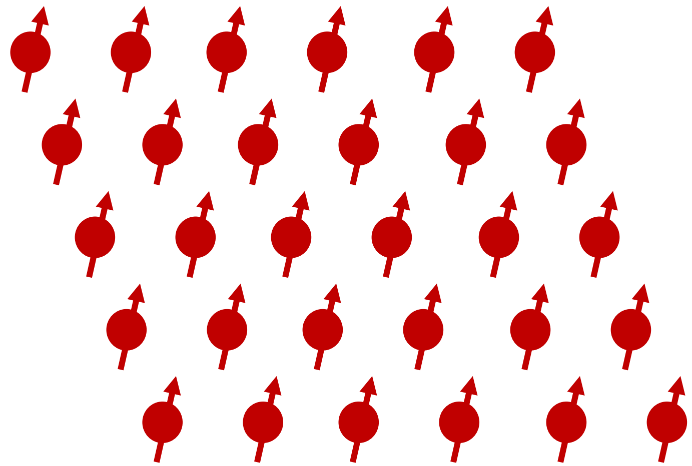
Counting without Sampling:

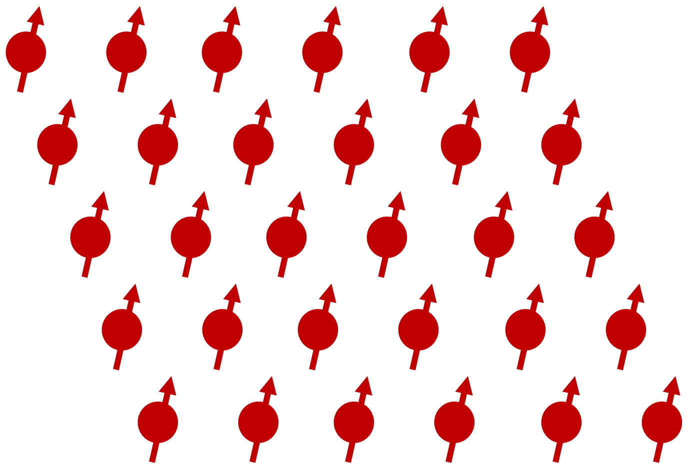
Approximation Algorithms for Quantum Many-Body Systems at *Finite Temperatures*

Mehdi Soleimanifar (MIT)

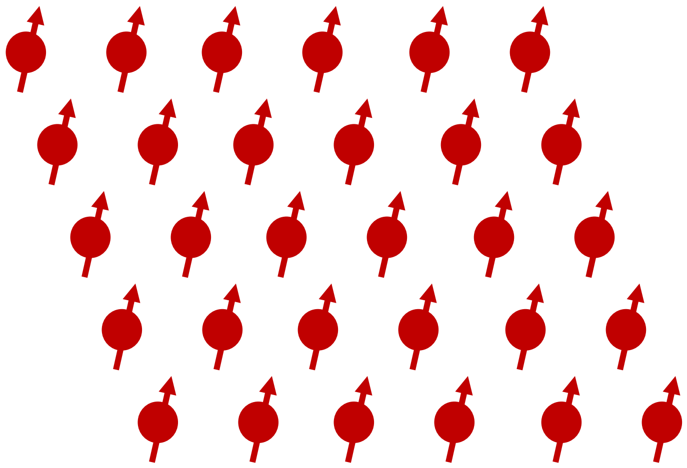
Joint work with

Aram Harrow and Saeed Mehraban (MIT)





n qudits (or spins) on a lattice



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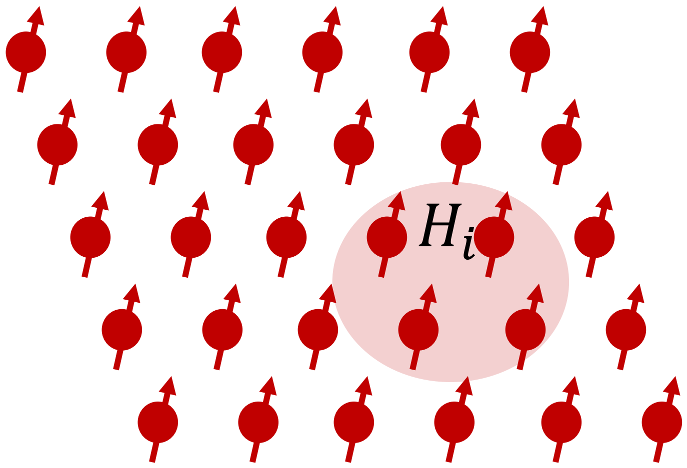
Interactions described by $H = \sum_i H_i$



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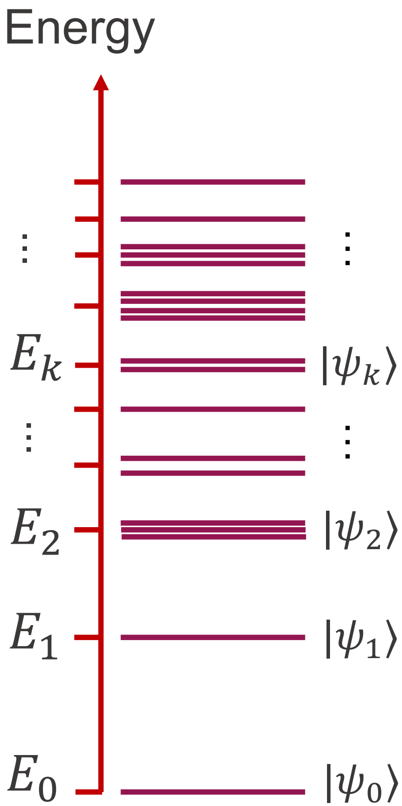
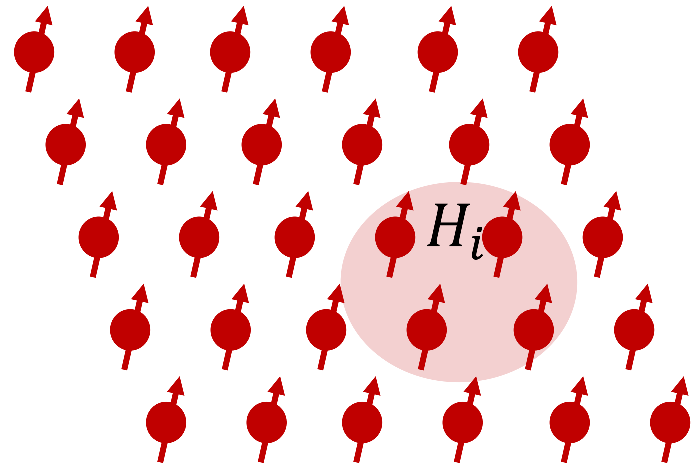
Interactions described by $H = \sum_i H_i$

H_i acting on a geometrically-local region





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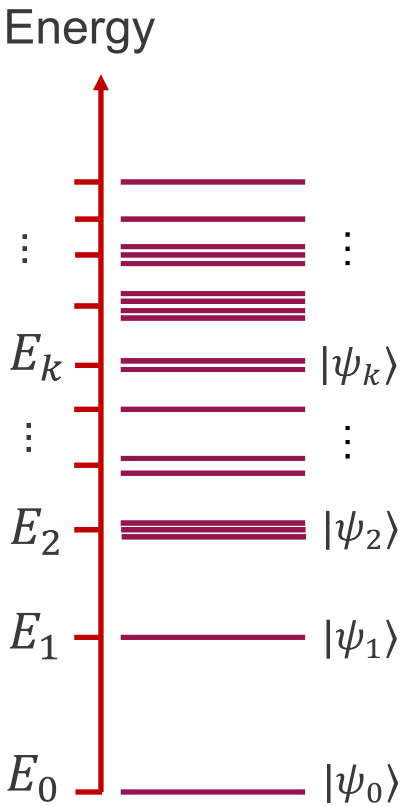

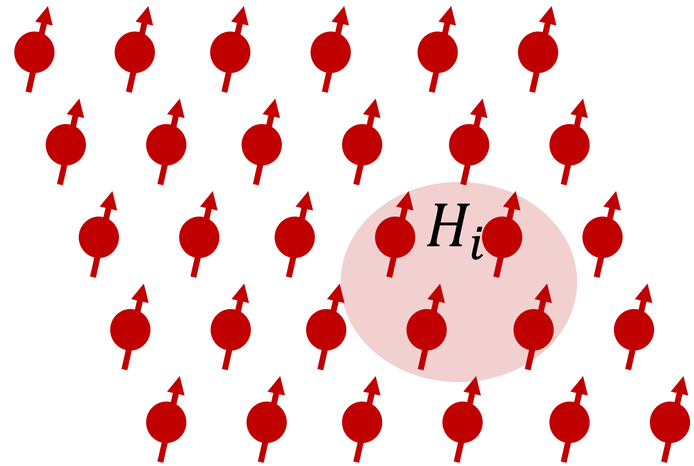

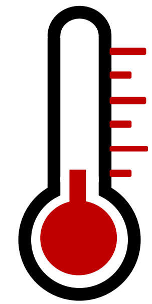

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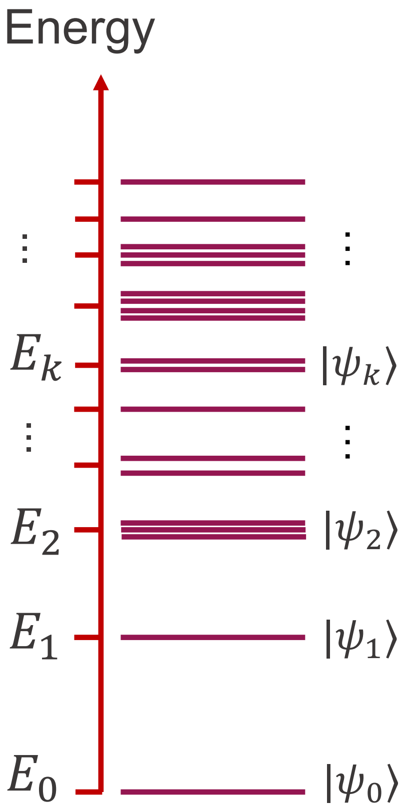
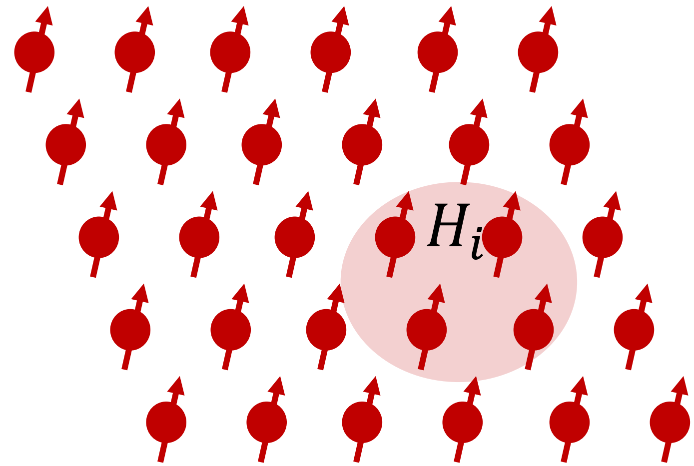
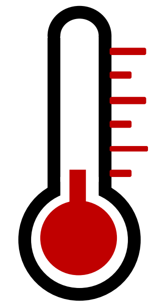
At zero temperature







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Interactions described by $H = \sum_i H_i$

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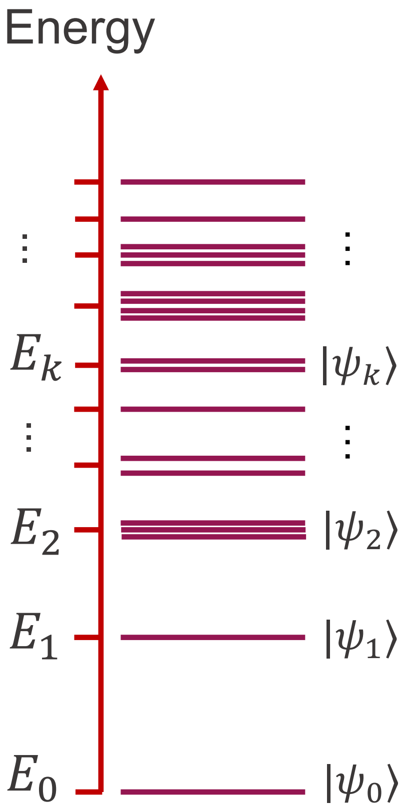
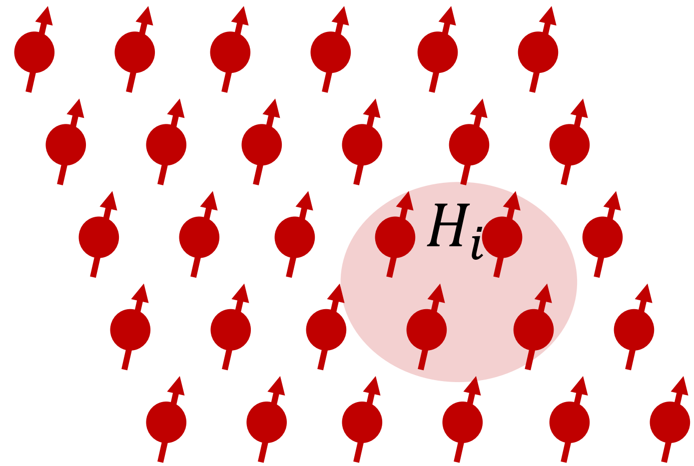
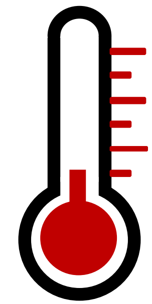
At zero temperature, in the ground state $|\psi_0\rangle$







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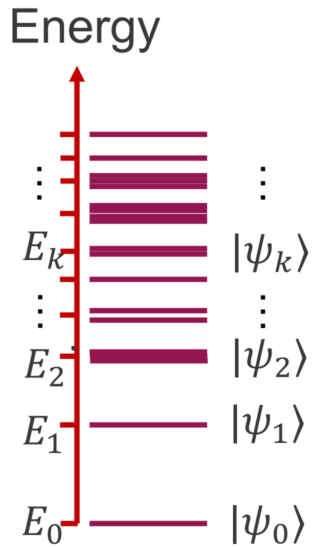
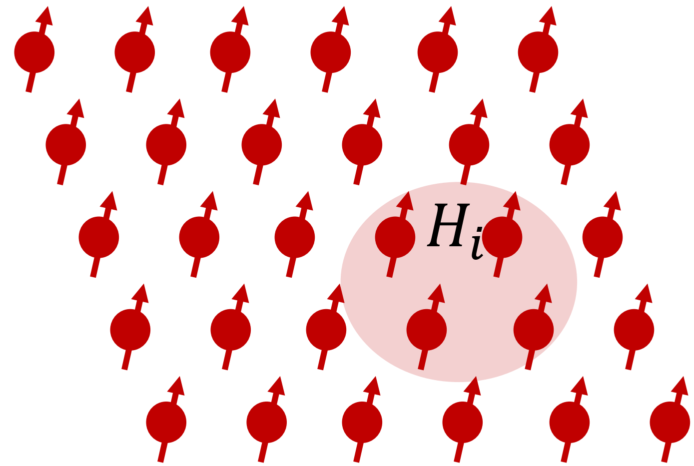
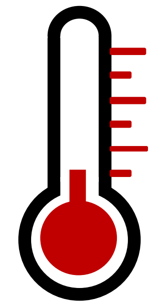
At zero temperature, in the ground state $|\psi_0\rangle$ with energy E_0







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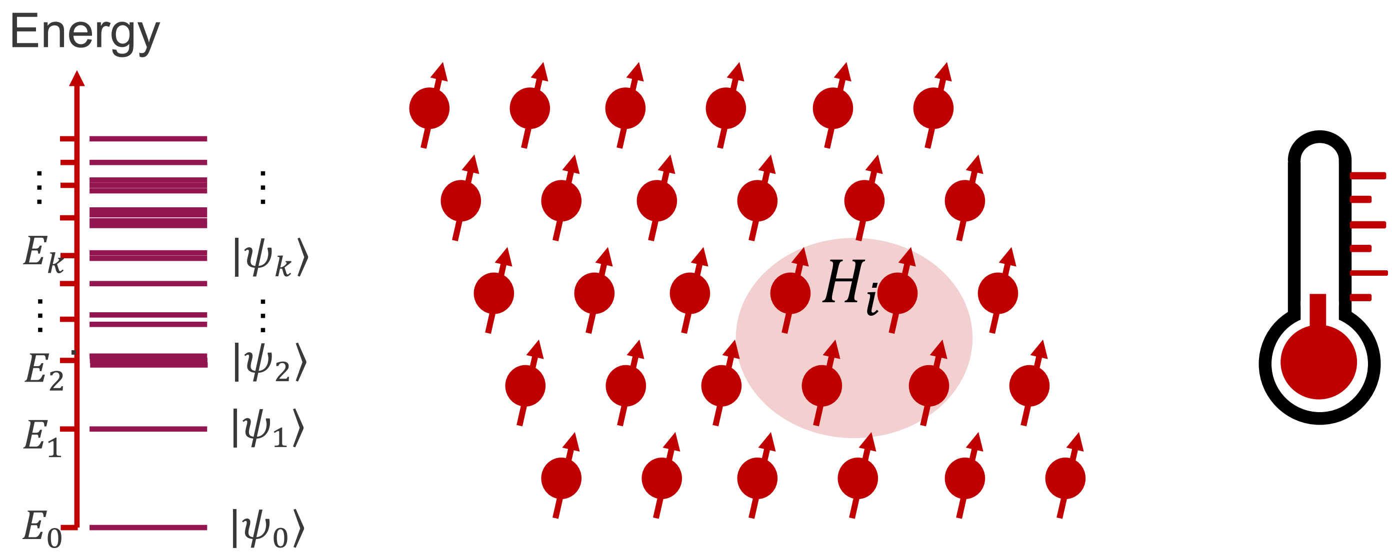
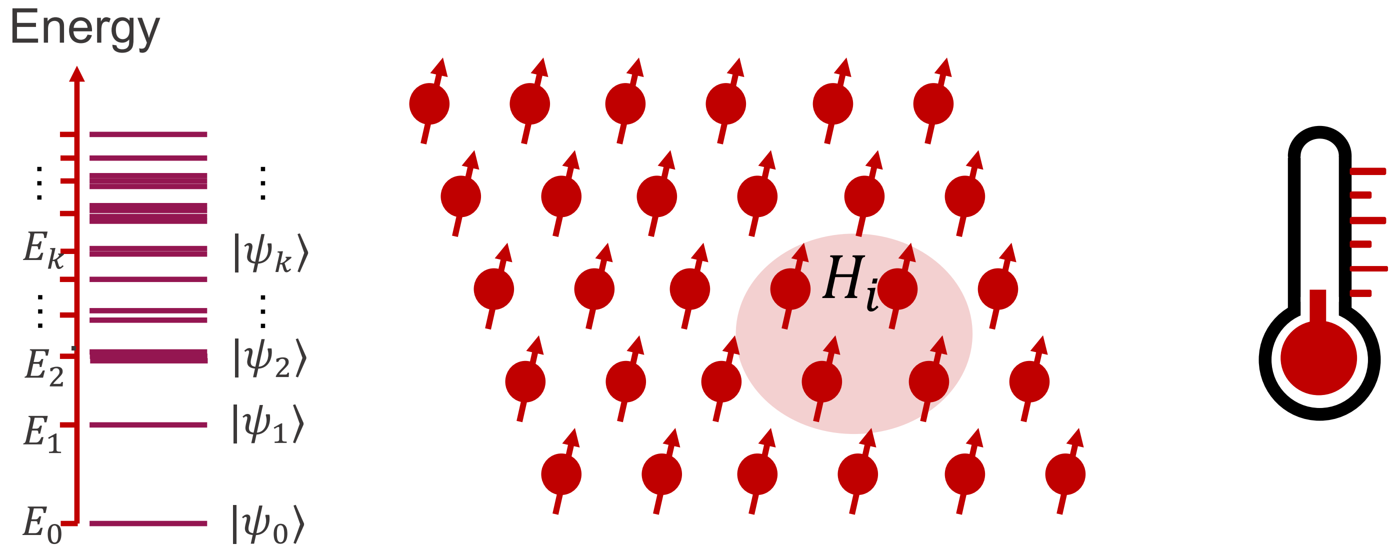


How hard is it to approximate E_0 in the worst case?



