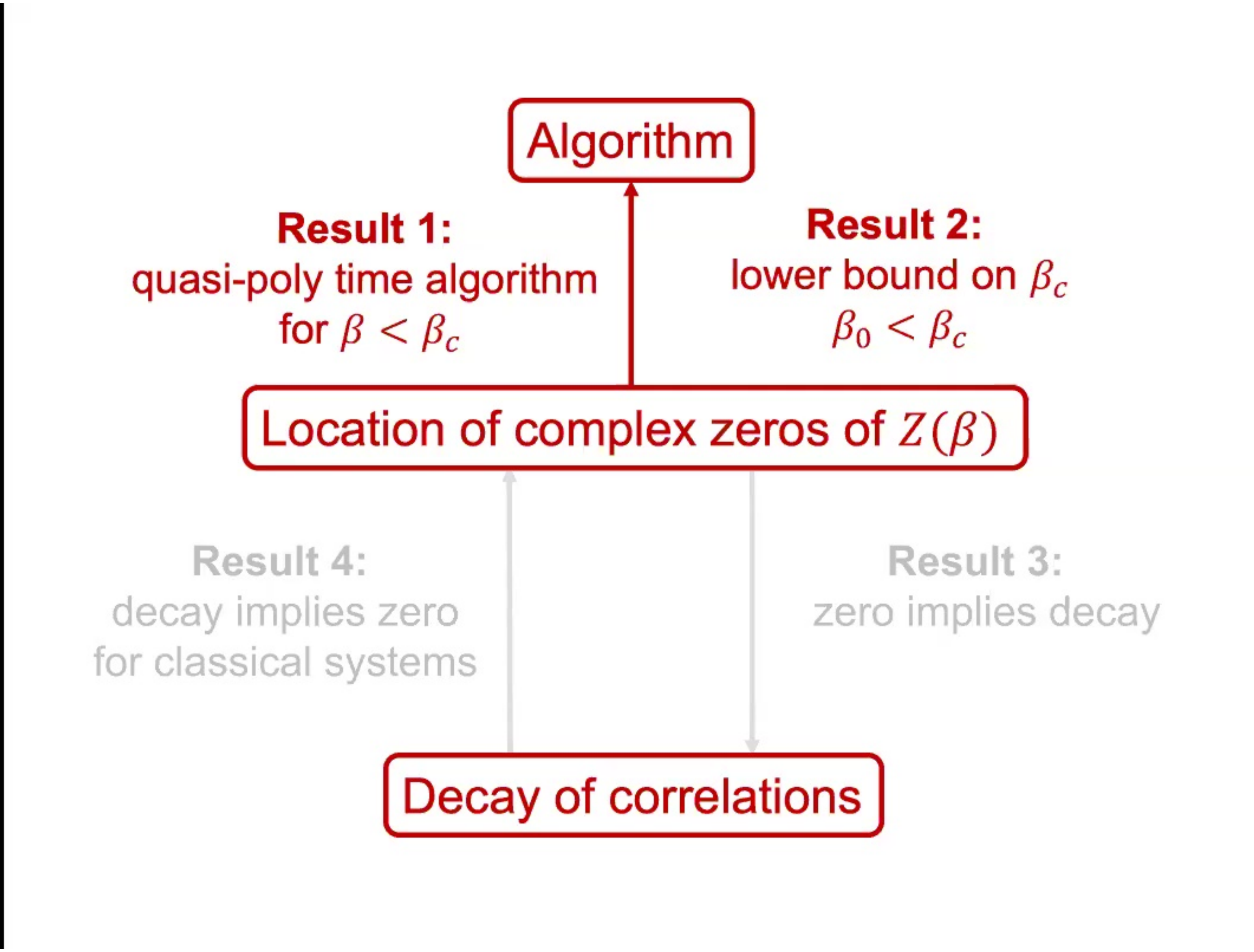
Mixing in time = Mixing in space

Mixing in time ↓ efficient sampling algorithm

Mixing in space ↓ exponential decay of correlations

- General Hamiltonians [BK'16]

Mixing in time ← Mixing in space + Decay of quantum CMI "Markov property"


Algorithm
Result 1:
quasi-poly time algorithm
for $\beta < \beta_c$
Result 2:
lower bound on β_c
$\beta_0 < \beta_c$
Location of complex zeros of $Z(\beta)$
Result 4:
decay implies zero
for classical systems
Result 3:
zero implies decay
Decay of correlations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What is the relation between
zeros of $Z(\beta)$ and decay of correlations?