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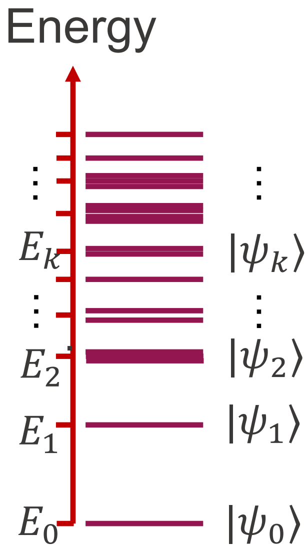
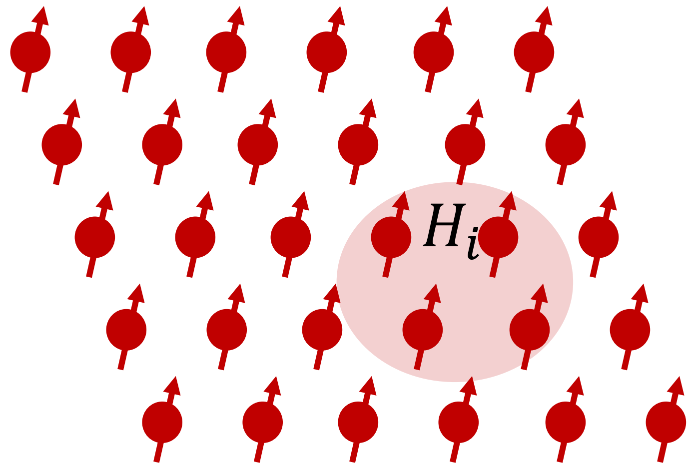
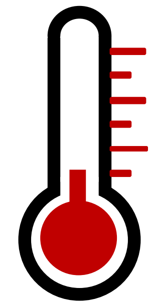
It is QMA-complete [K'02, KKR'05, …]







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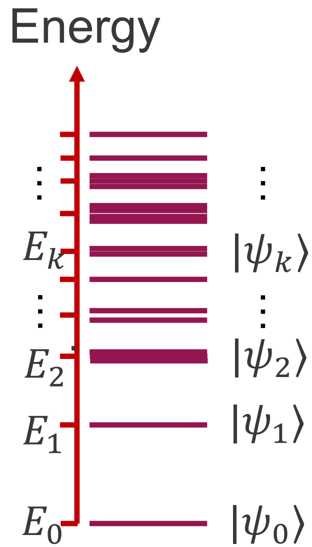

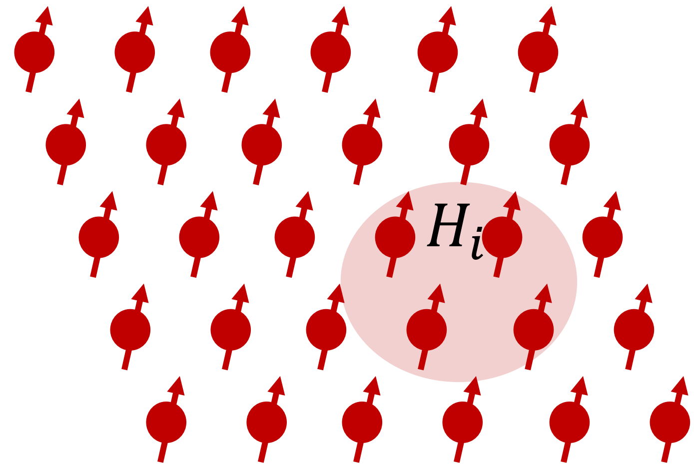

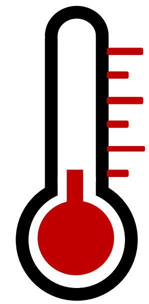

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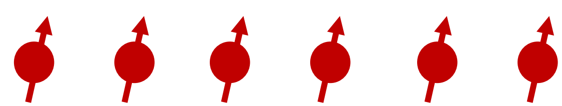
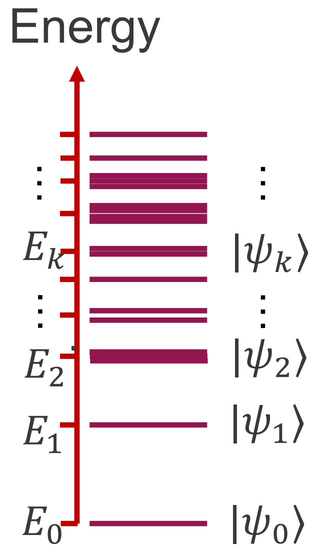
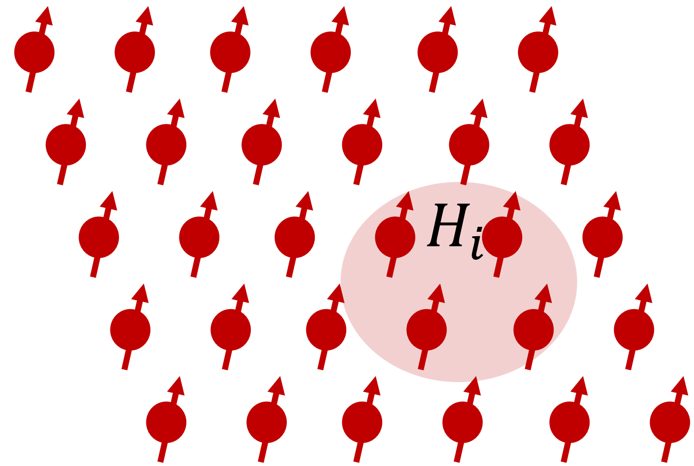
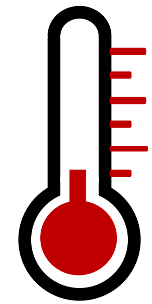
1D Lattice
H gapped









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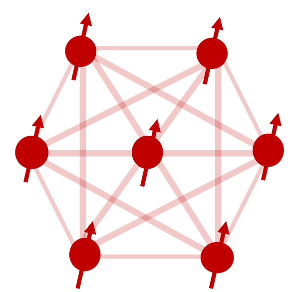
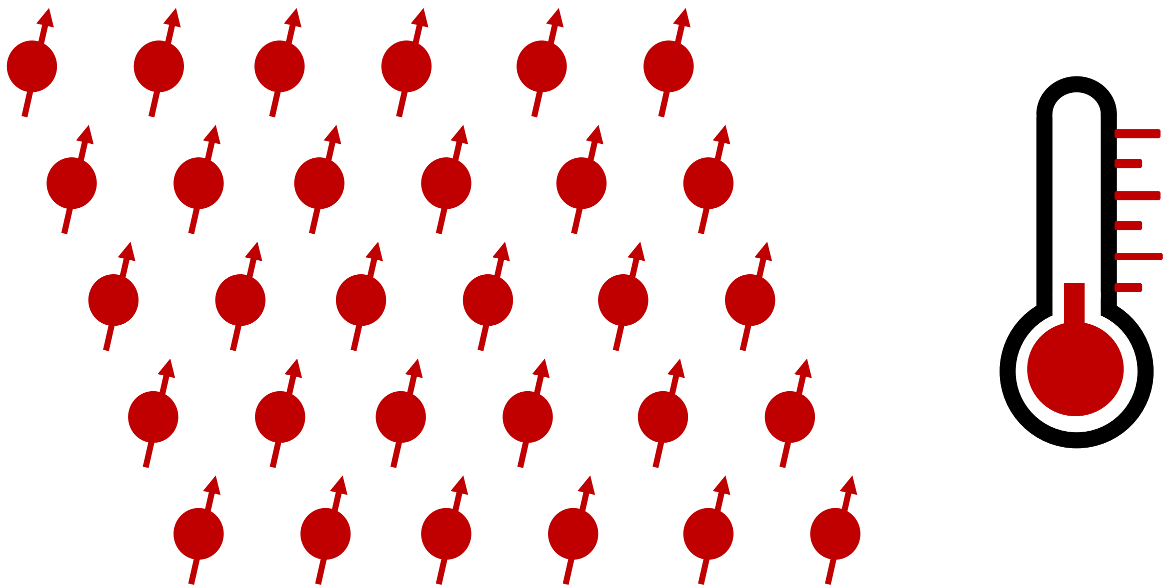
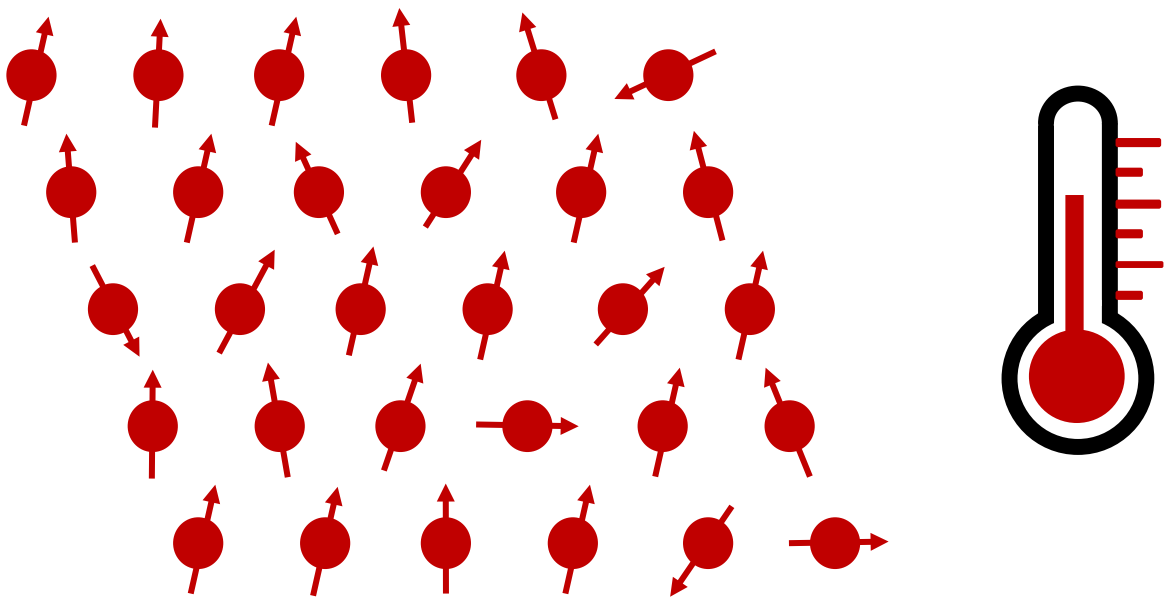
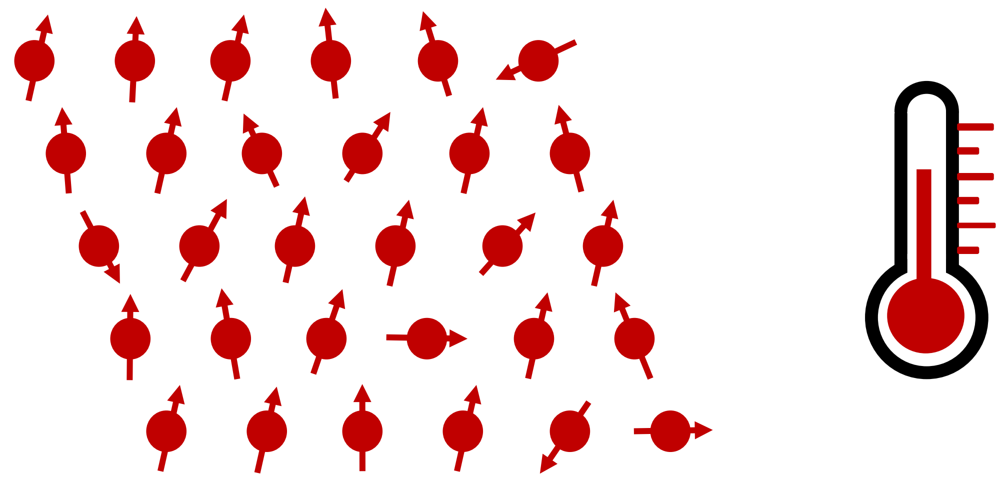
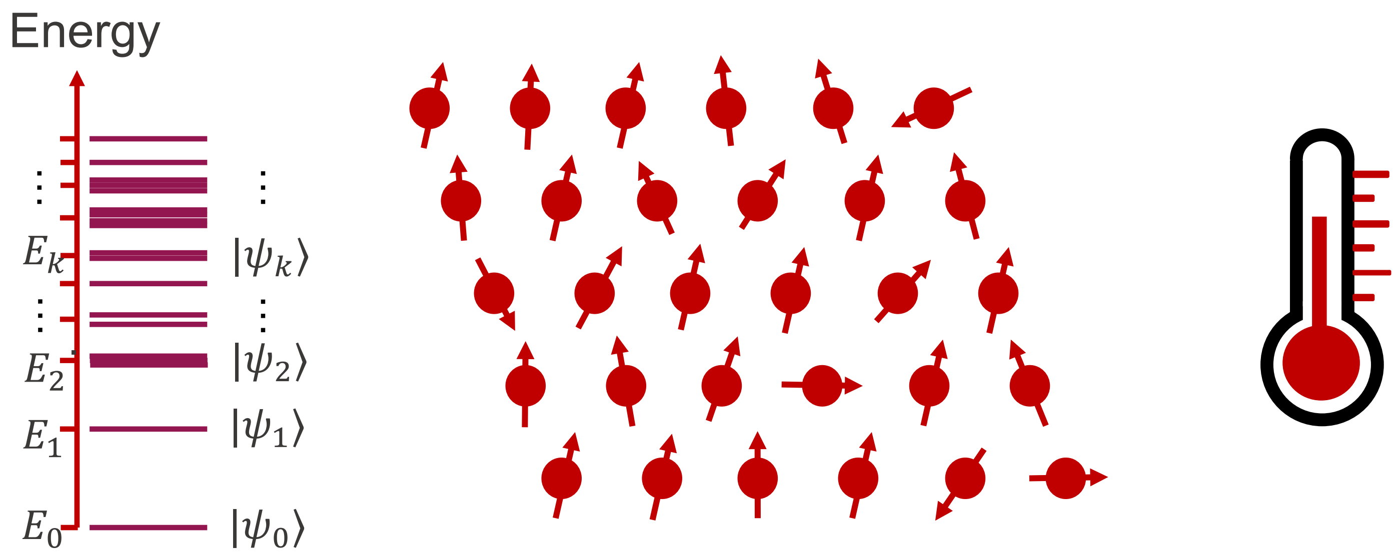
Dense Lattice



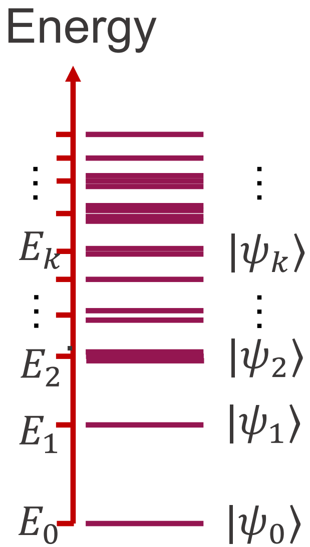


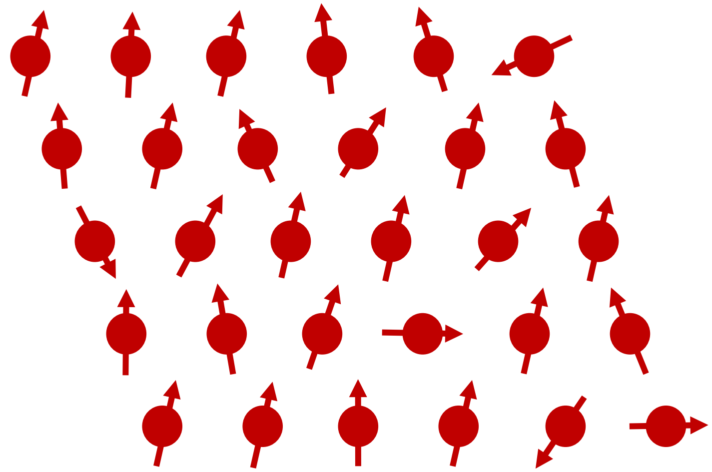


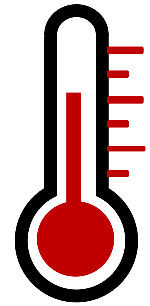




At non-zero temperature $T = 1/\beta$

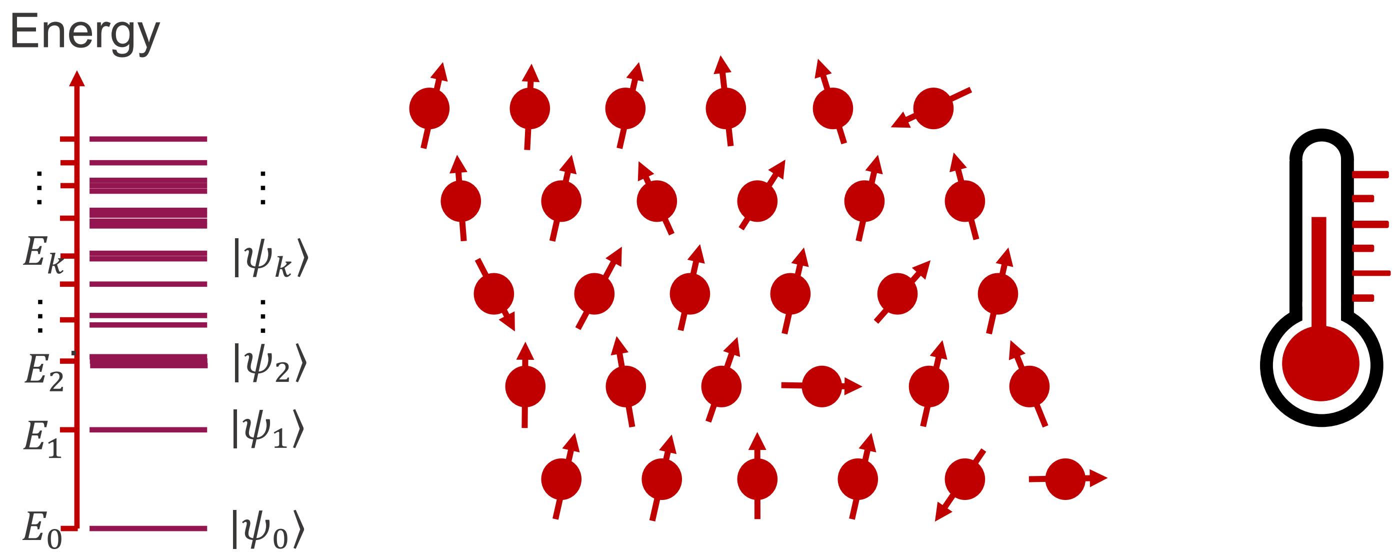






At non-zero temperature $T = 1/\beta$, system in state

$$\rho \propto \sum_k e^{-\beta E_k} |\psi_k\rangle\langle\psi_k|$$



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

Gibbs state

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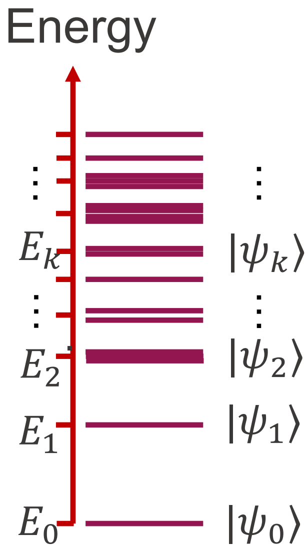
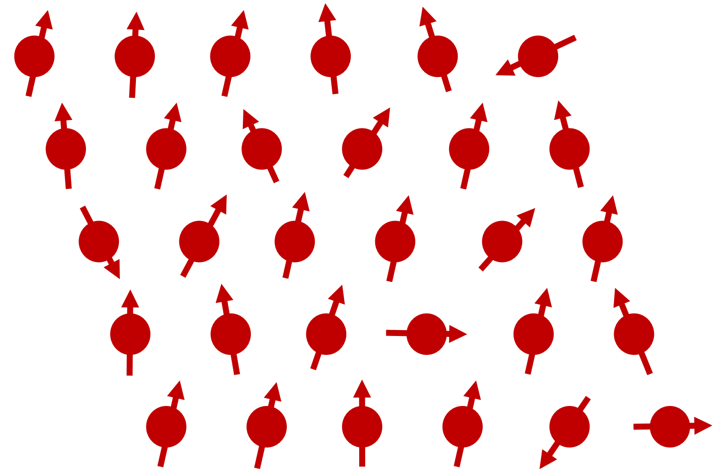
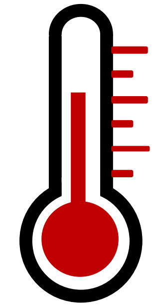




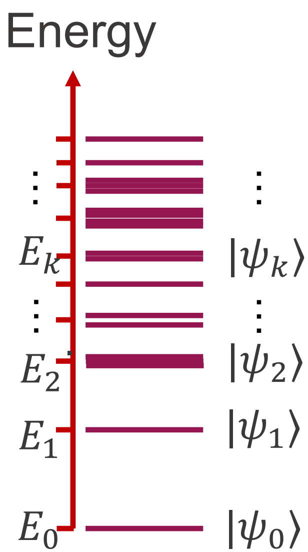


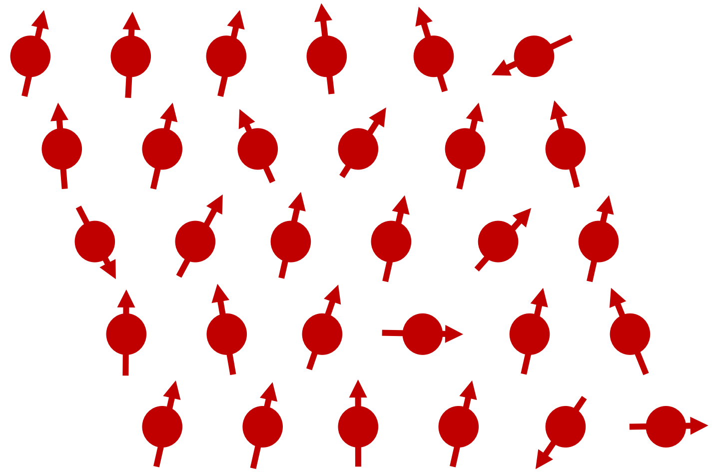
At non-zero temperature $T = 1/\beta$, system in state

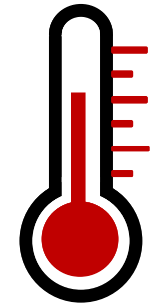
Gibbs state

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

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







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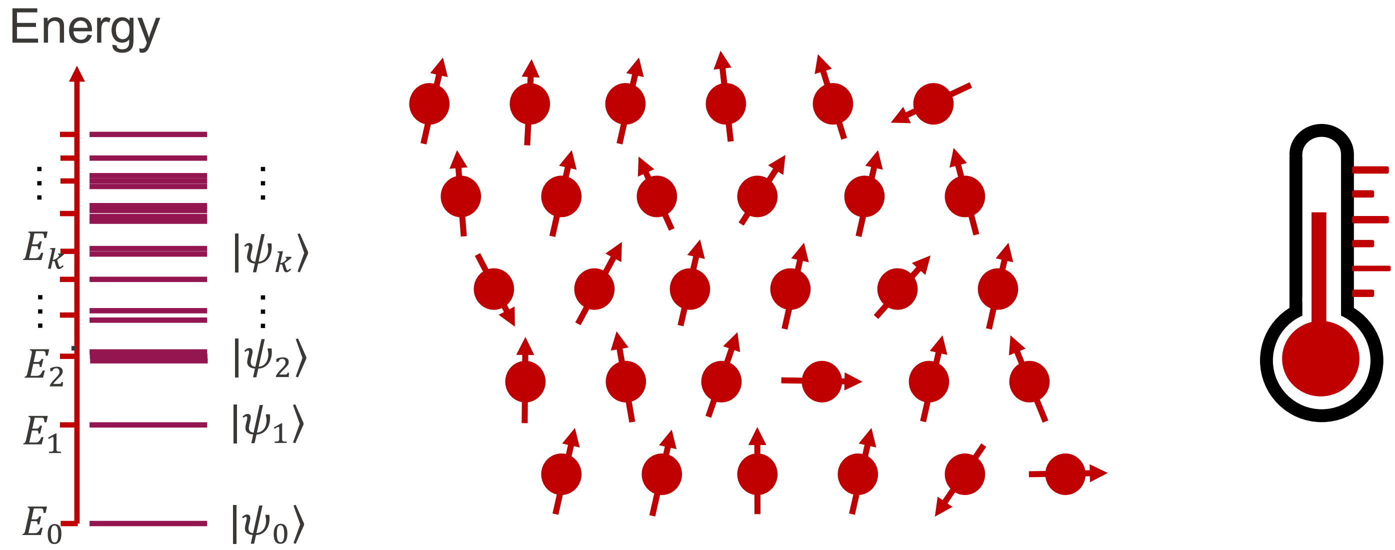
Partition function $Z(\beta) = \sum_k e^{-\beta E_k} = \mathrm{Tr}[e^{-\beta H}]$



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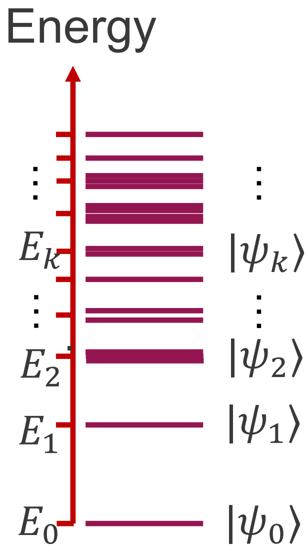

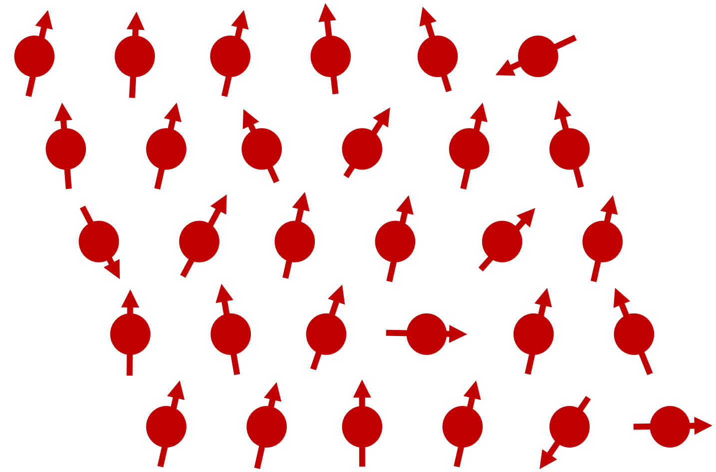

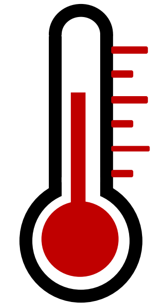

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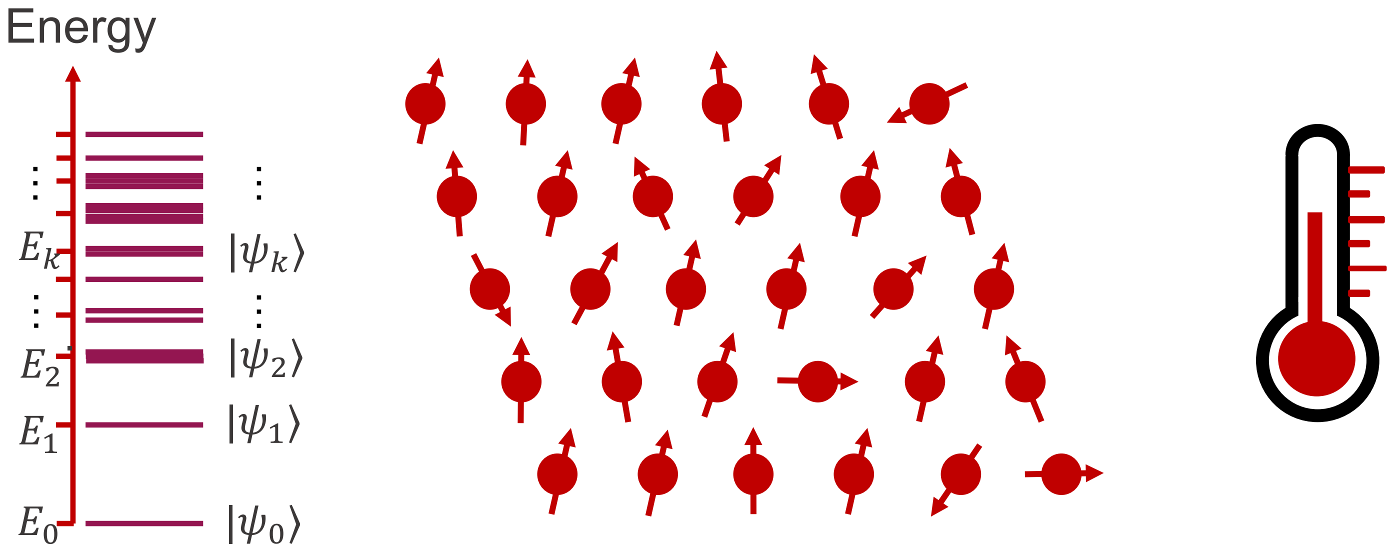

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Free energy

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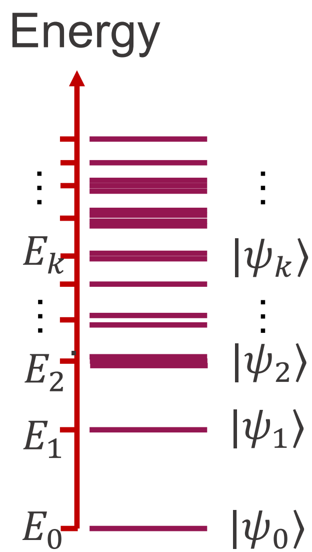

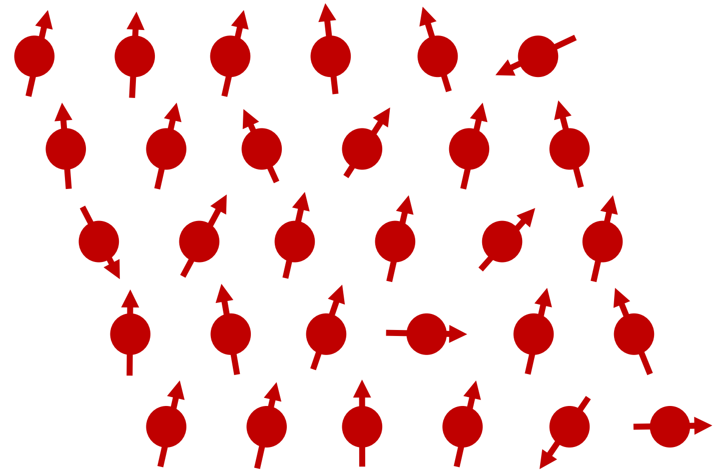

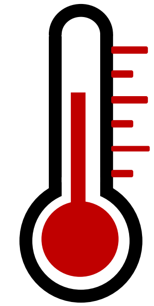

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Finding $Z(\beta)$ exactly is $\#\mathrm{P}$-hard [Val'79]

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Goal: design an algorithm that

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Input:

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$$|\log Z(\beta) - \log \hat{Z}(\beta)| \leq 1/\mathrm{poly(n)}$$

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Goal: design an algorithm that

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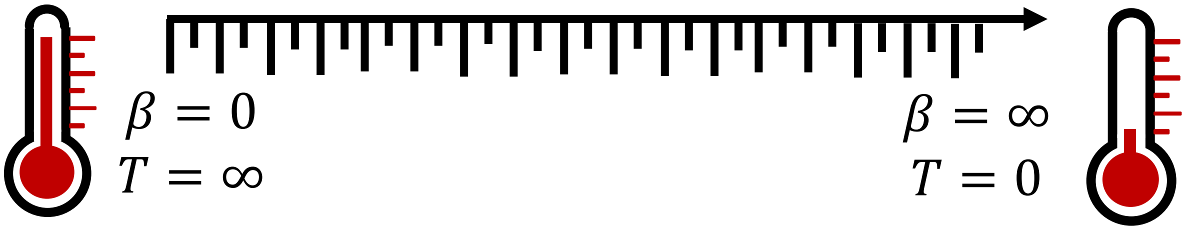
Hardness depends on temperature



$\beta = 0$
$T = \infty$
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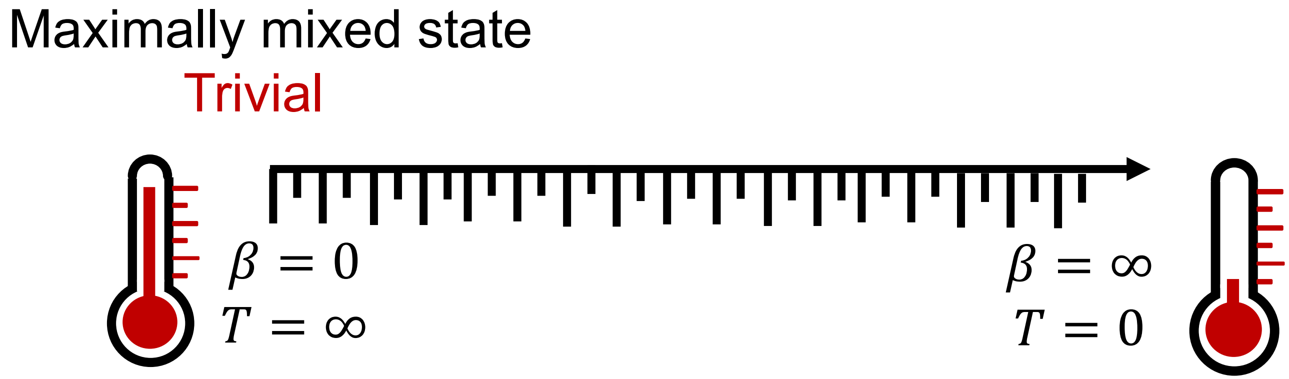
Maximally mixed state
Trivial
$\beta = 0$
$T = \infty$
$\beta = \infty$
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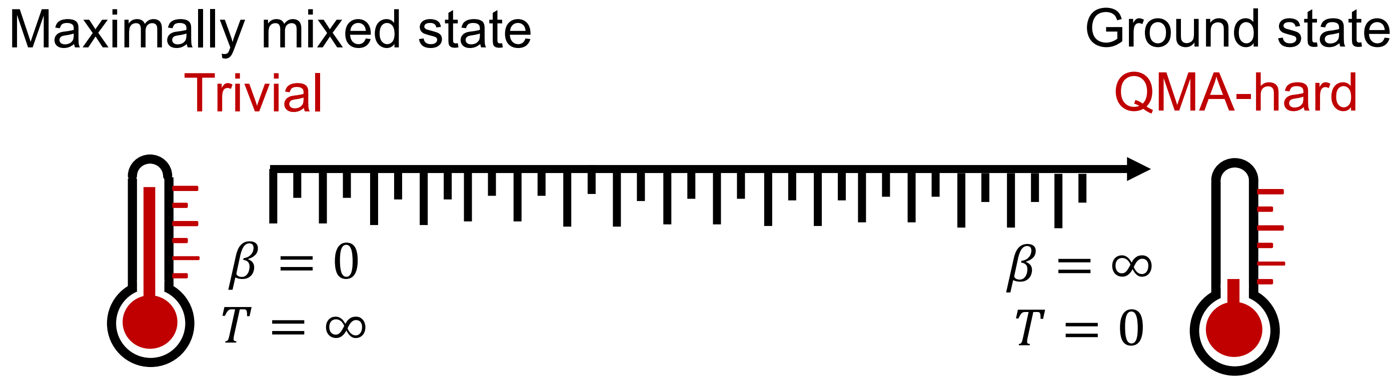
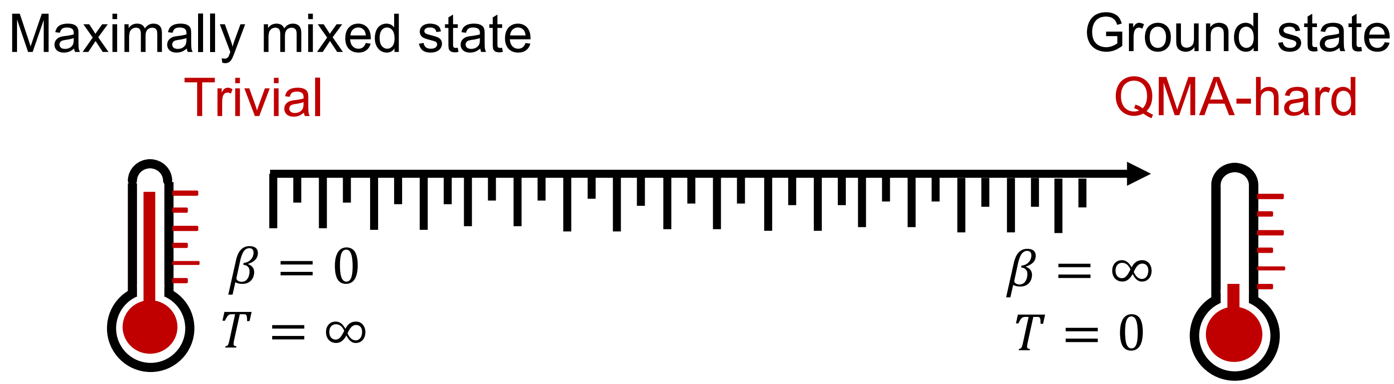


Maximally mixed state
Trivial
$\beta = 0$
$T = \infty$
Ground state
QMA-hard
$\beta = \infty$
$T = 0$



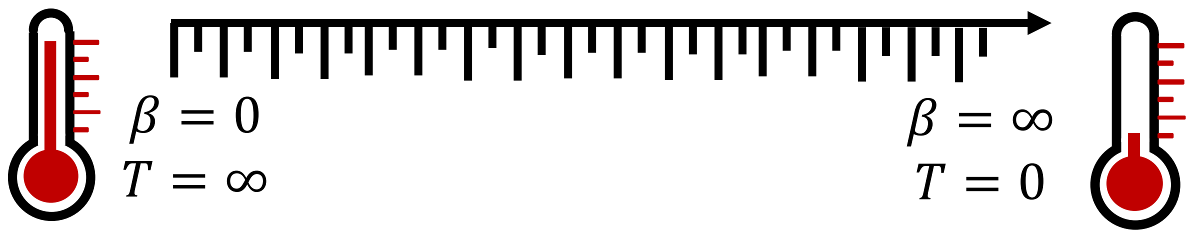
Transition in the hardness

Maximally mixed state

Trivial

Ground state

QMA-hard



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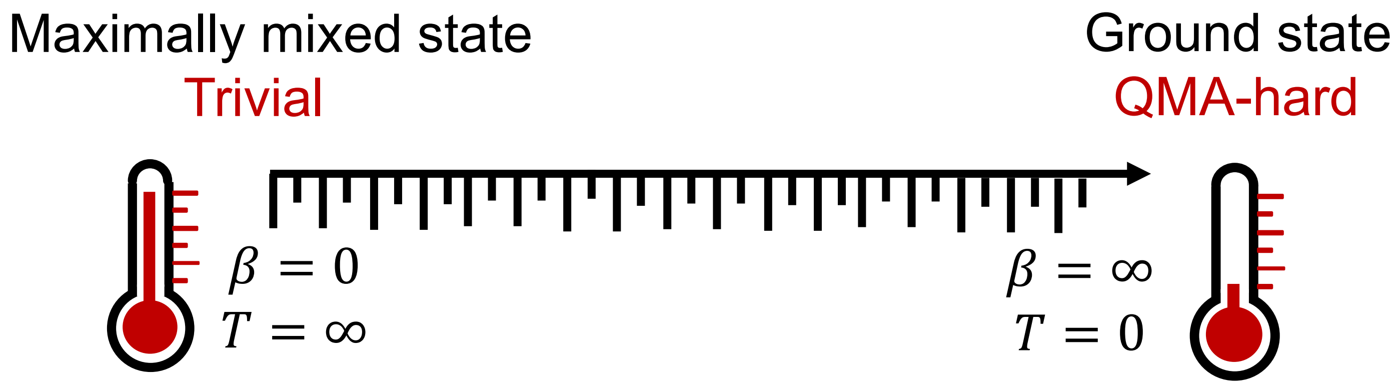

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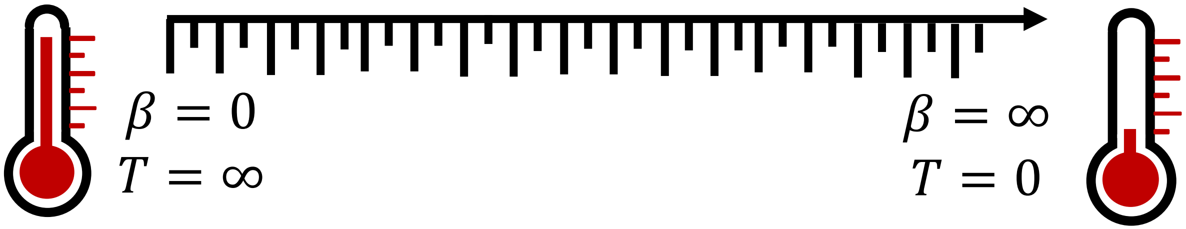

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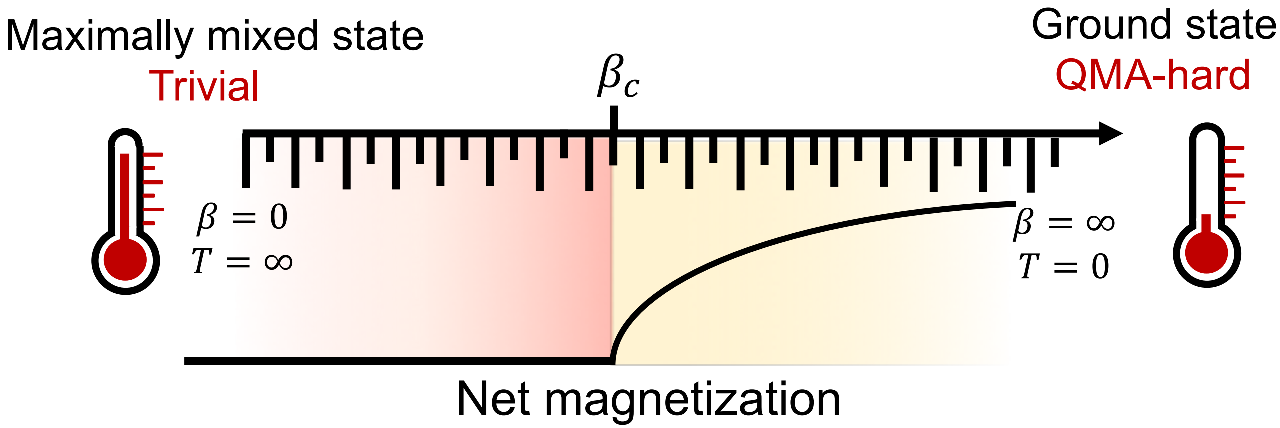
Physical properties abruptly change



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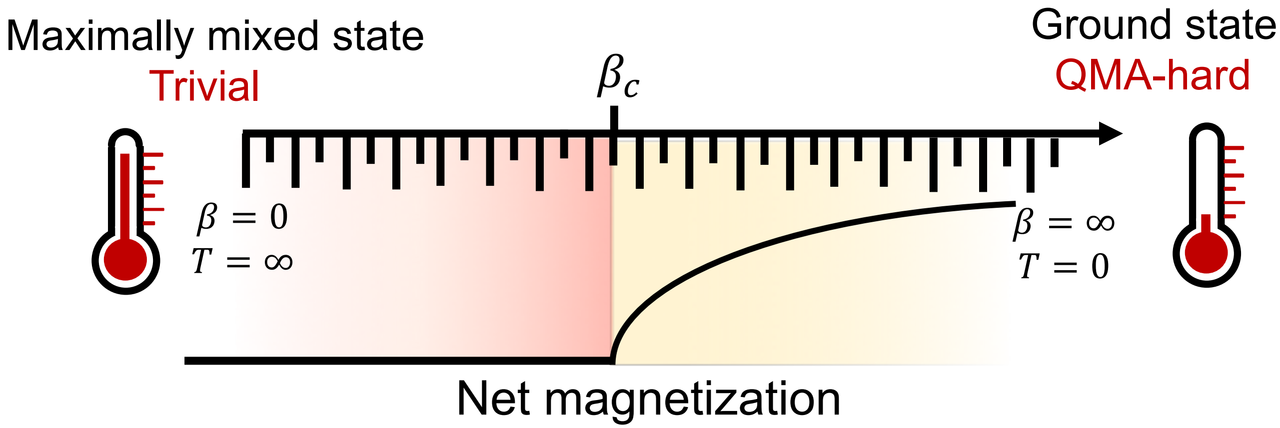

Transition in the hardness

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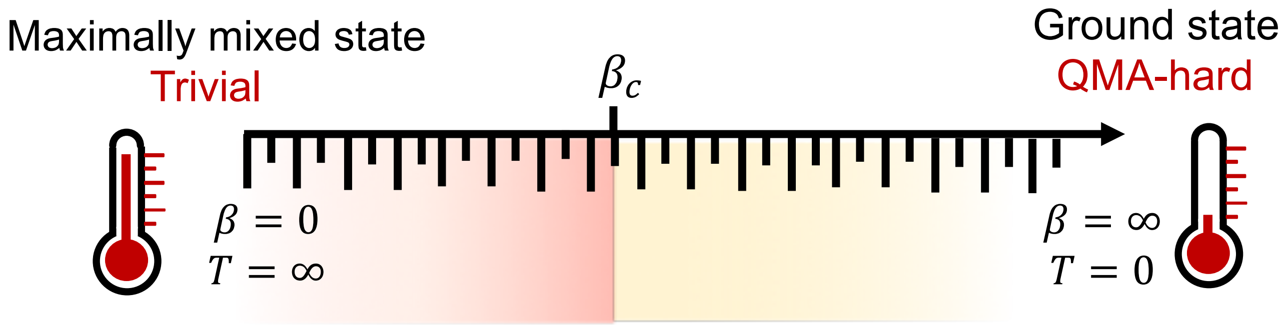
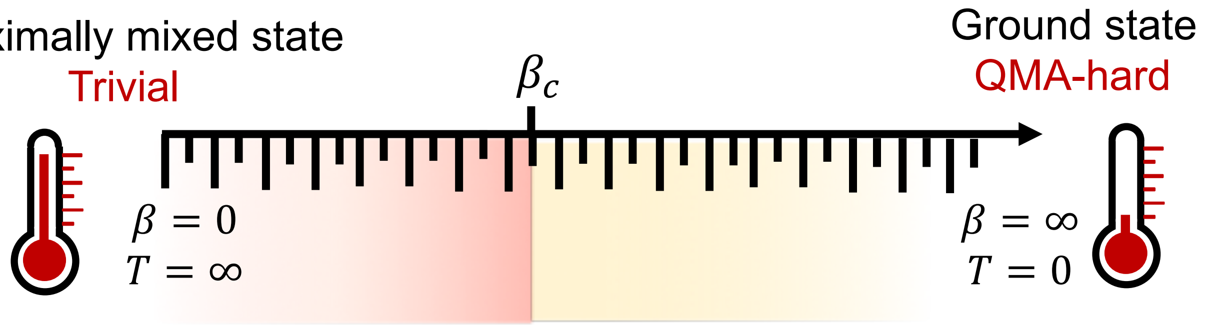
Transition in the phase

Physical properties abruptly change

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

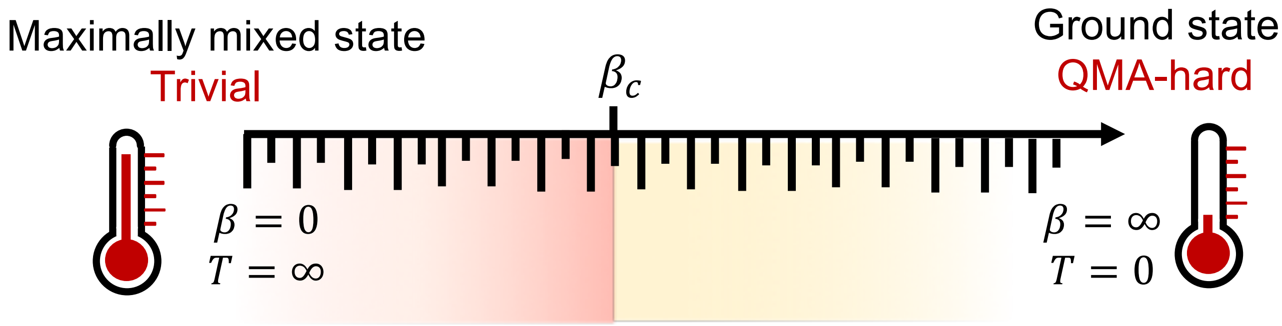


For **classical** Ising model



For **classical** Ising model

- Above T_c there is a polynomial time algorithm



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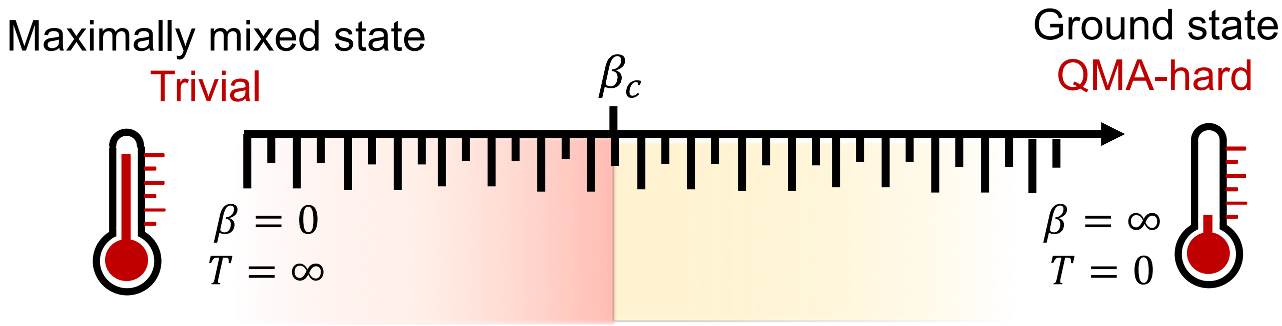
- Above T_c there is a polynomial time algorithm
- Below T_c no efficient algorithm unless $\mathrm{NP} = \mathrm{RP}$ [Sly'10]