For translationally-invariant ***classical***
system proved to be equivalent [DS'85]

How about quantum systems?

Result 3

We show absence of zeros near real axis implies exponential decay of correlations

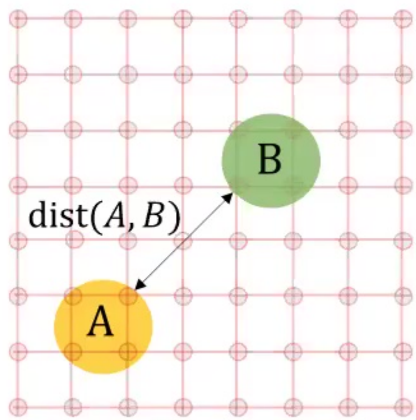
When

- For any quantum system if $\mathrm{dist}(A, B) = \Omega(\log n)$
- H consists of commuting terms $H = \sum_i H_i$, $[H_i, H_j] = 0$
- General H on a one-dimensional chain

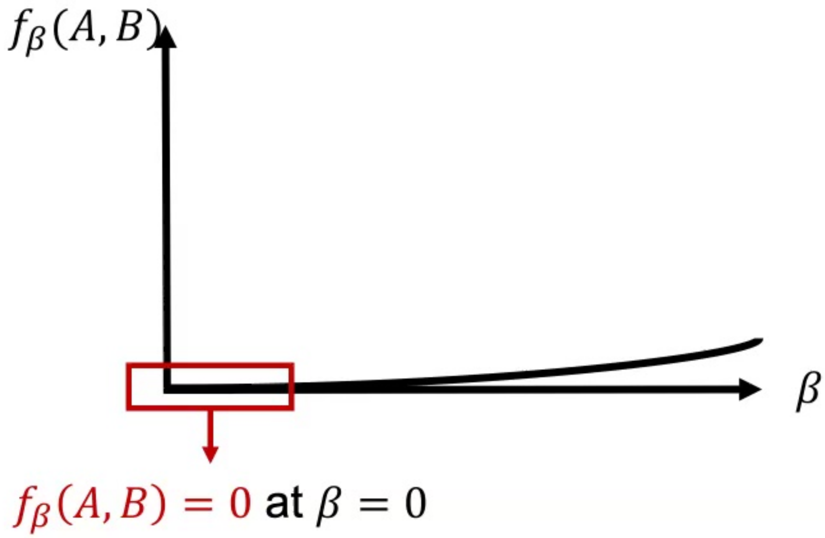
Proof: Similar to the extrapolation idea in our algorithm and the one used in [DS'85]

- Define a function that measures correlations btw A, B

$$f_\beta(A, B)$$



We show



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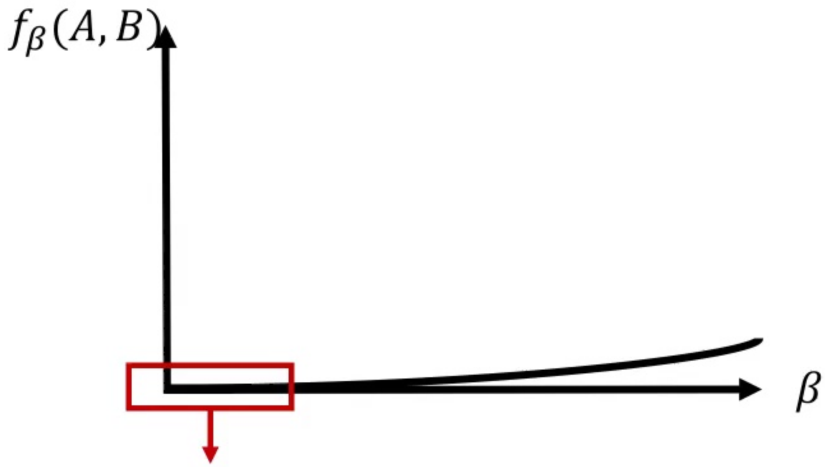
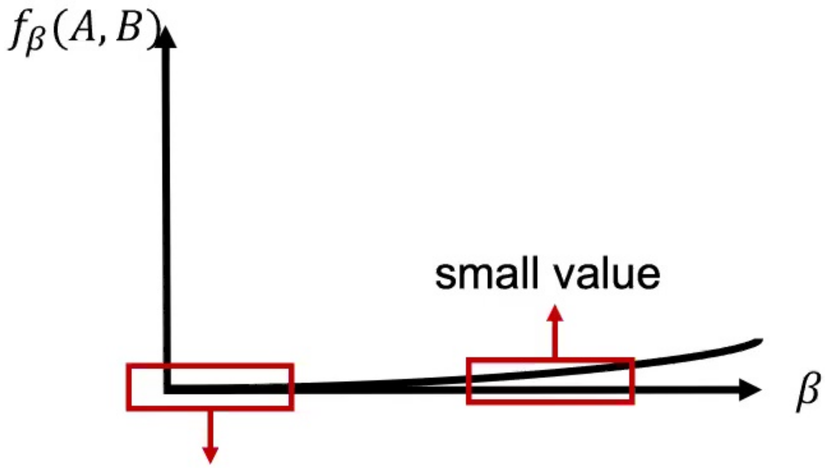