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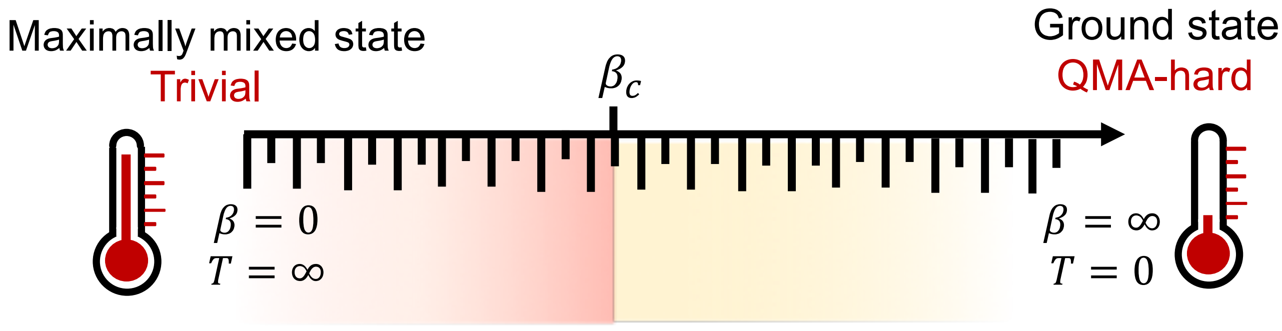
Computational phase transition
matches
Physical phase transition



To design approximation algorithms good to understand why physical phase transition happens

Two ways to study phase transition

Two ways to study phase transition

Location of complex zeros of $Z(\beta)$

Two ways to study phase transition

Location of complex zeros of $Z(\beta)$

Decay of correlations

Algorithm

Location of complex zeros of $Z(\beta)$

Decay of correlations

Algorithm

Location of complex zeros of $Z(\beta)$

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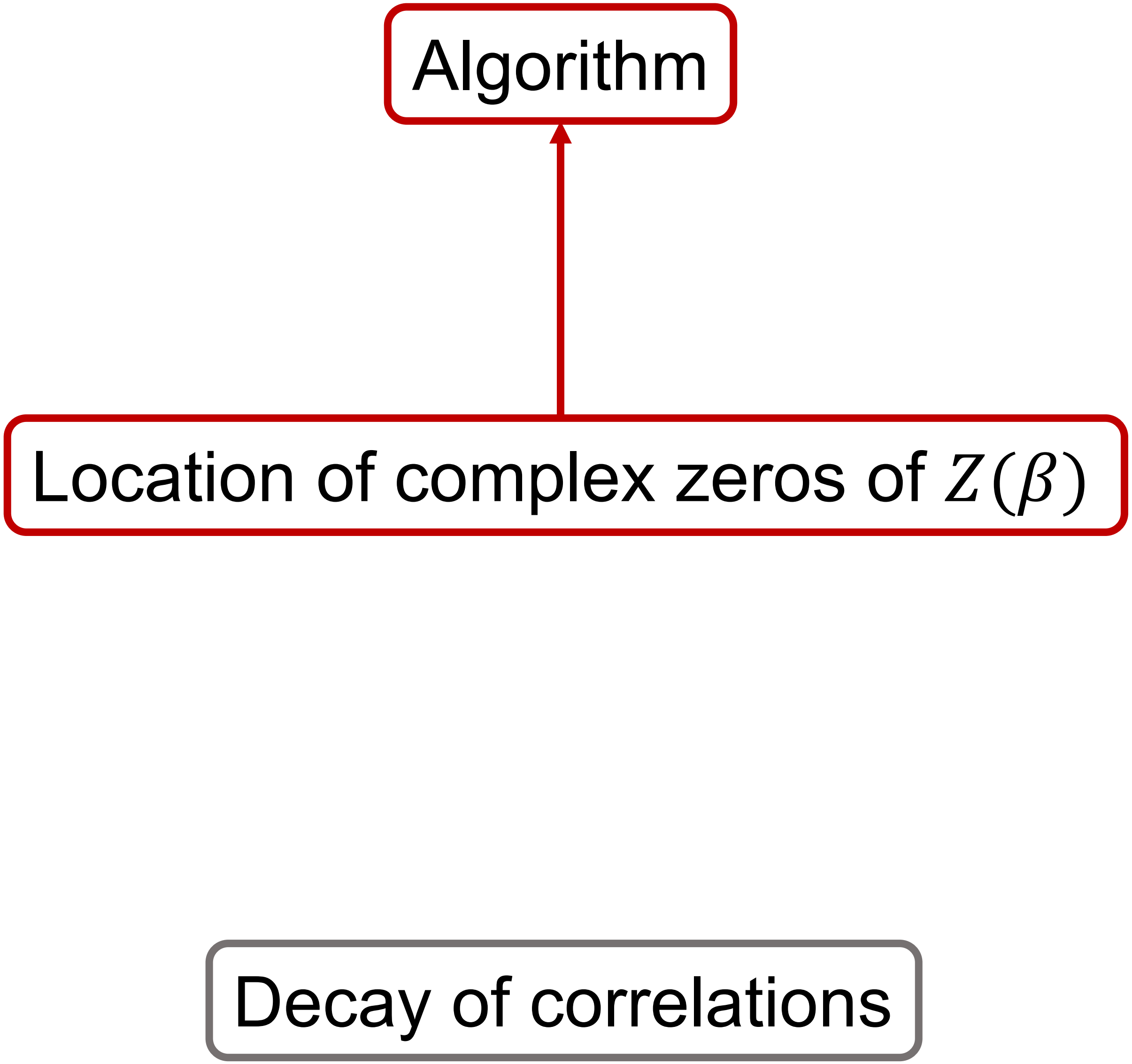
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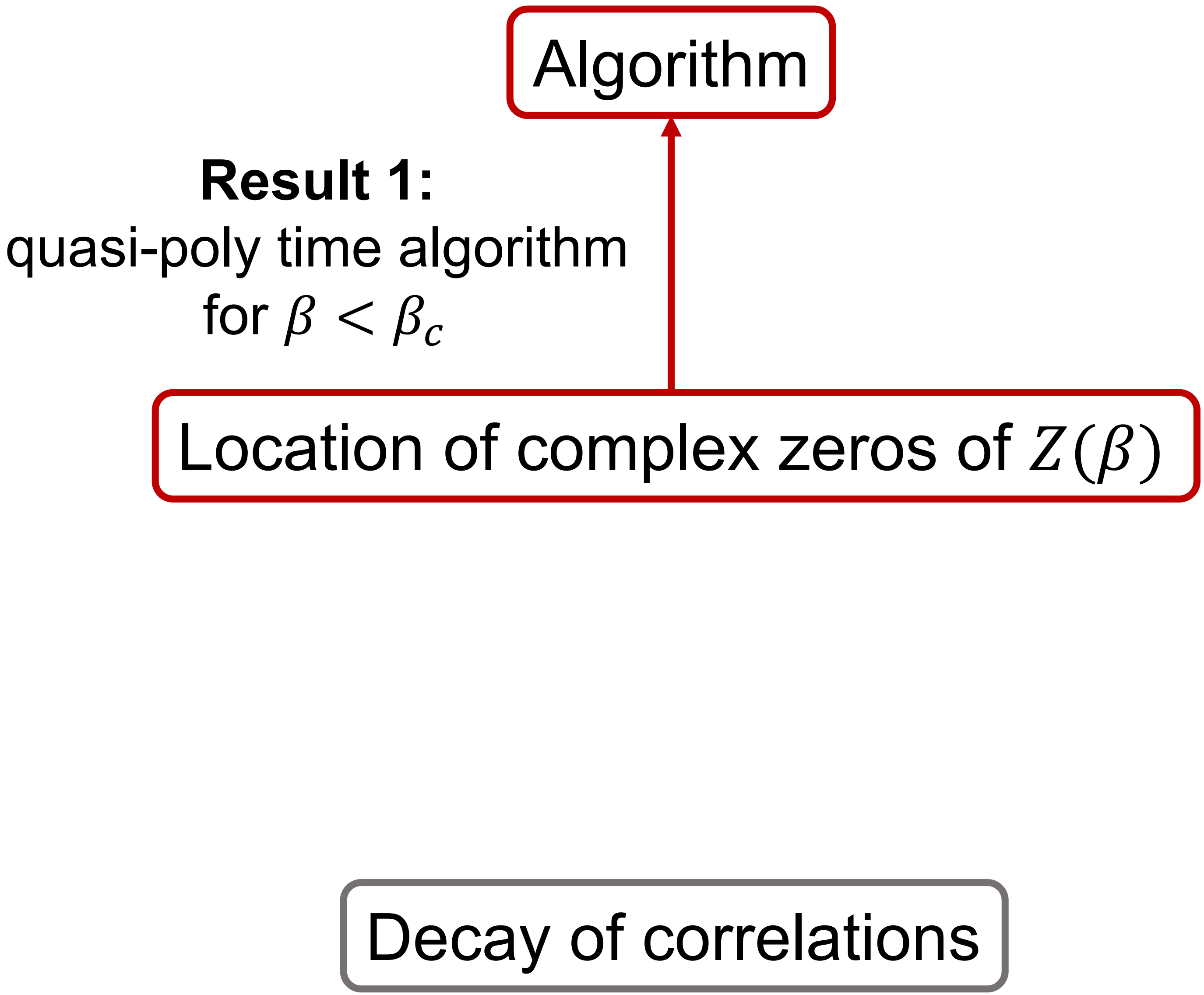
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Location of complex zeros of $Z(\beta)$
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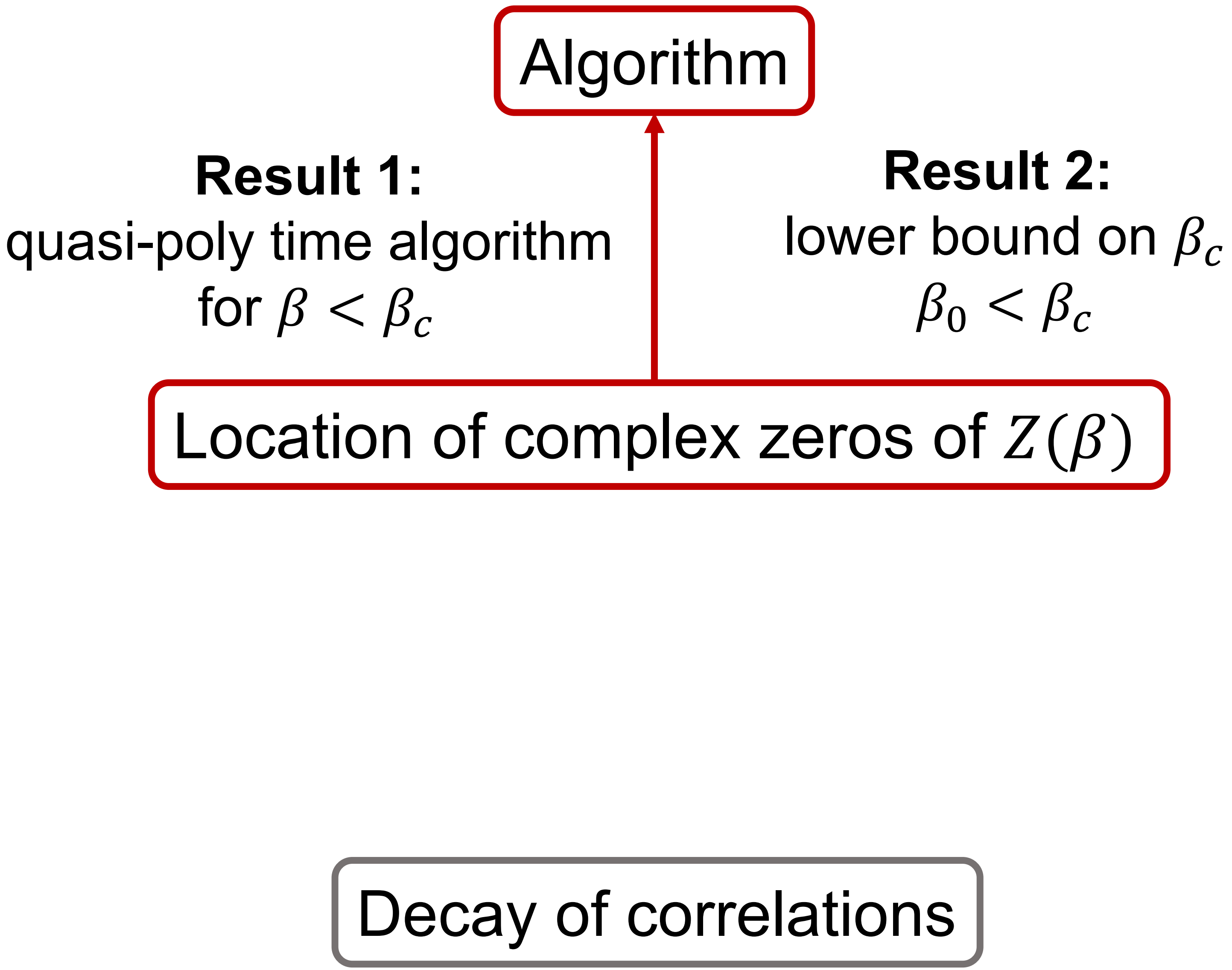

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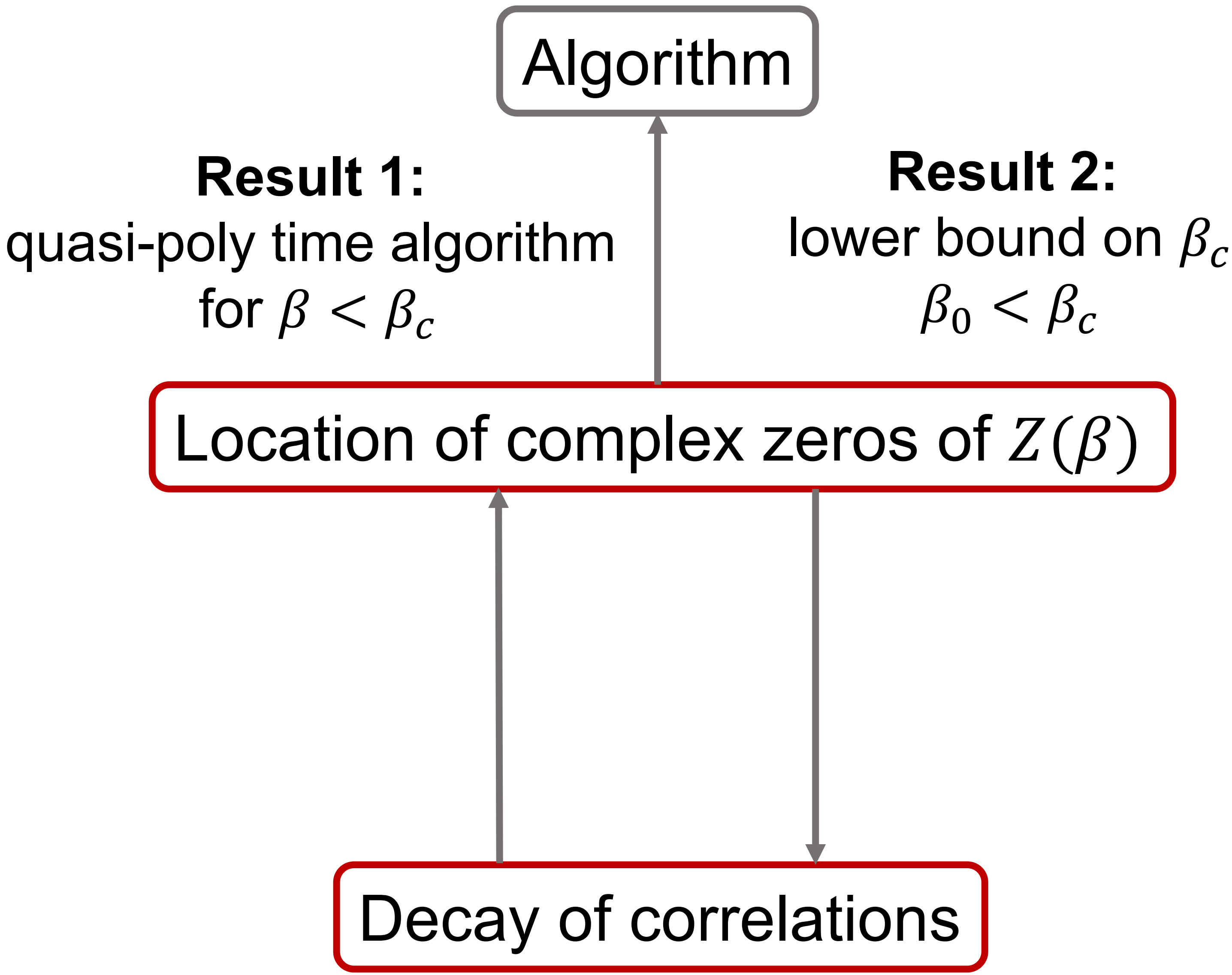
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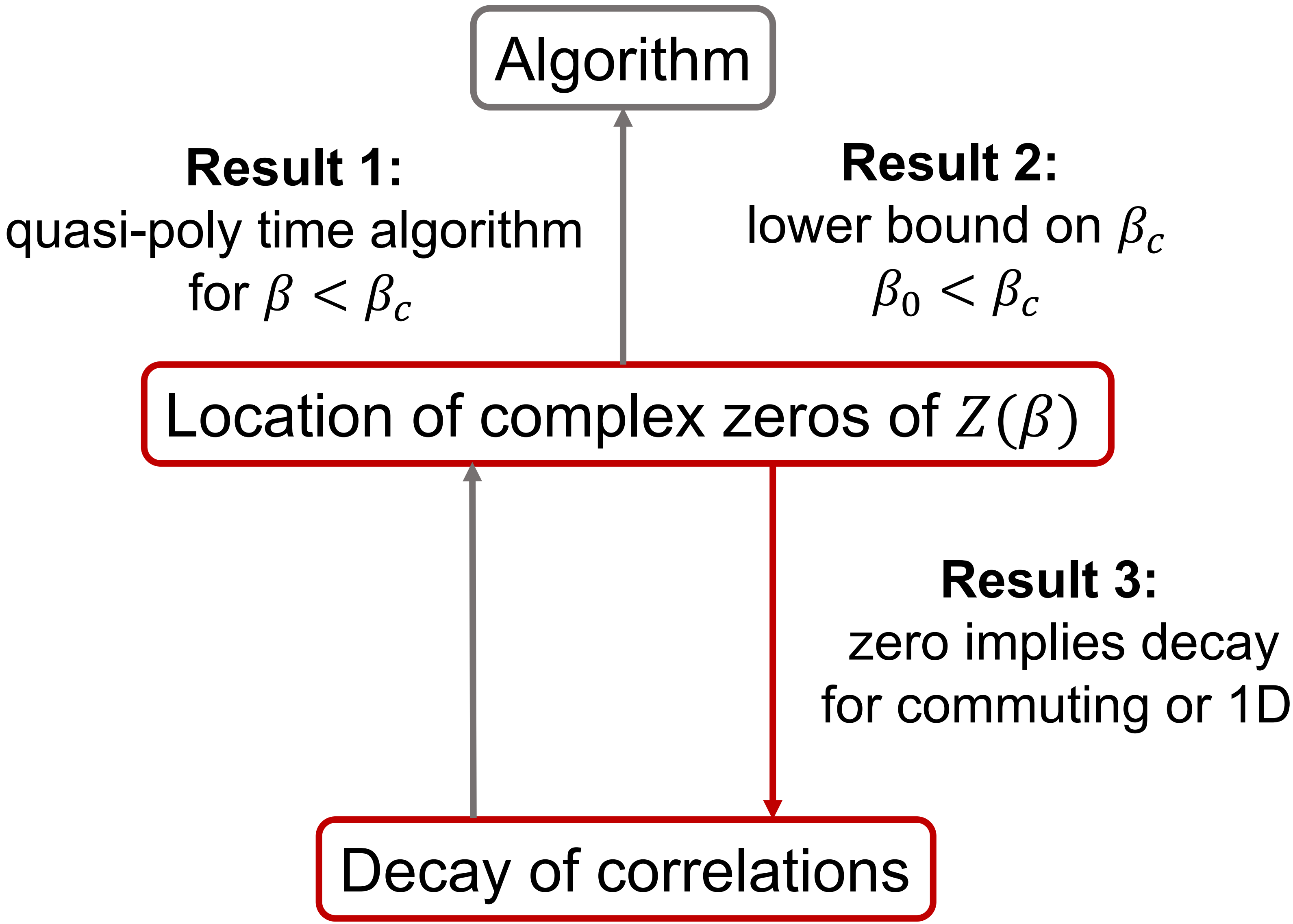
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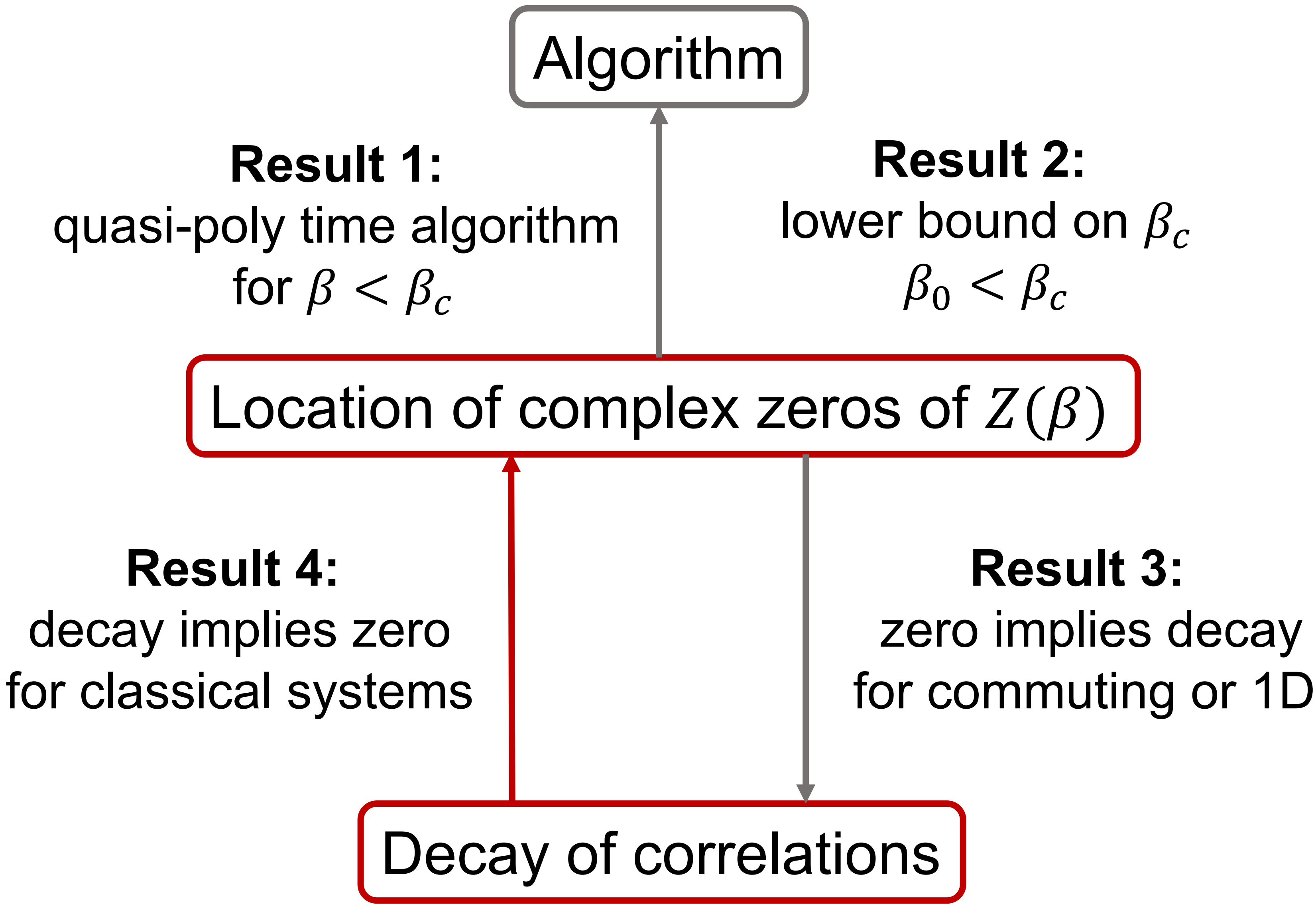
Decay of correlations