$f_\beta(A,B) = 0$ at $\beta = 0$

$\frac{d^m}{d\beta^m} f_\beta(A,B) = 0$ for $m < O(\text{dist}(A,B))$

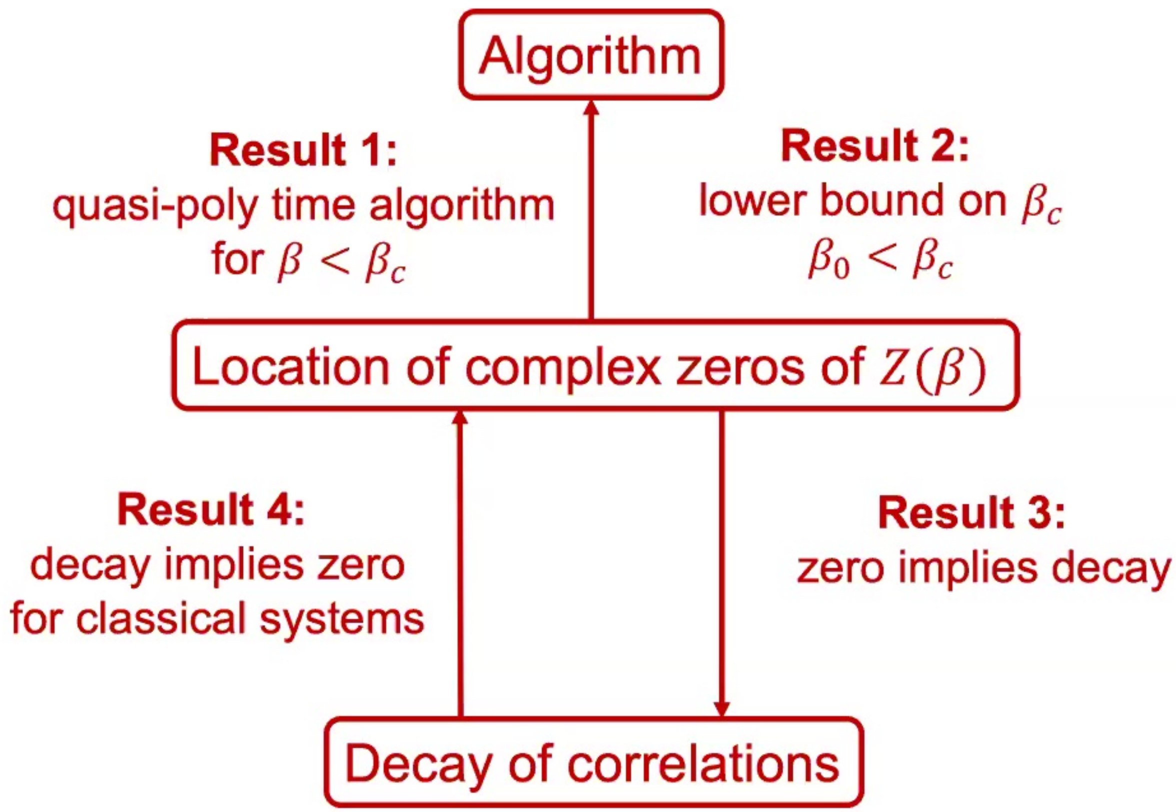
We show



$f_\beta(A, B) = 0$ at $\beta = 0$

\+ $f_\beta(A, B)$ analytic

$$\frac{d^m}{d\beta^m} f_\beta(A, B) = 0 \text{ for } m < O(\mathrm{dist}(A, B))$$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Result 4:

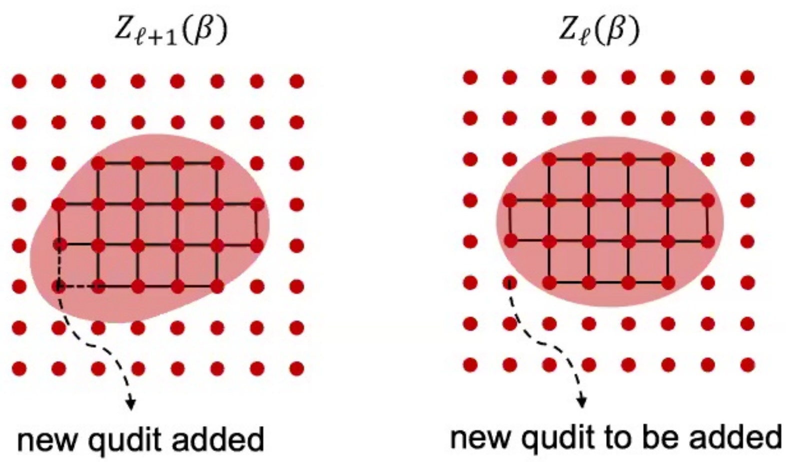
Decay of correlations at real temperature β

implies no zeros close to real axis at β

- Proved for translationally-invariant classical systems [DS'85]
- We can extend their proof for general classical systems