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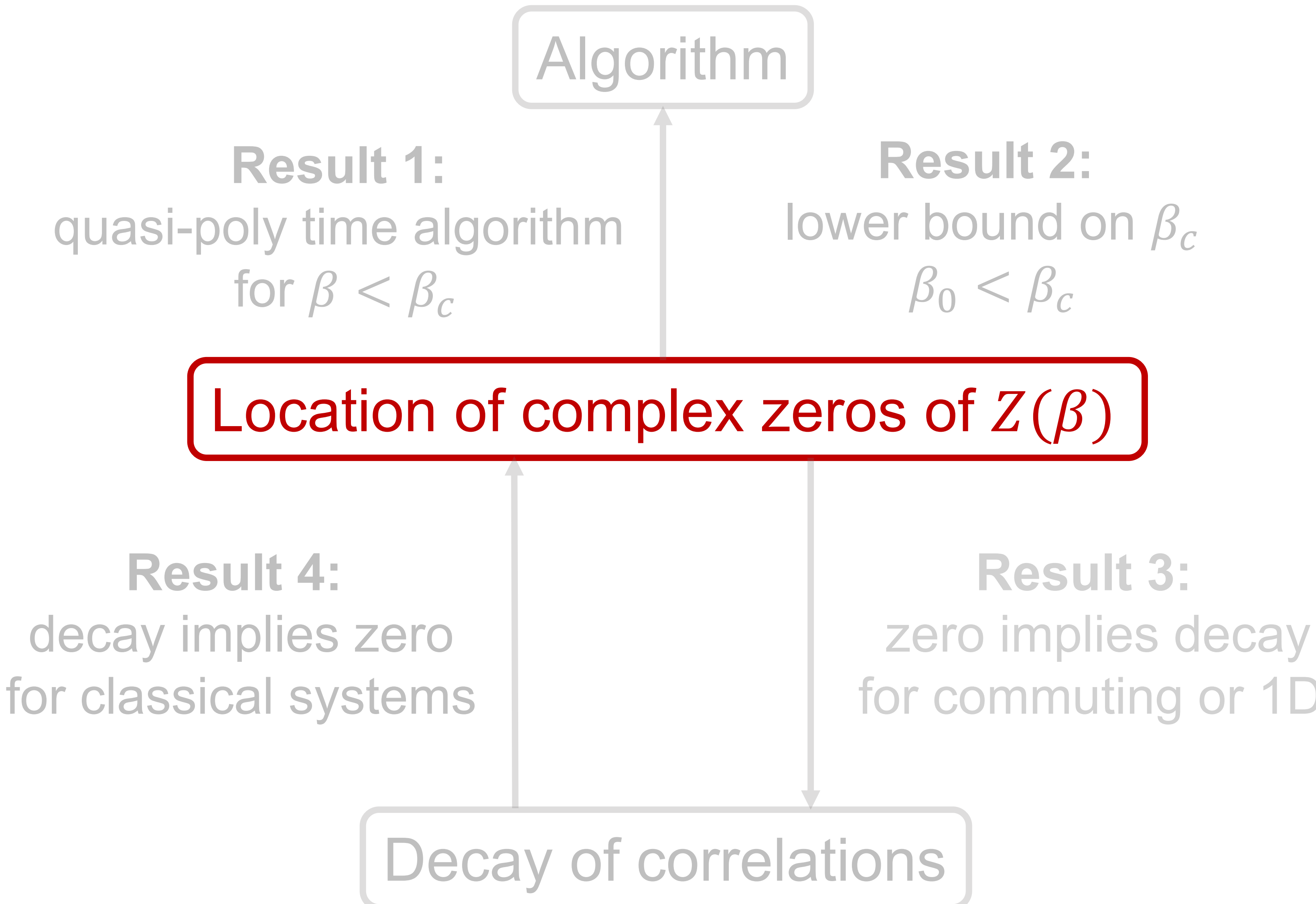

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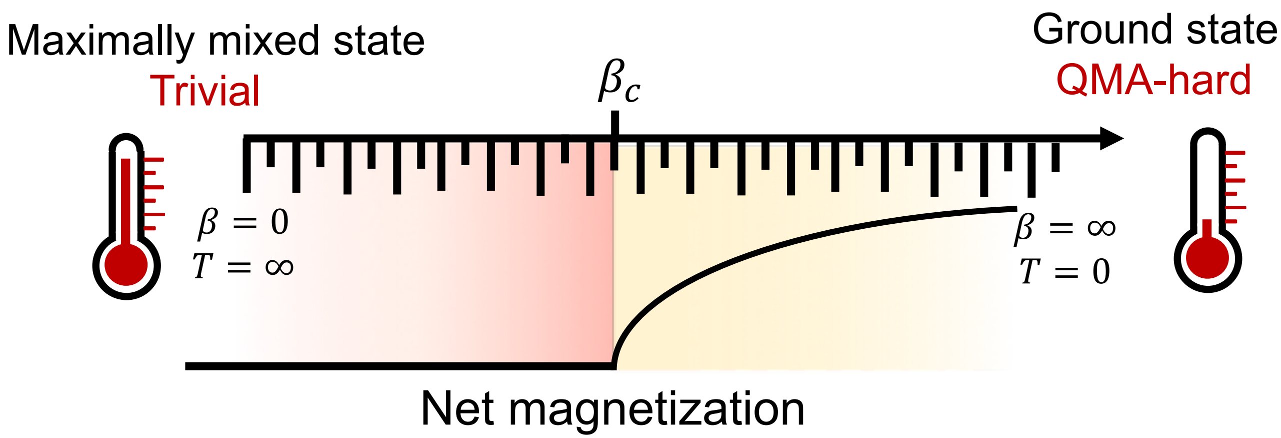
Complex zeros vs phase transition



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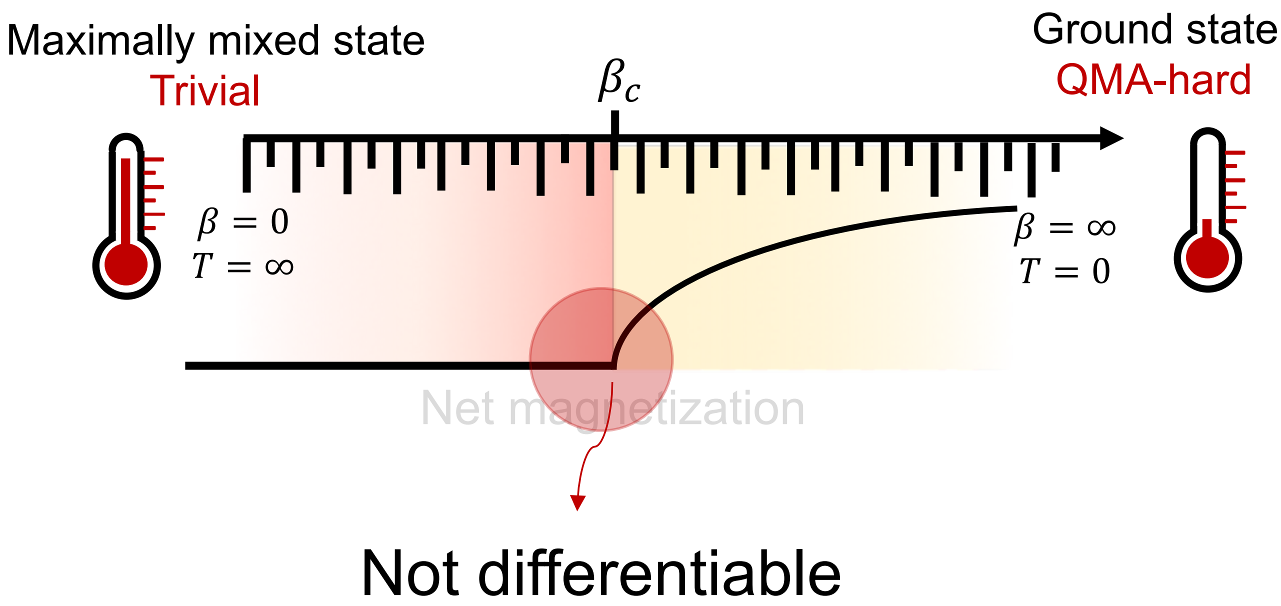
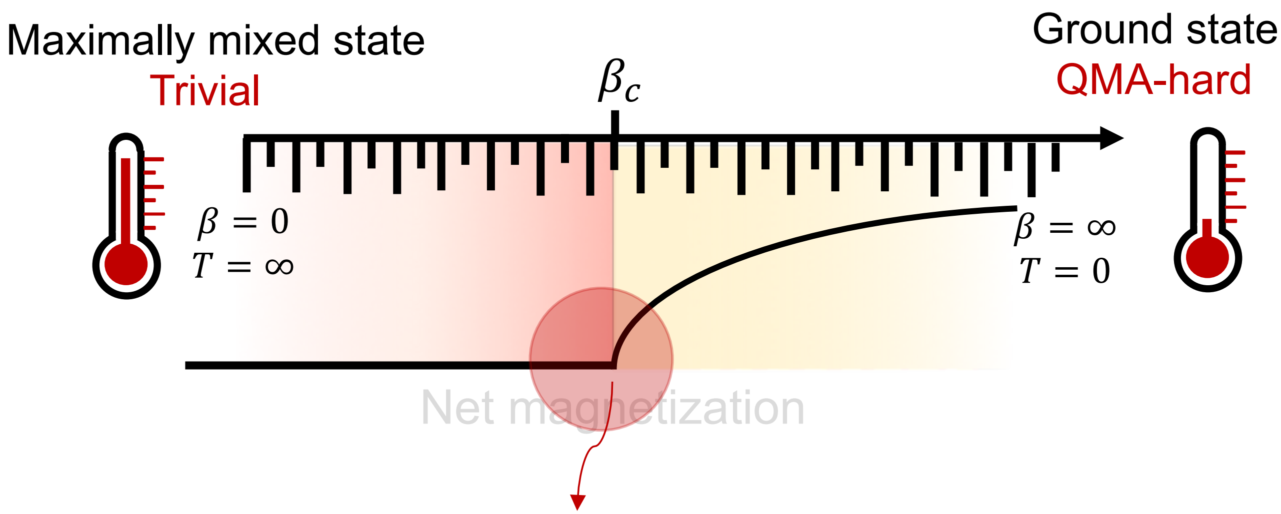


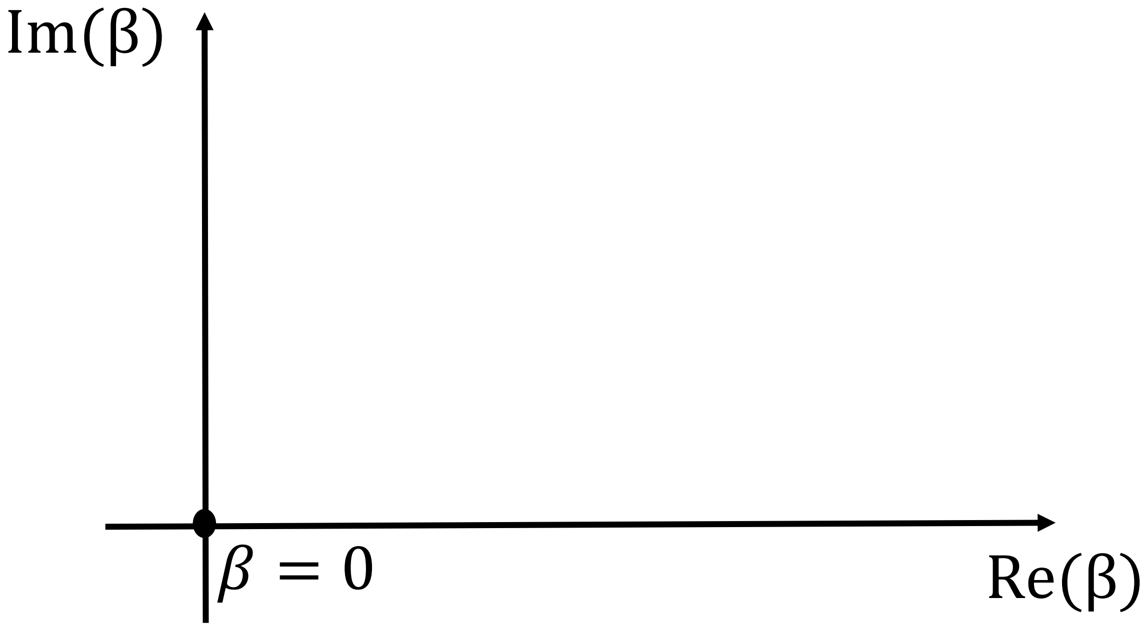
Complex zeros vs phase transition



Not differentiable

Singularities at β_c

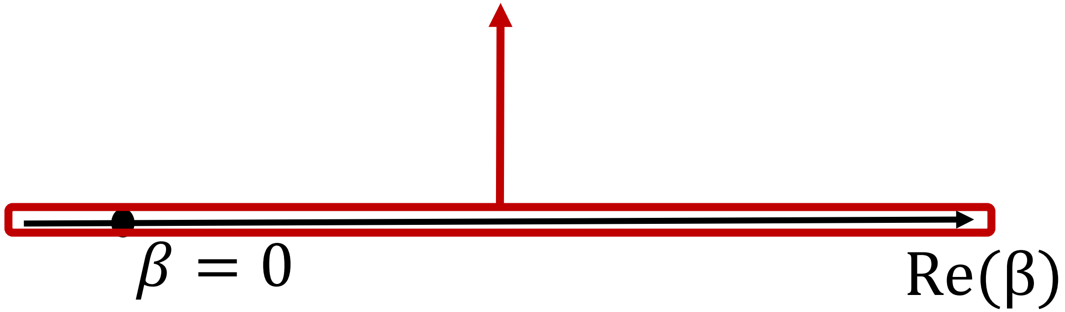
Complex zeros vs phase transition



Complex zeros vs phase transition

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

Sum of strictly positive terms

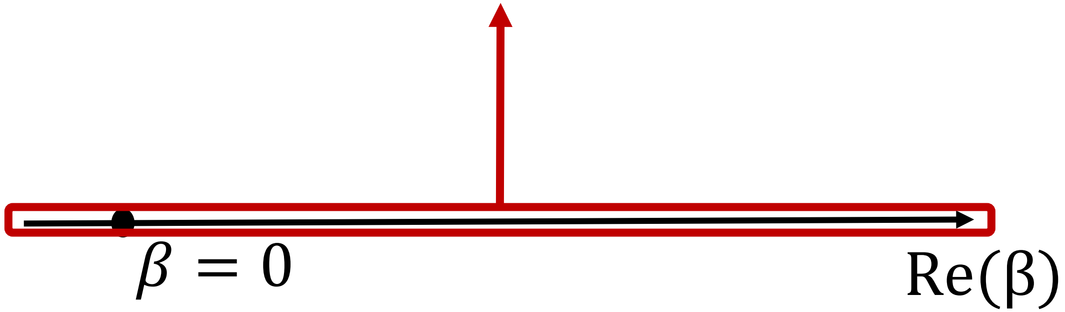


Complex zeros vs phase transition

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

Sum of strictly positive terms

No singularities for free energy



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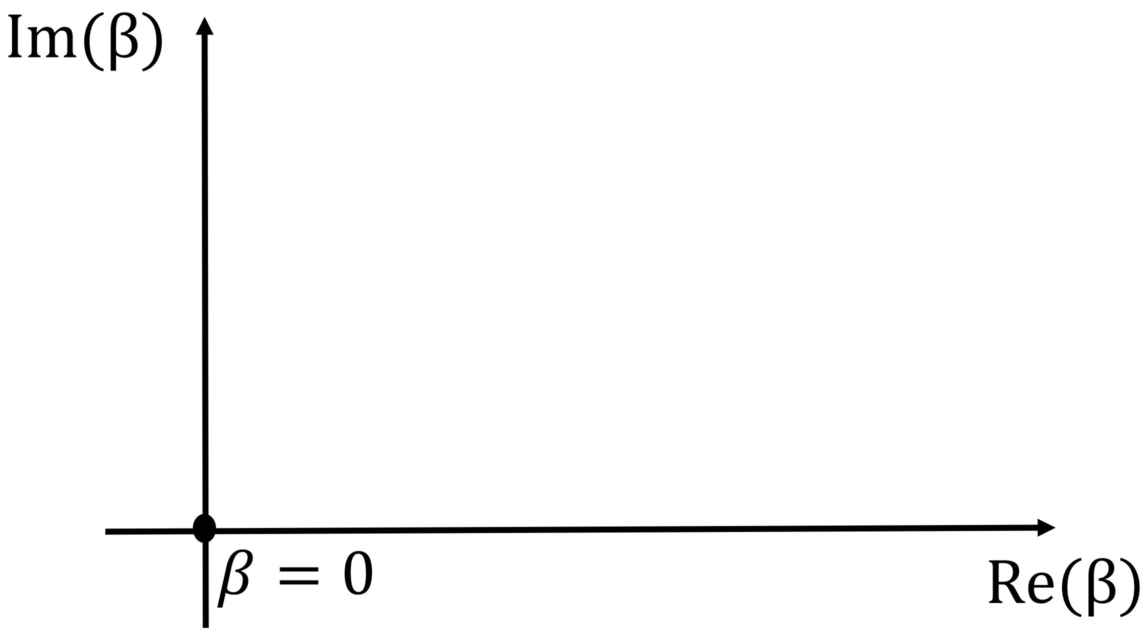
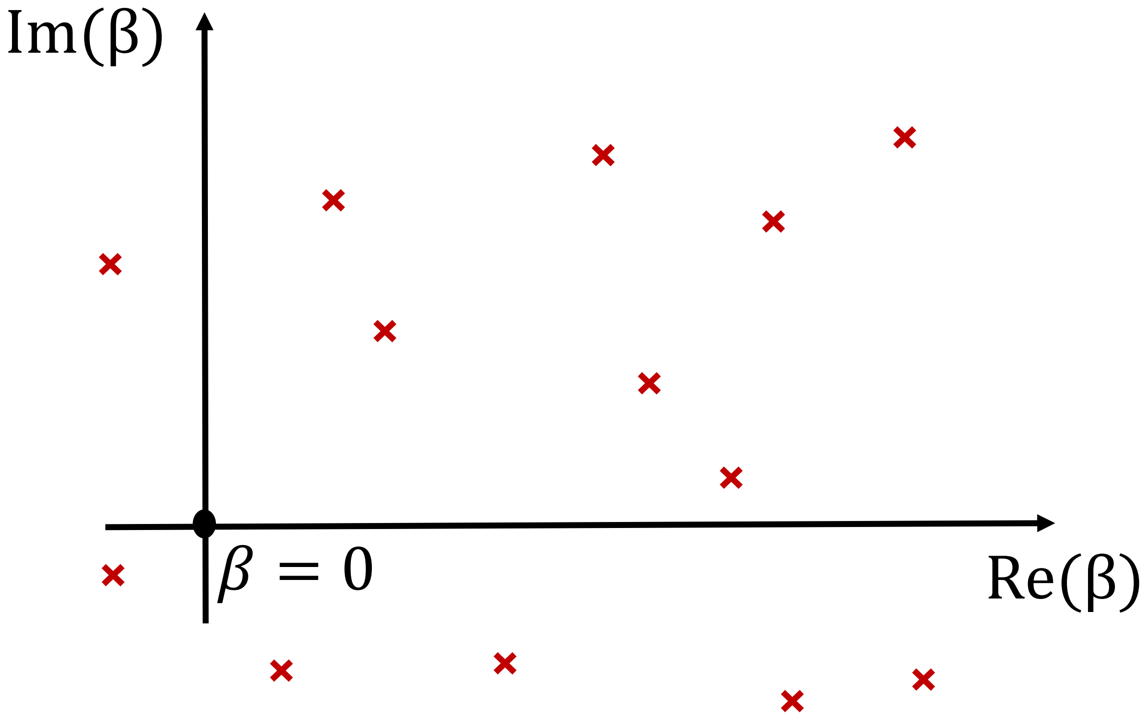


Complex zeros vs phase transition

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



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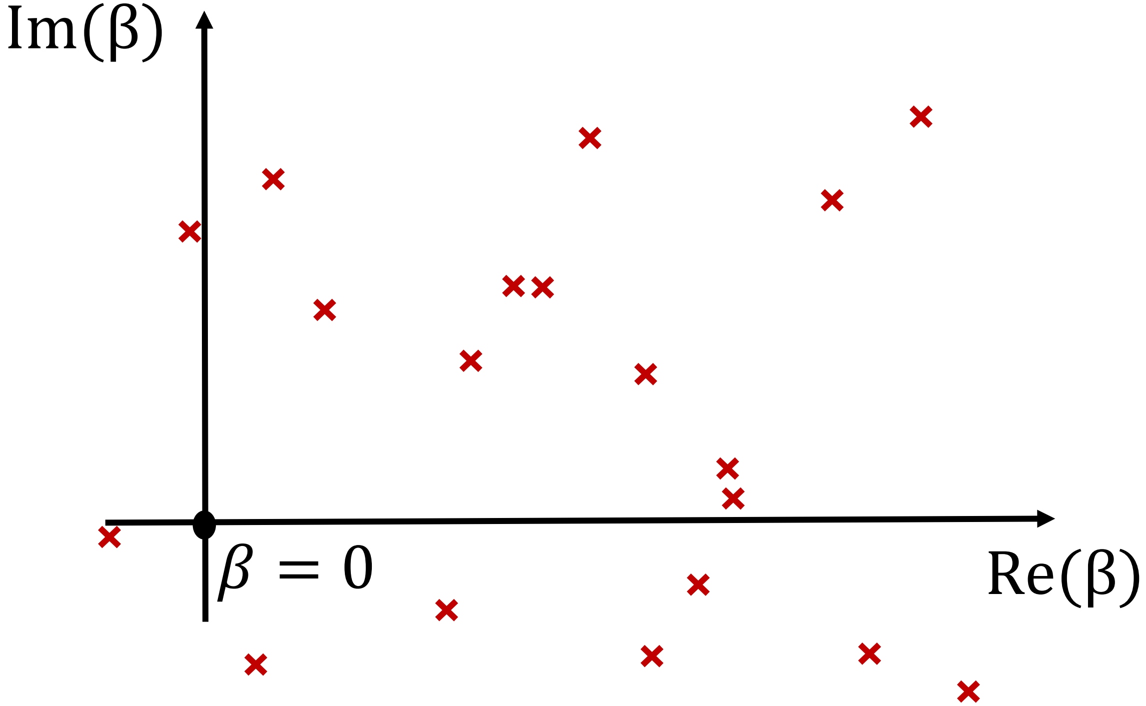

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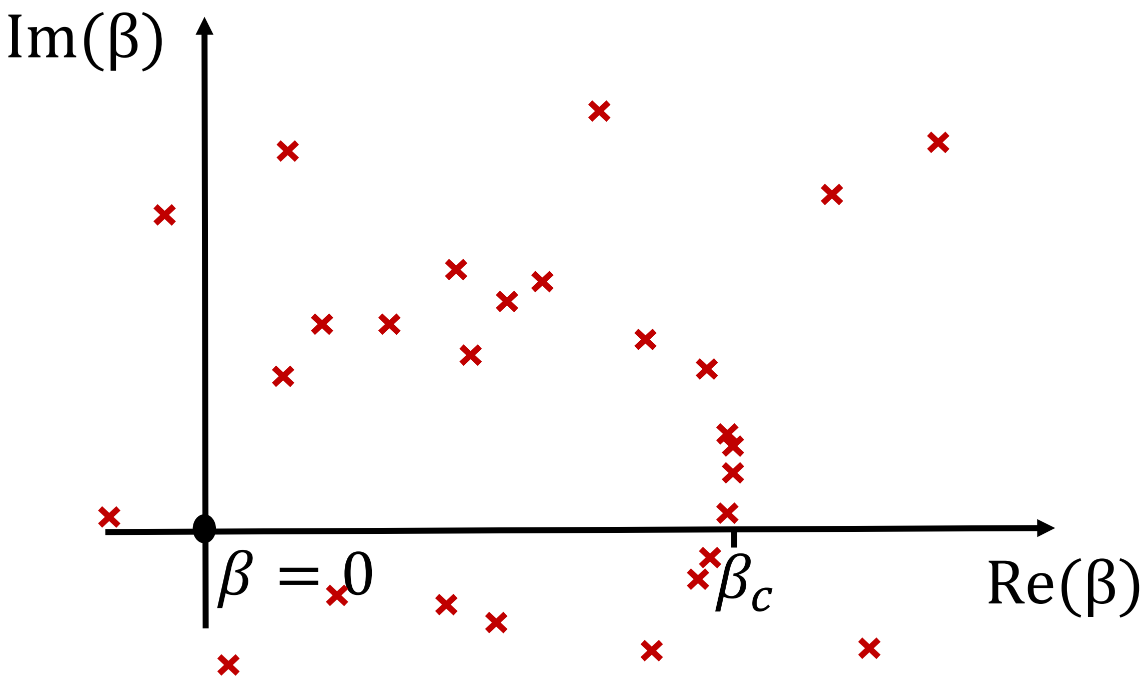

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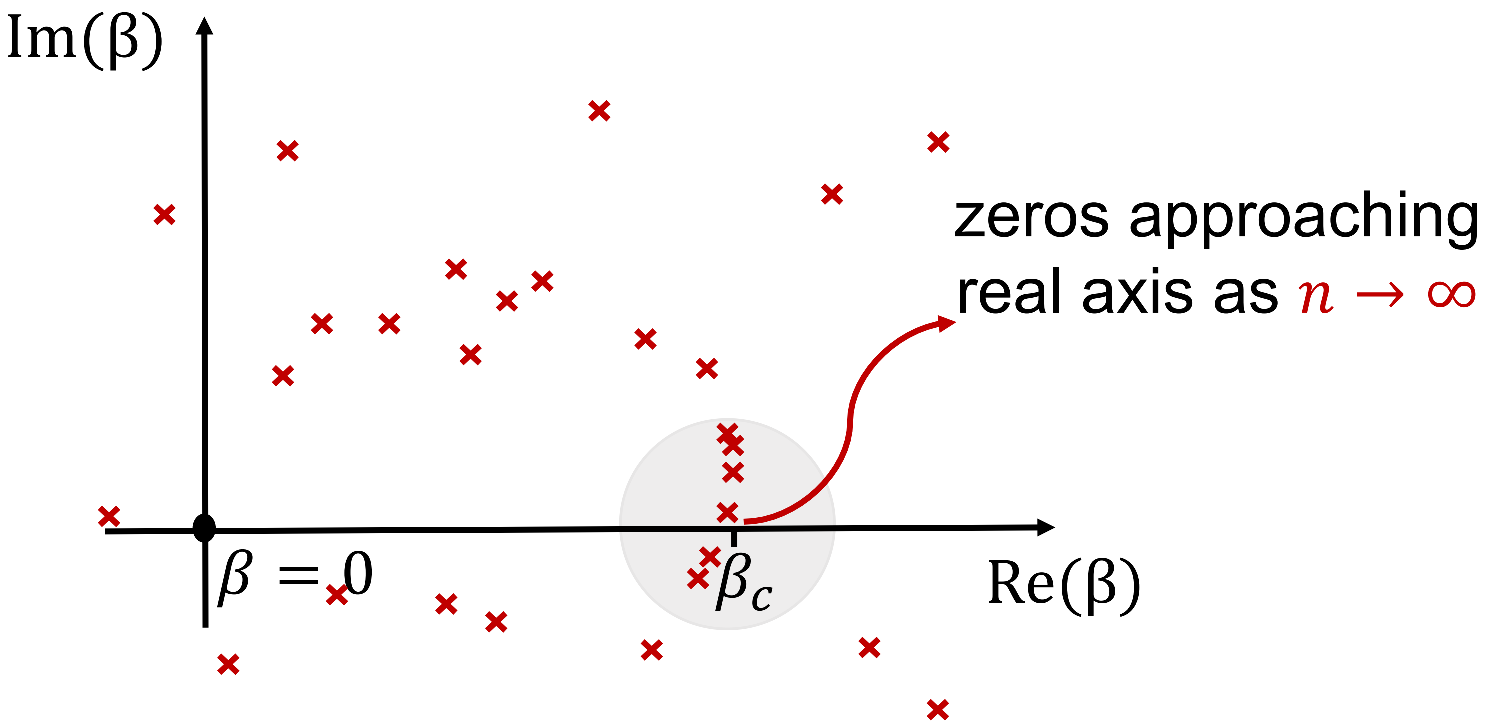

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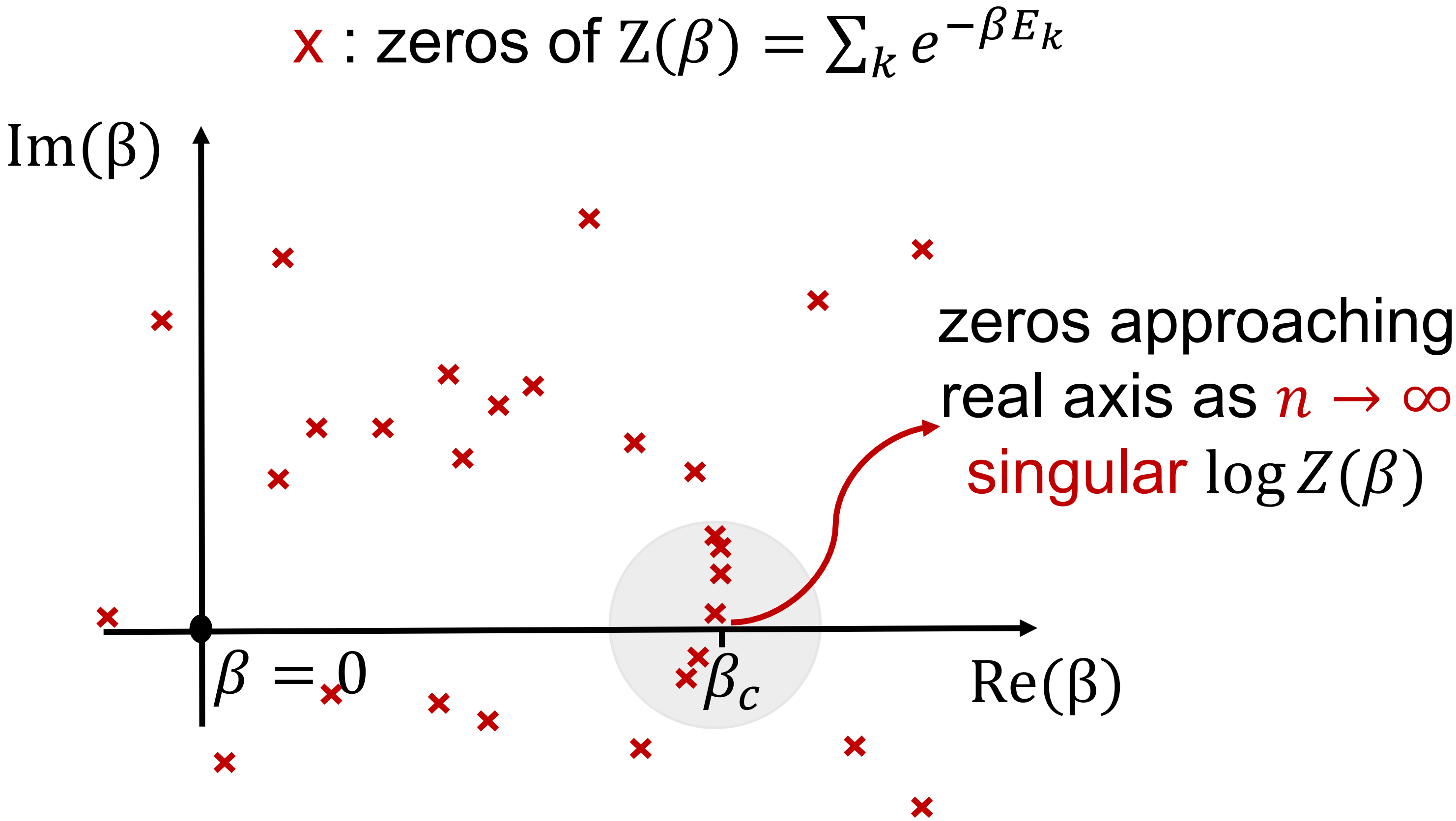

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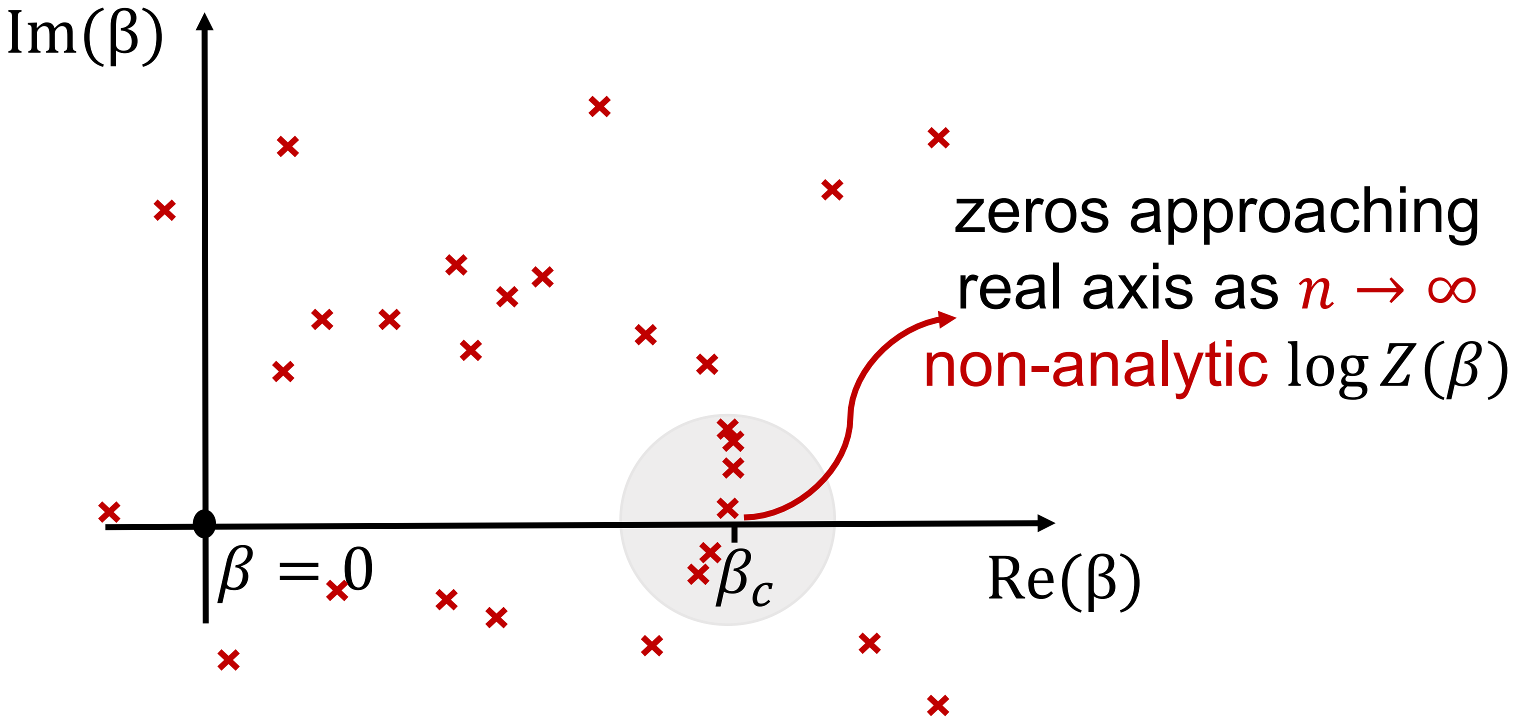
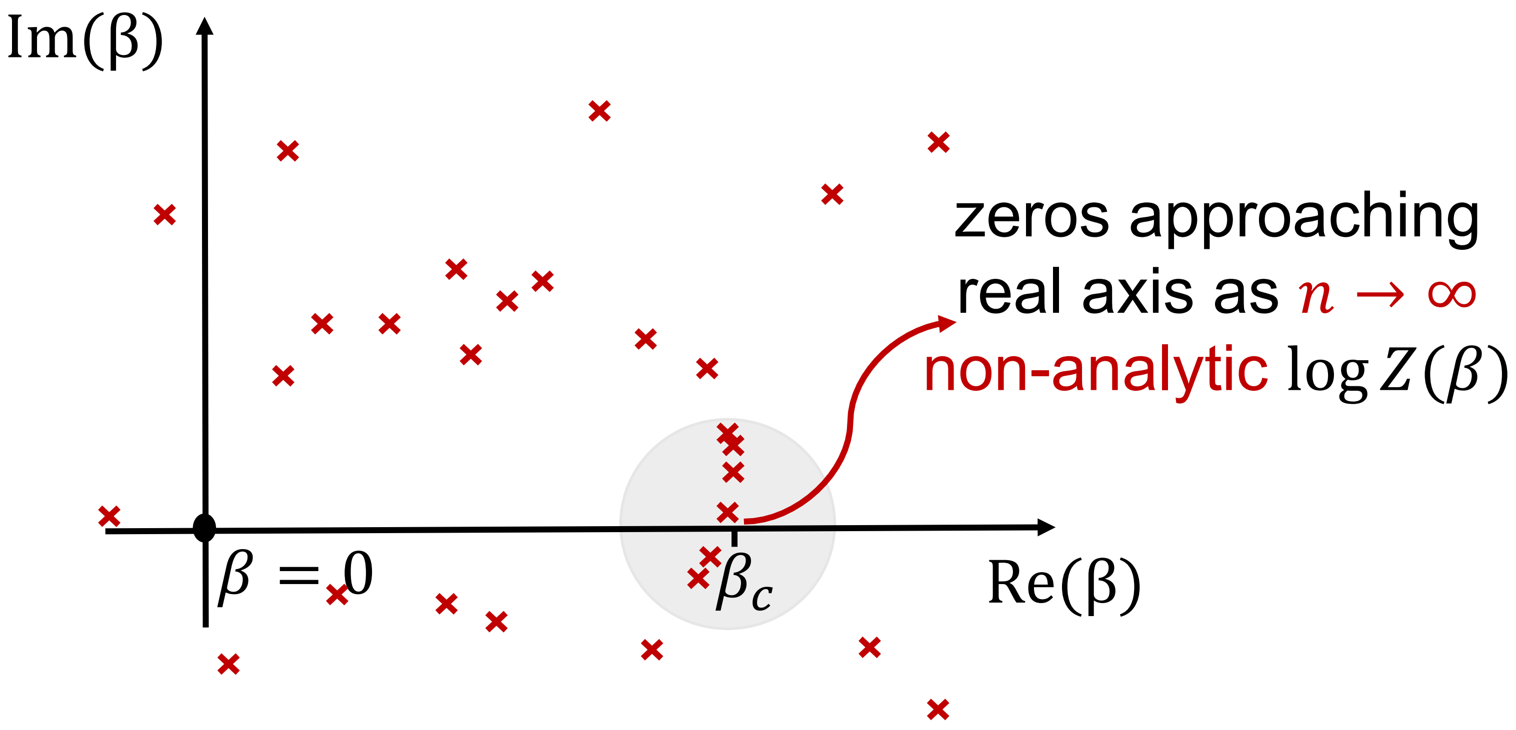


Complex zeros vs phase transition

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]

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

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

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

To Recap

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We made two observations

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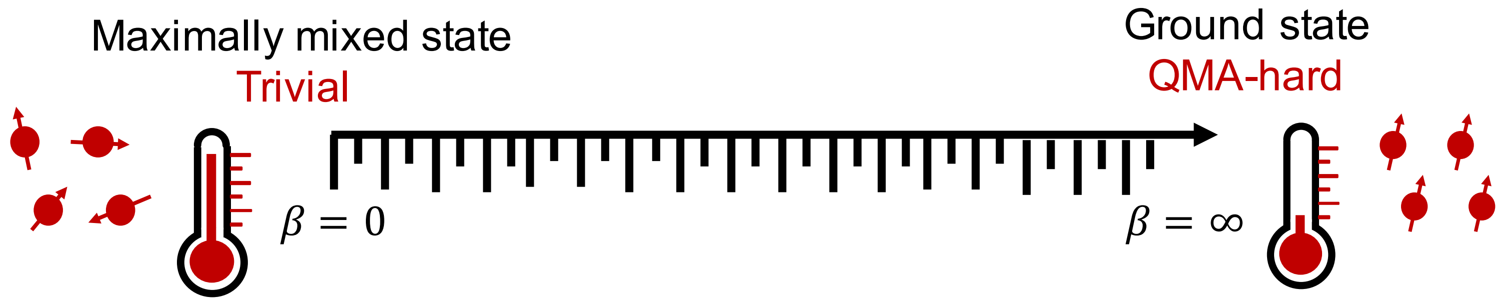
1)



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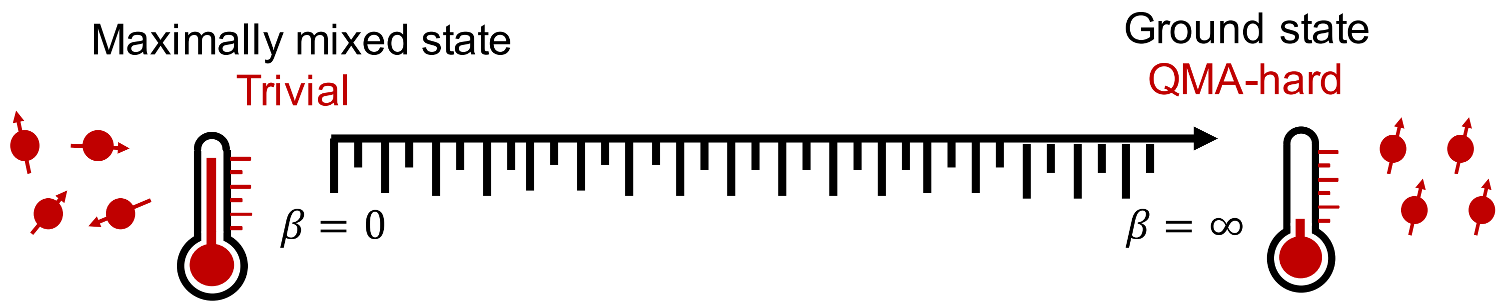

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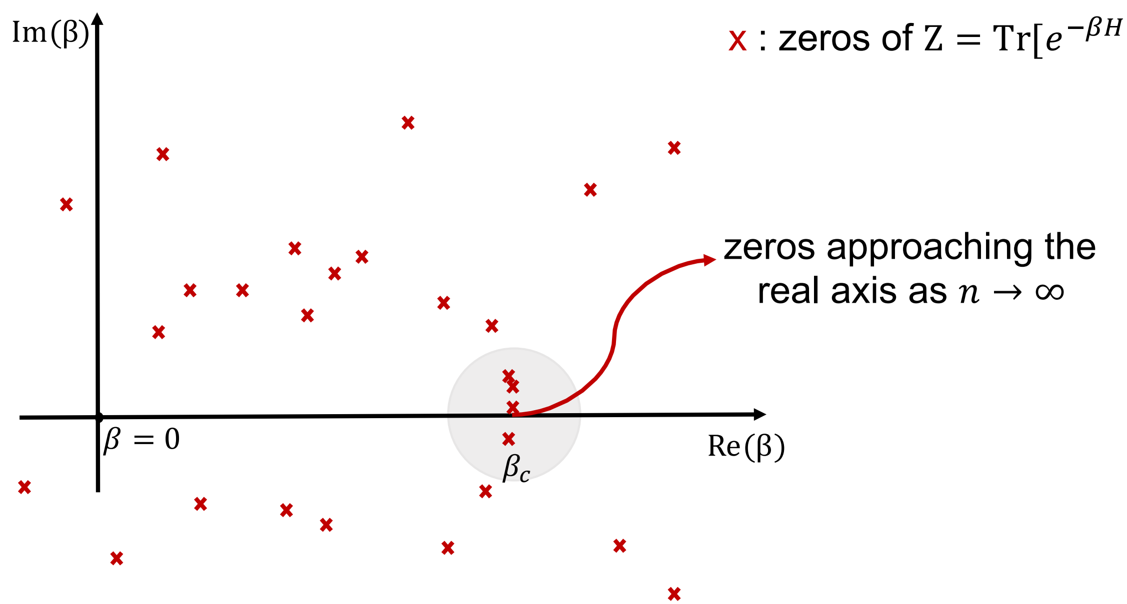