Rough high level idea

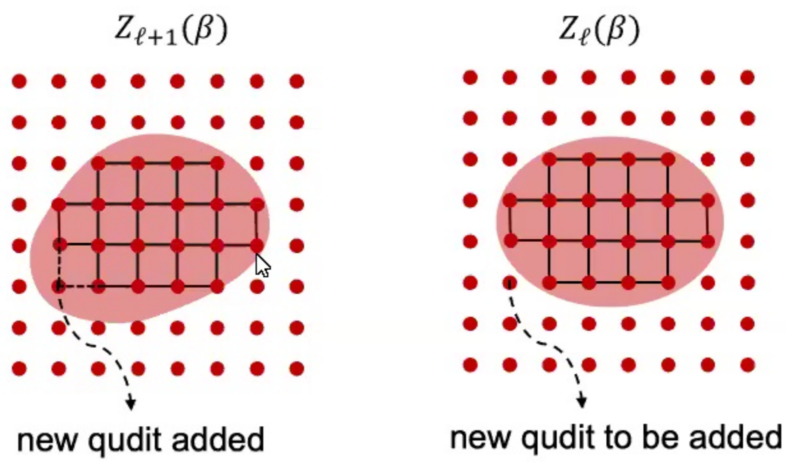
Similar to **Result 2**

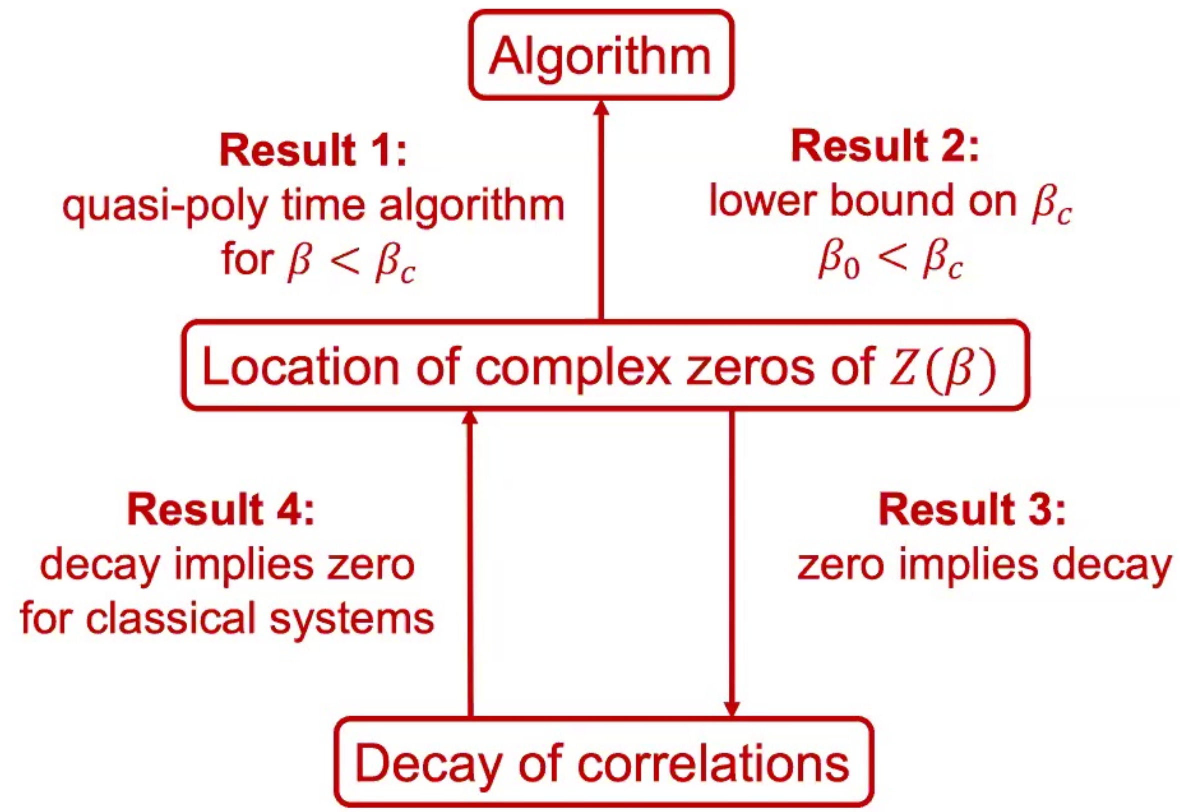


Rough high level idea

Similar to **Result 2**

Instead of cluster expansions use decay of correlations

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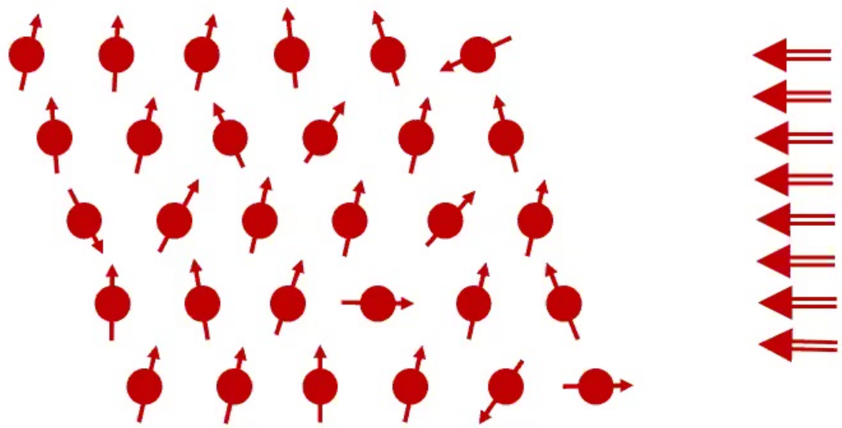
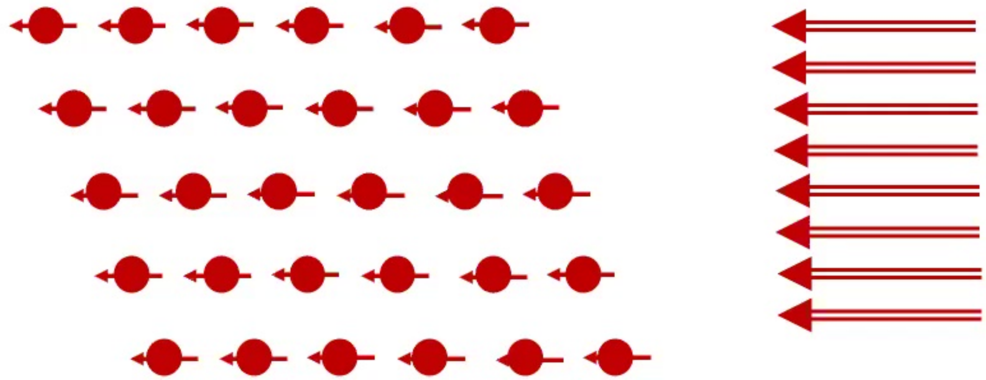
Extrapolating in external field



Extrapolating in external field



Easy regime

Result 5:

Ferromagnetic Heisenberg model

$$H = -\sum_{ij} K_{ij} Z_i Z_j - \sum_{ij} J_{ij}\left(X_i X_j + Y_i Y_j\right) - \sum_i J_i Z_i$$