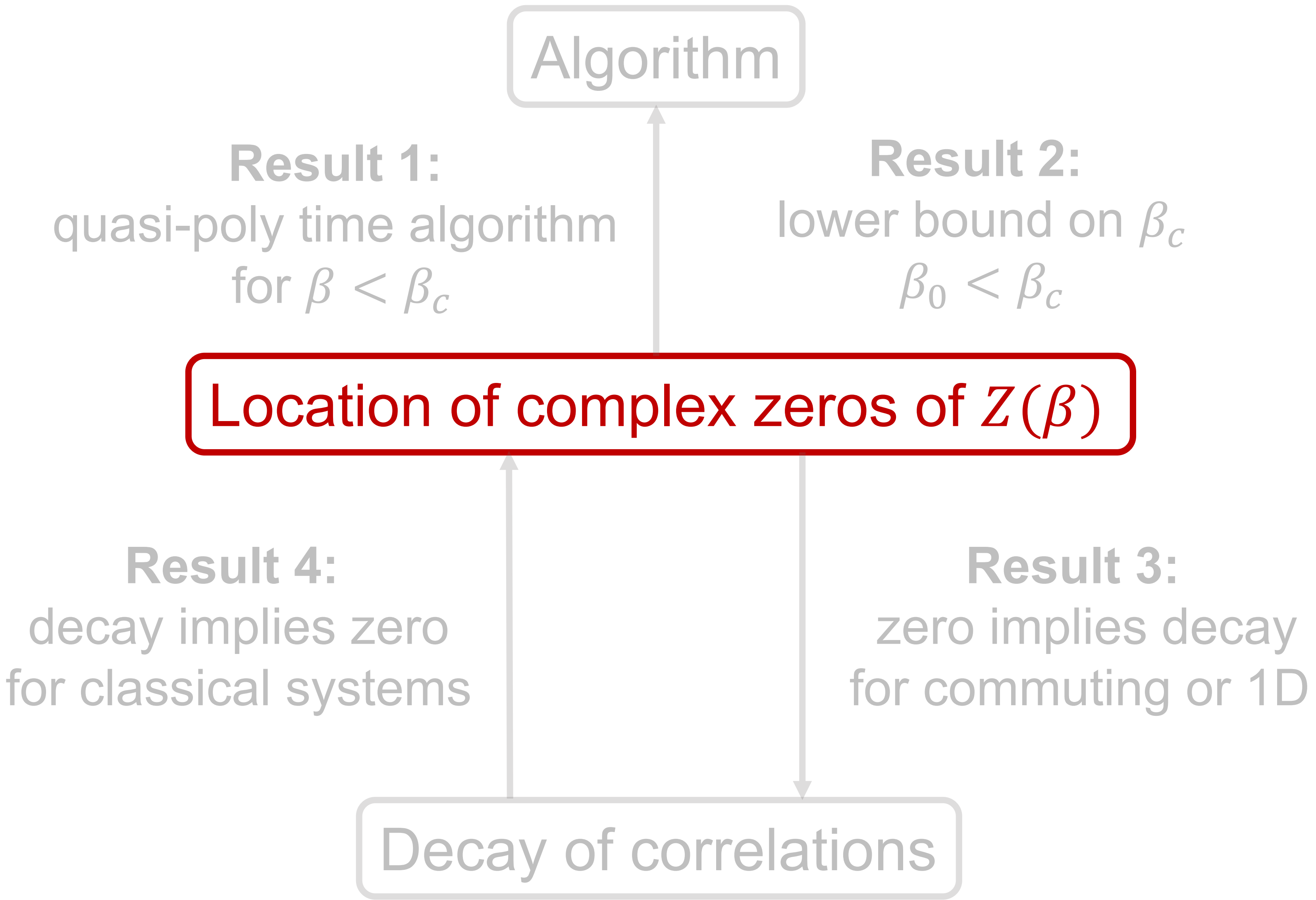
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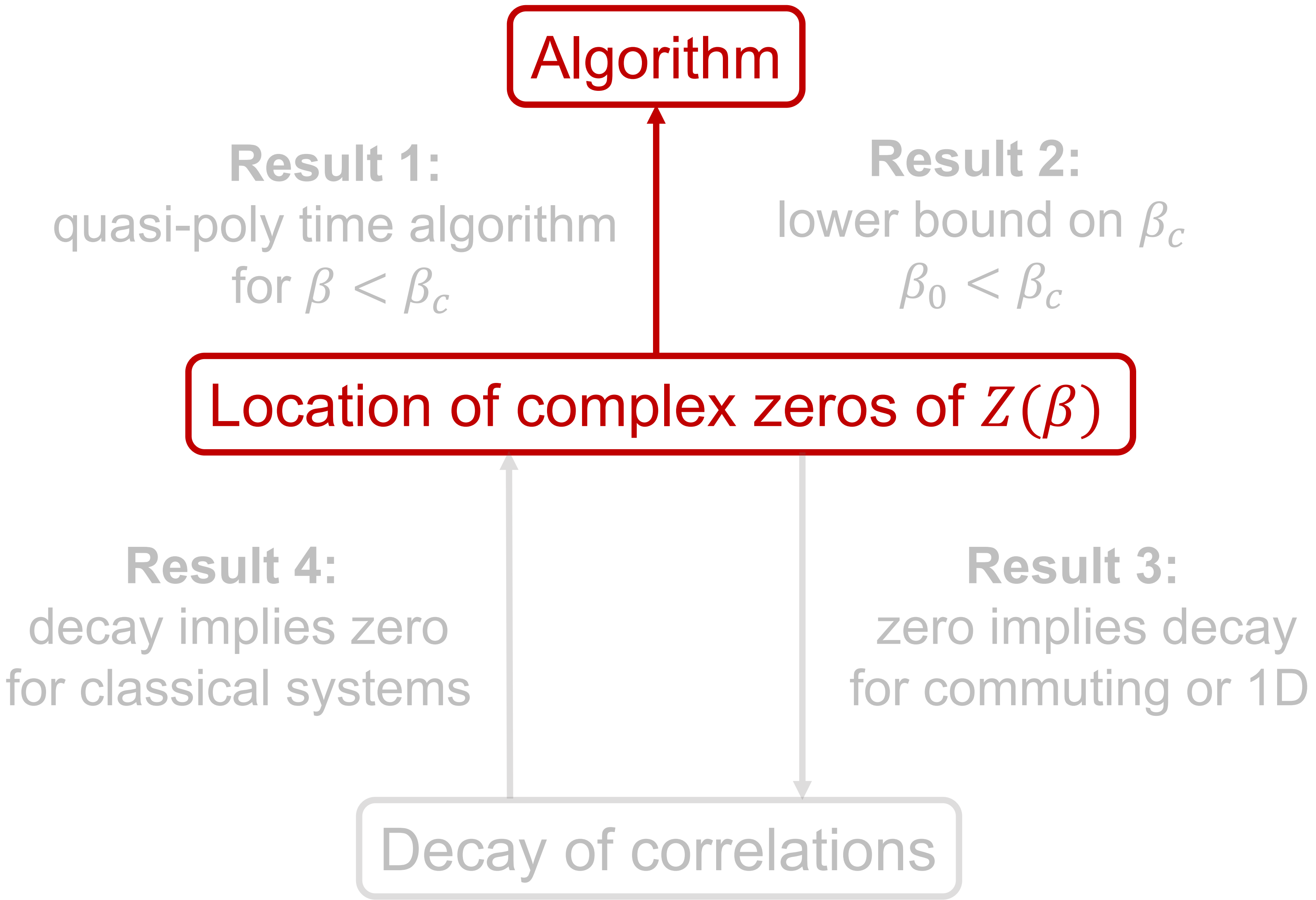
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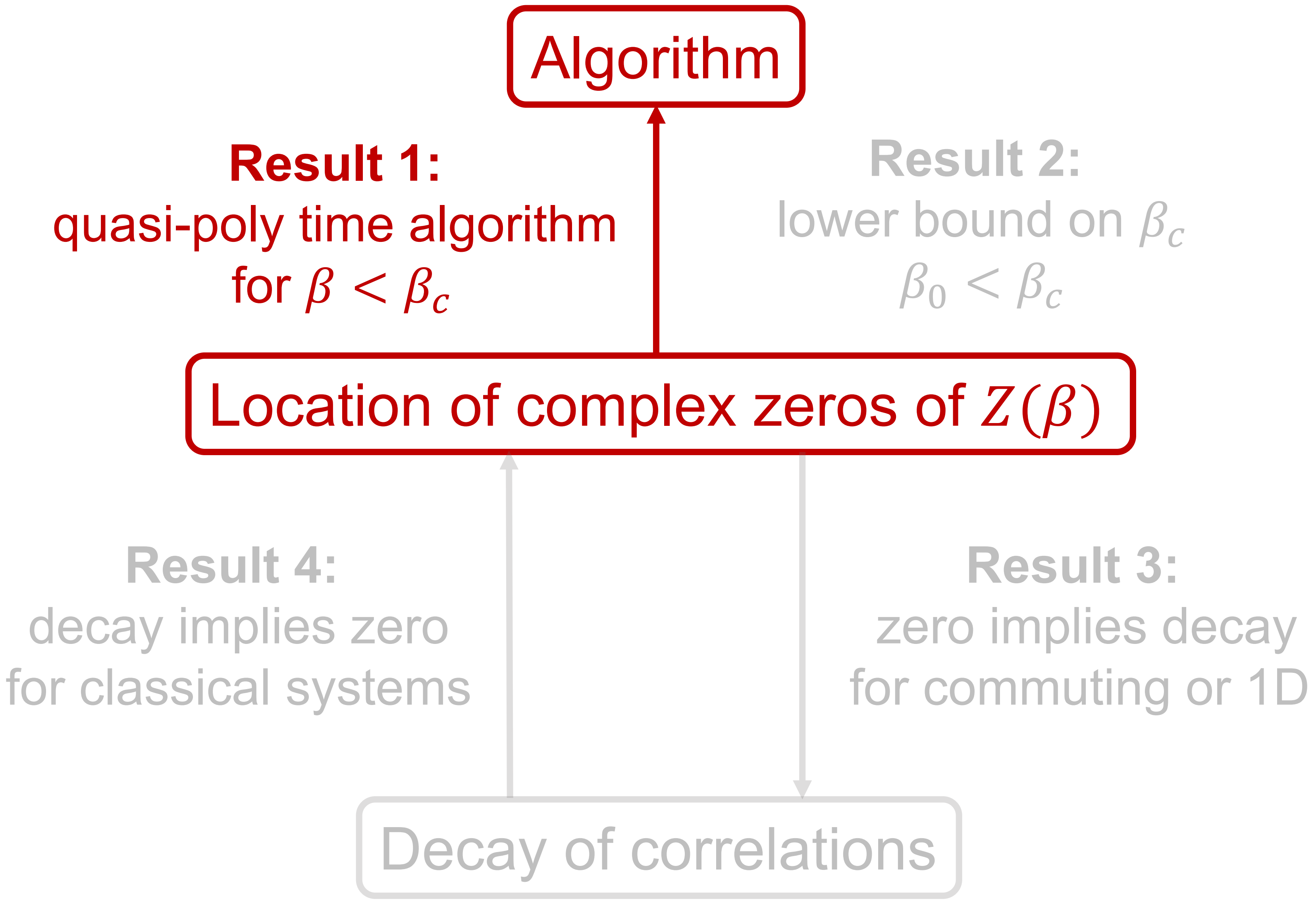
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Goal: design an algorithm that

Input: H, β, ε

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

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

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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*

Goal: design an algorithm that

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Result 1:

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

Analysis:

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The idea is to

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Extrapolate the solution in the easy regime (high T)

Analysis:

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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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Taylor expanding $\log Z(\beta)$

Keeping first few terms of expansion

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

Taylor expanding $\log Z(\beta)$

Keeping first few terms of expansion

Need to make sure Taylor expansion converges

Extrapolating $\log Z(\beta)$

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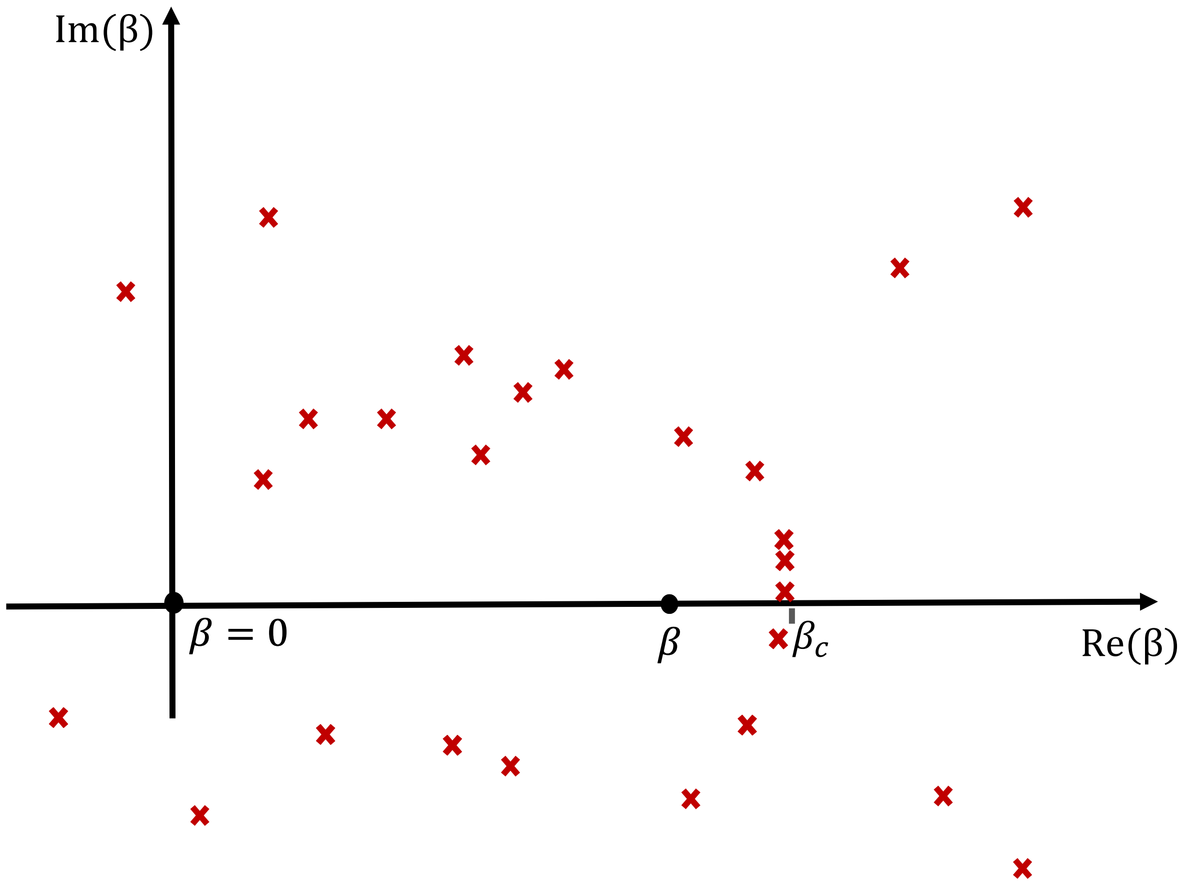
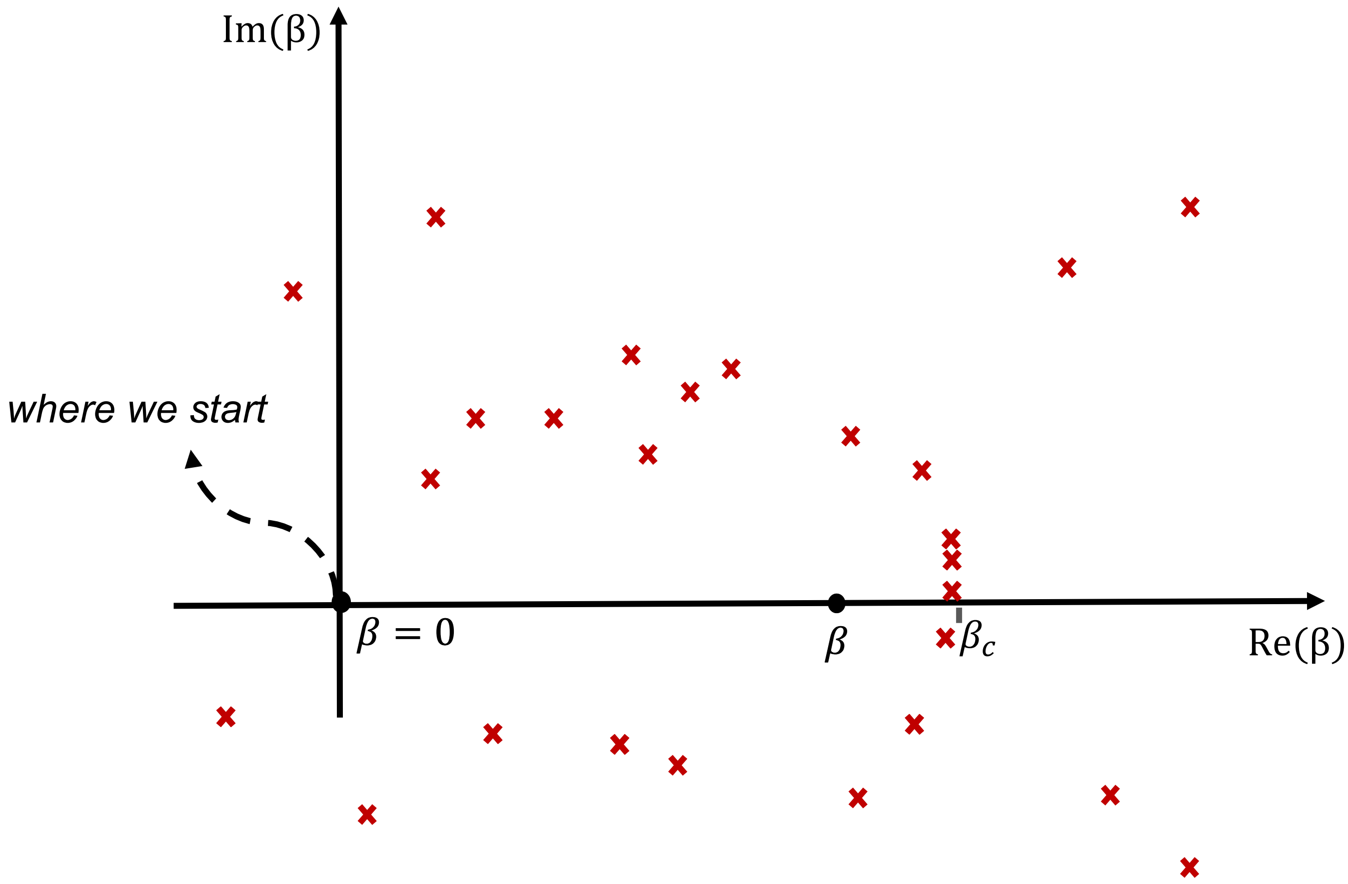


Extrapolating $\log Z(\beta)$



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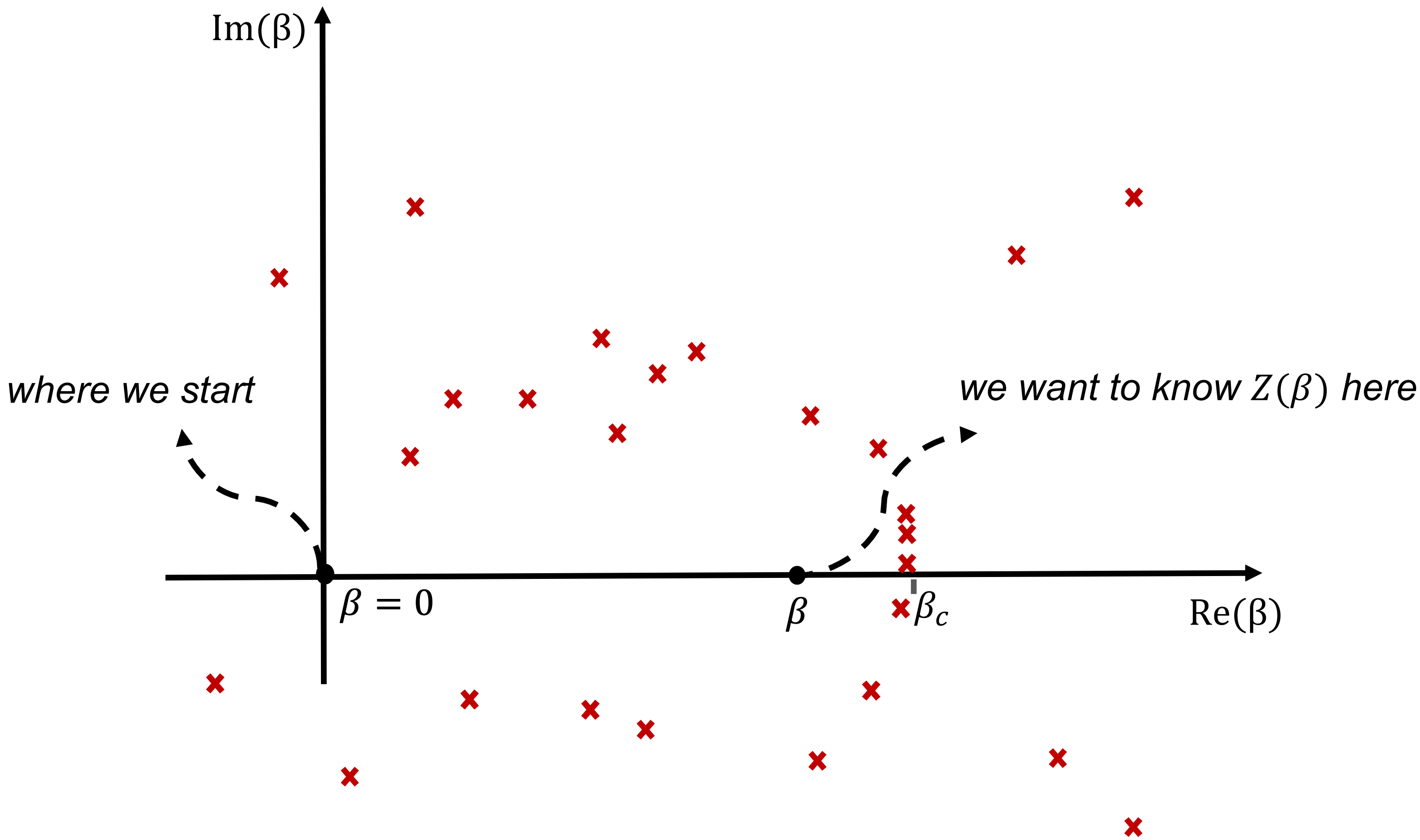

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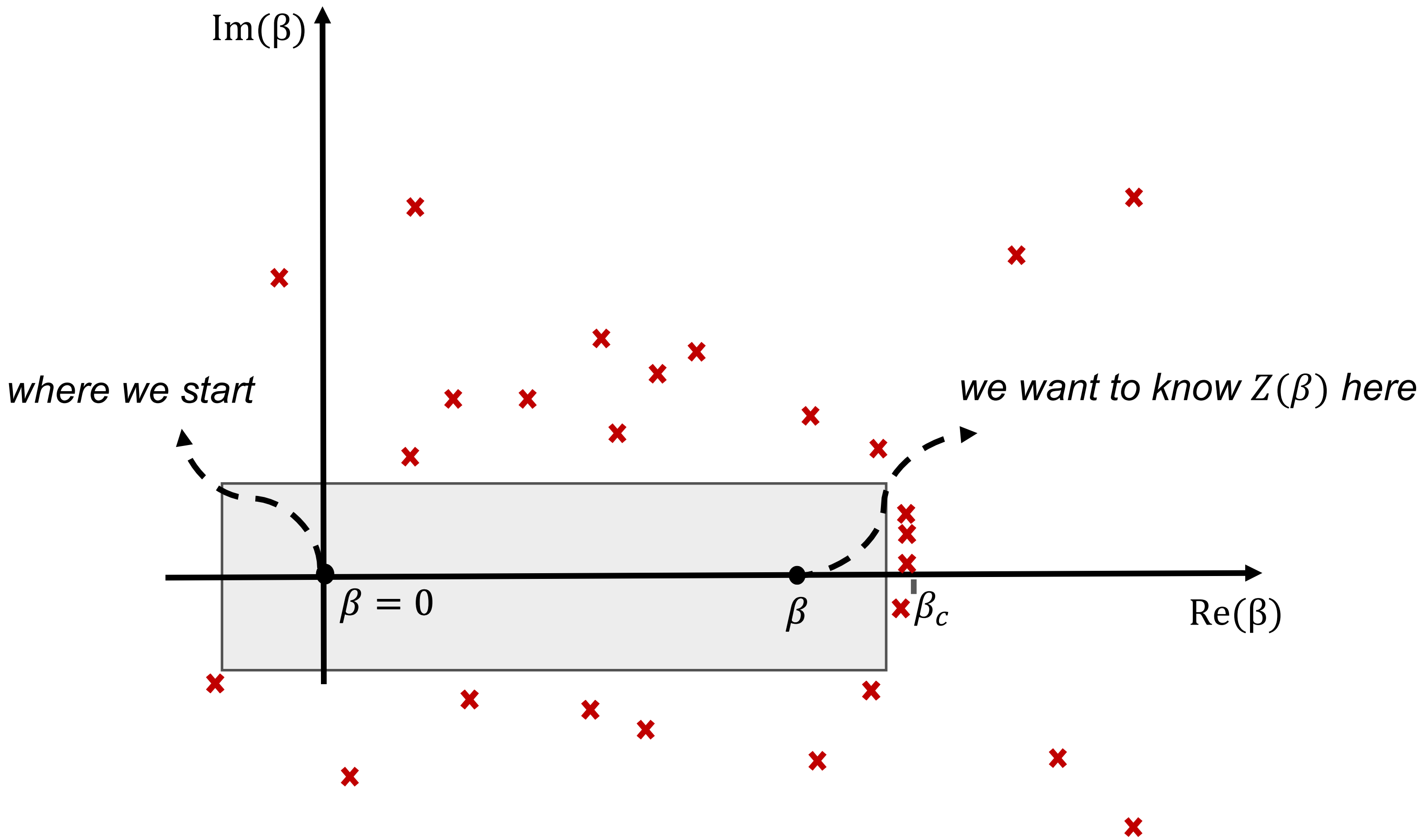