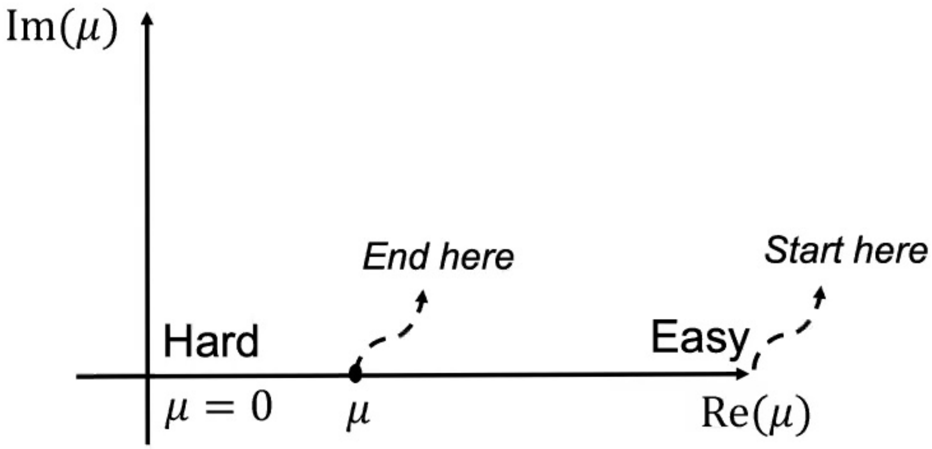
$$K_{ij} \geq |J_{ij}|$$

Result 5:

Ferromagnetic Heisenberg model

$$H = -\sum_{ij} K_{ij} Z_i Z_j - \sum_{ij} J_{ij}\left(X_i X_j + Y_i Y_j\right) - \mu \sum_i J_i Z_i$$

$$K_{ij} \geq |J_{ij}|$$



Result 5:

Ferromagnetic Heisenberg model

$$H = -\sum_{ij} K_{ij} Z_i Z_j - \sum_{ij} J_{ij}\left(X_i X_j + Y_i Y_j\right) - \mu \sum_i J_i Z_i$$

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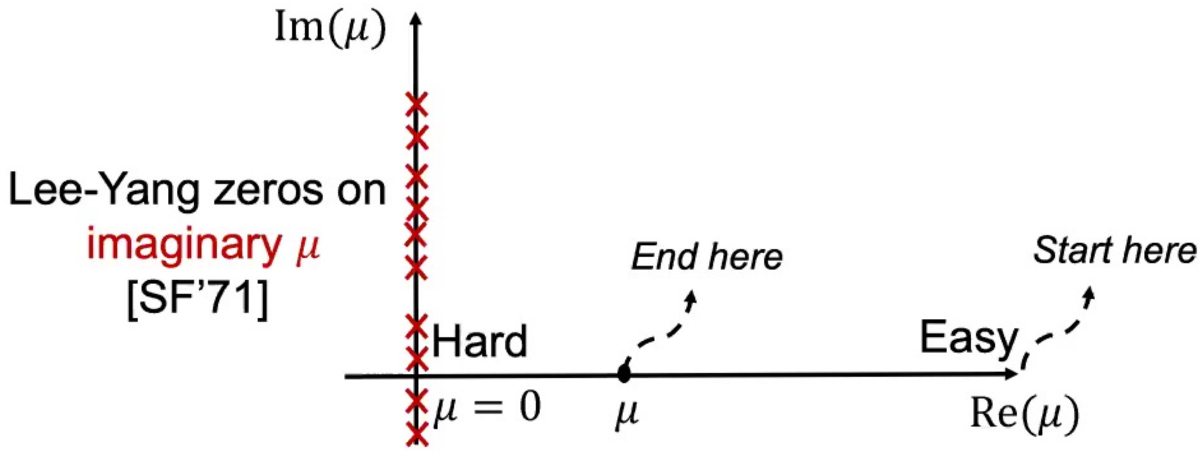


Previously, polynomial time algorithm for ferromagnetic XY model [BG'17]

$$H = -\sum_{ij} b_{ij} X_i X_j - \sum_{ij} c_{ij} Y_i Y_j - \sum_i d_i Z_i$$

$$b_{ij} \geq |c_{ij}|$$

Solved by reducing to counting perfect matchings

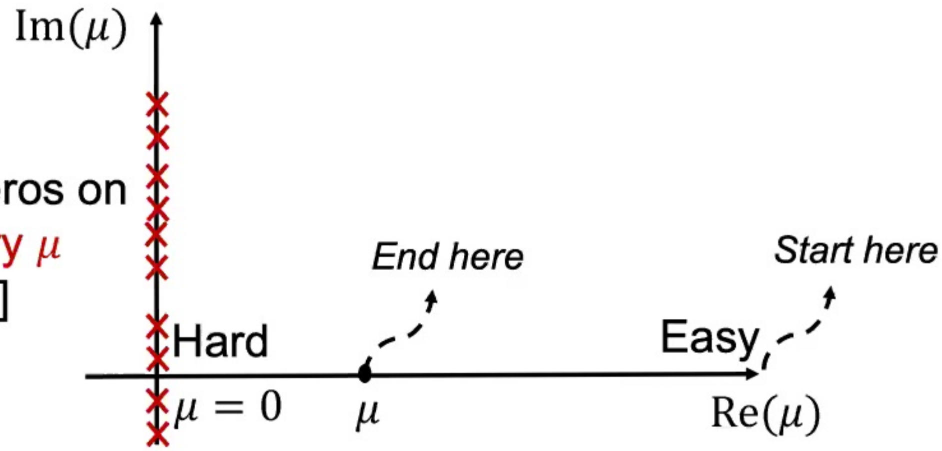
Result 5:

Ferromagnetic Heisenberg model

$$H = -\sum_{ij} K_{ij} Z_i Z_j - \sum_{ij} J_{ij}\left(X_i X_j + Y_i Y_j\right) - \mu \sum_i J_i Z_i$$

$$K_{ij} \geq |J_{ij}|$$

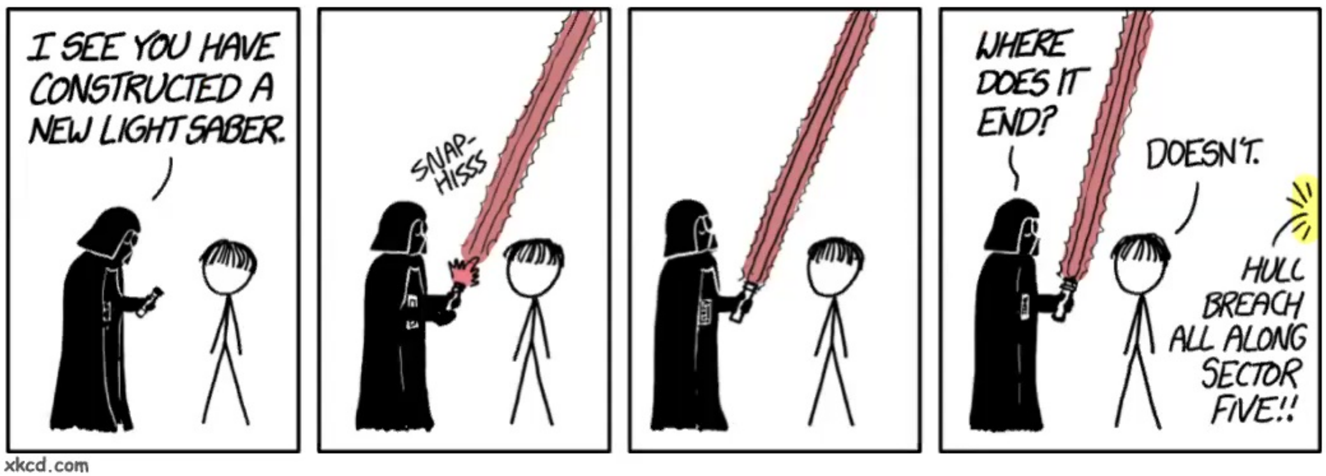
Lee-Yang zeros on imaginary μ [SF'71]



Open questions

- Fully establish the equivalence between absence of complex zeros and decay of correlations
- Absence of zeros implies decay of quantum CMI?
- A regime where quantum computer can't sample but extrapolation works?
- Other applications for extrapolation (avoiding sign problem, adiabatic algorithms,…)
- Other algorithms for $Z(\beta)$ like convex relaxations?

Thanks!


I SEE YOU HAVE CONSTRUCTED A NEW LIGHTSABER.
SNAP-HISSS
WHERE DOES IT END?
DOESN'T.
HULL BREACH ALL ALONG SECTOR FIVE!!
xkcd.com