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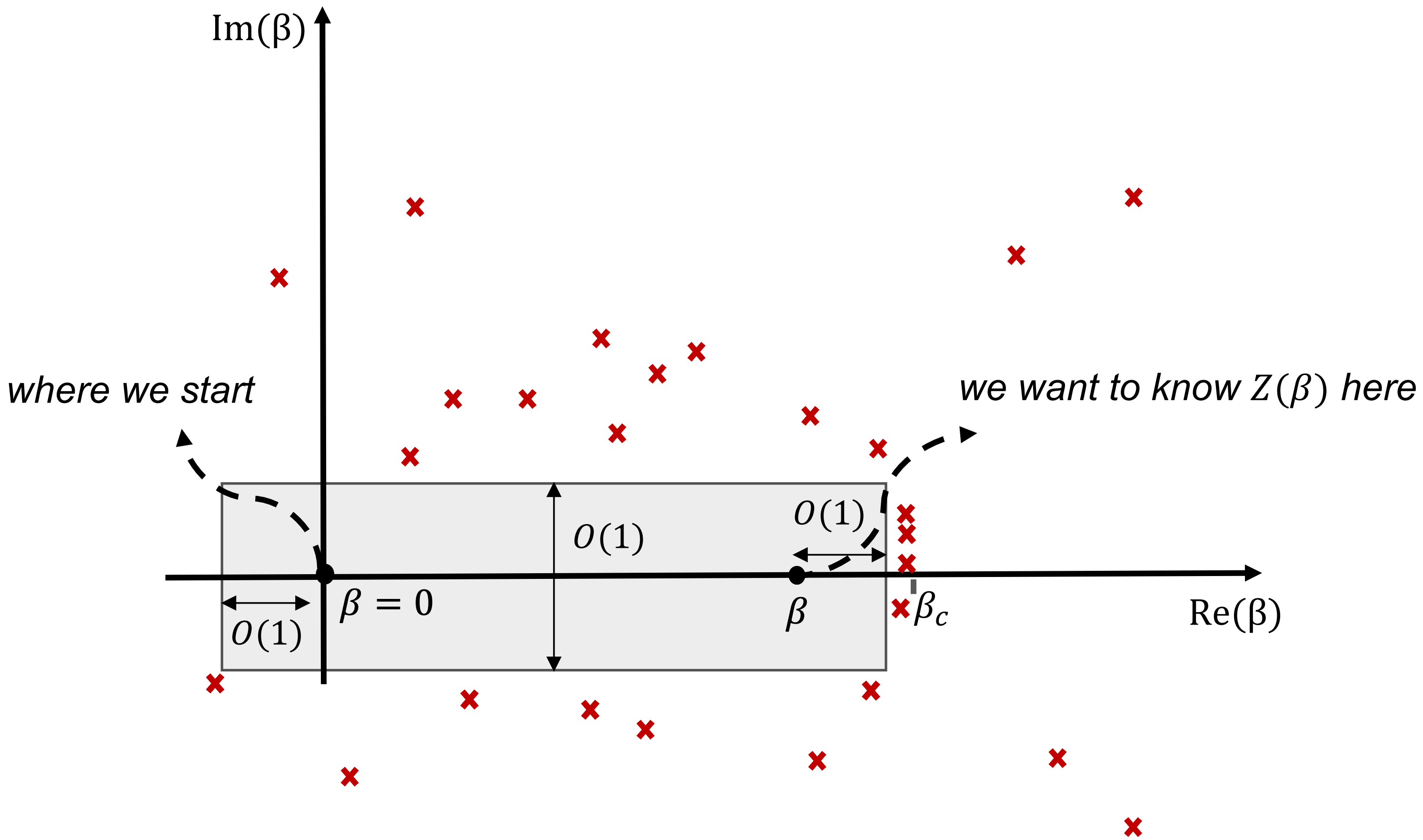

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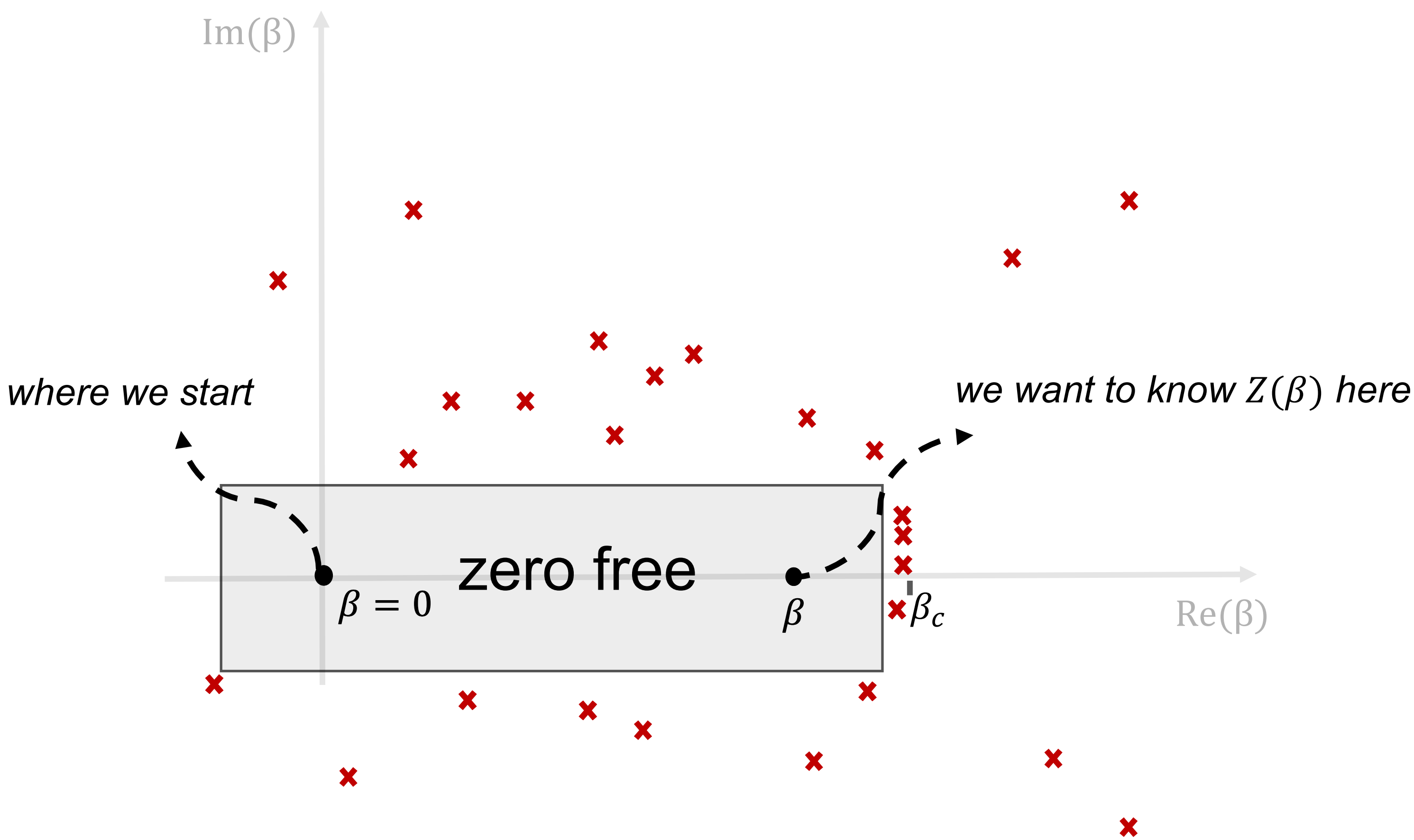
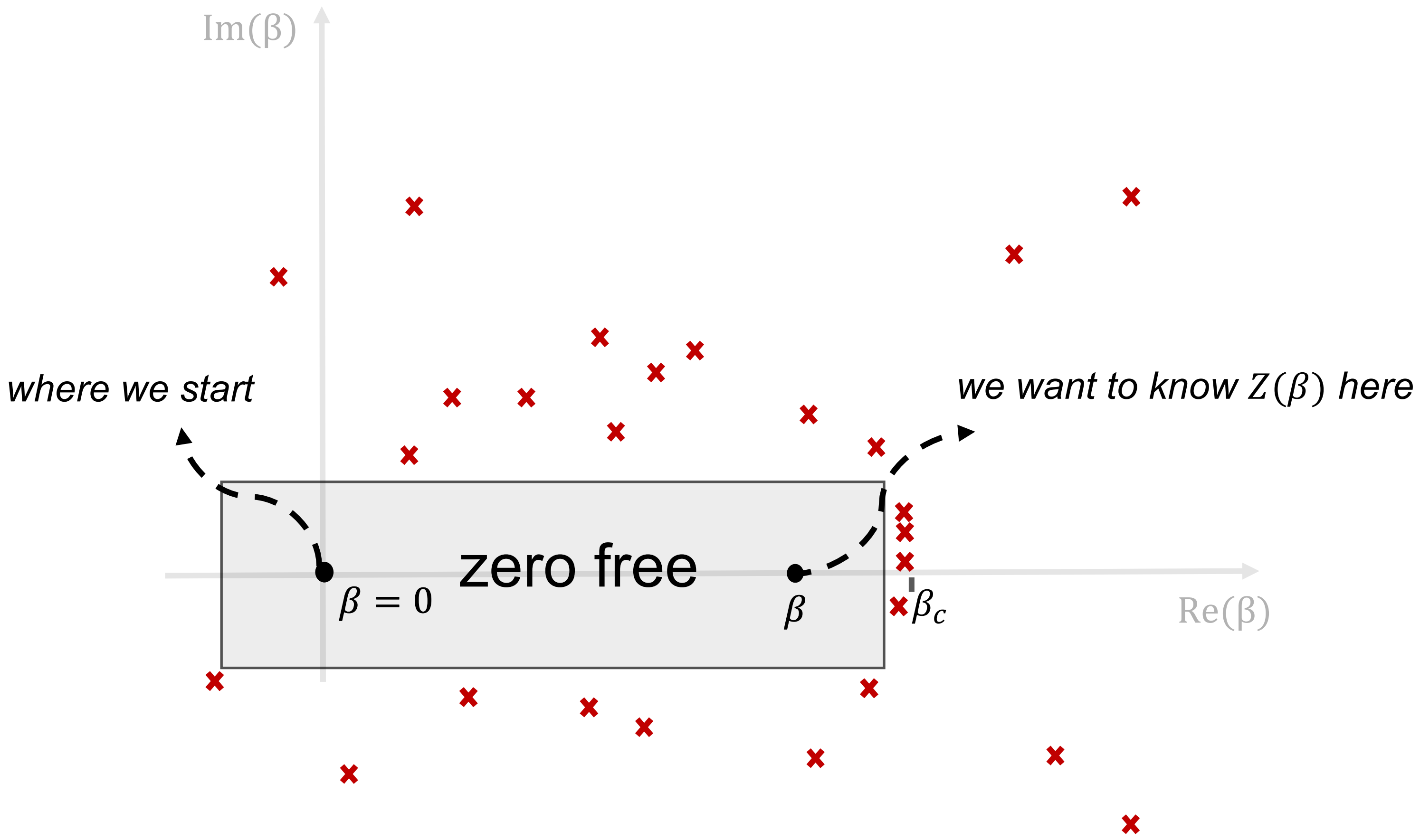


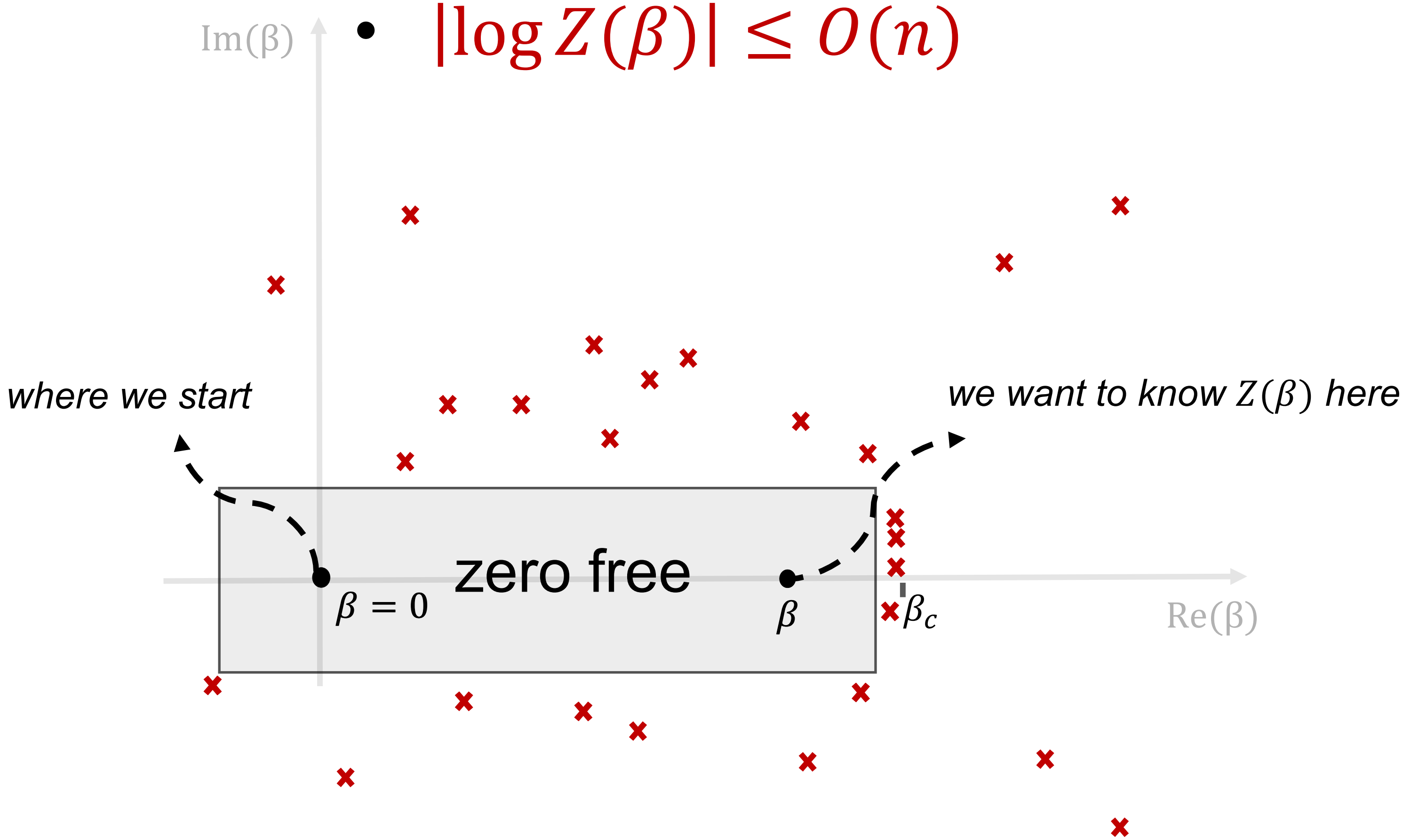
Extrapolating $\log Z(\beta)$

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



Extrapolating $\log Z(\beta)$

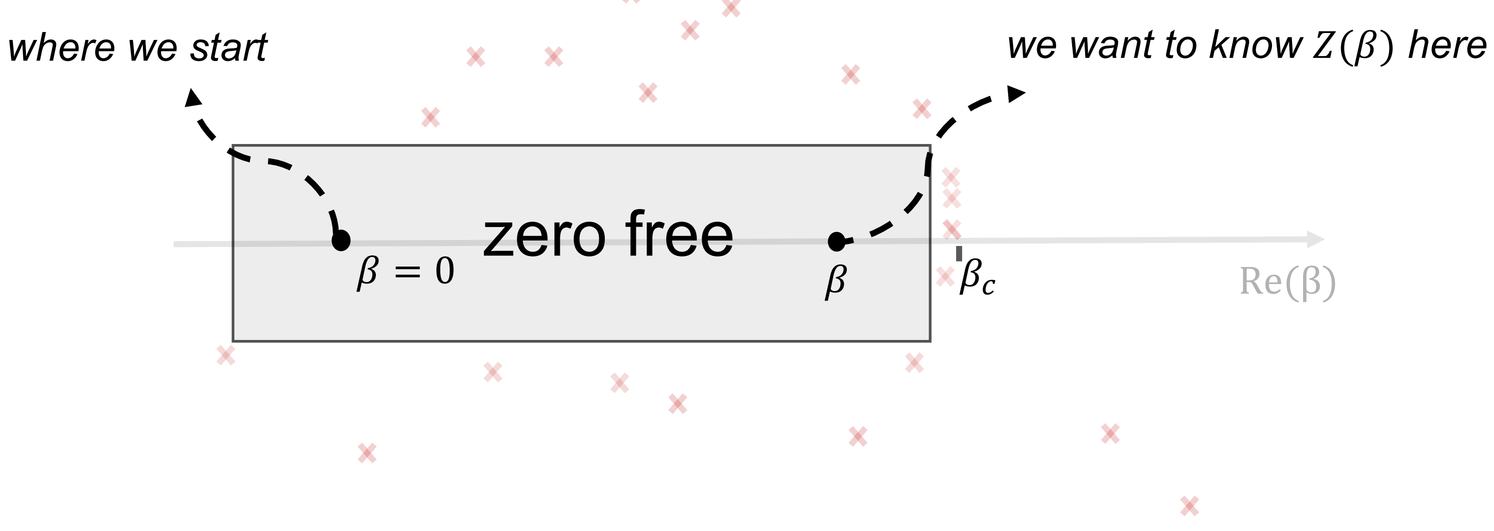
- $\log Z(\beta)$ is analytic in zero free region
  - $|\log Z(\beta)| \leq O(n)$



Extrapolating $\log Z(\beta)$

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

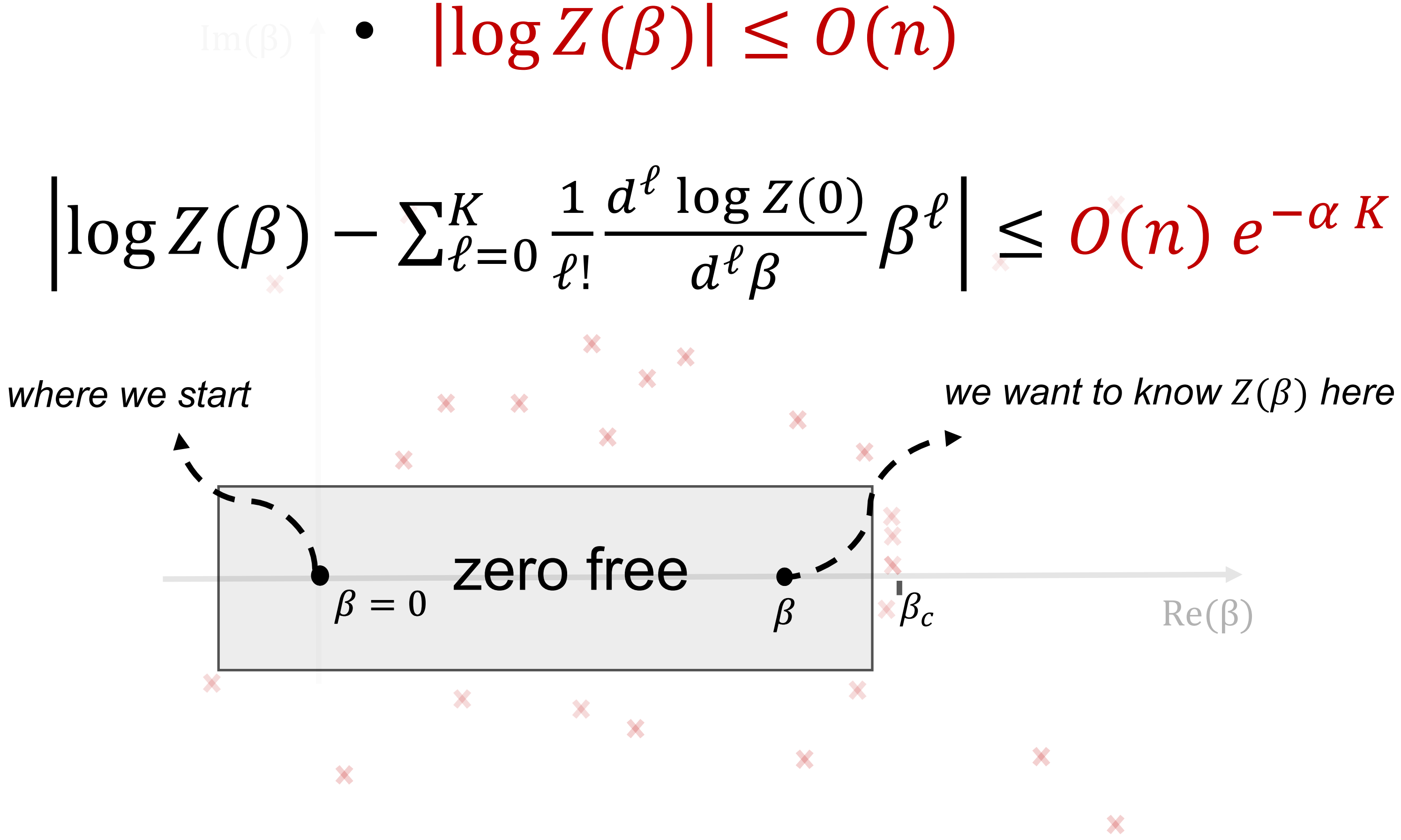
$$\sum_{\ell=0}^{K} \frac{1}{\ell!} \frac{d^\ell \log Z(0)}{d^\ell \beta} \beta^\ell$$



Extrapolating $\log Z(\beta)$

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

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



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

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

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

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

→ $1/\text{poly}(n)$

Extrapolating $\log Z(\beta)$

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

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

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

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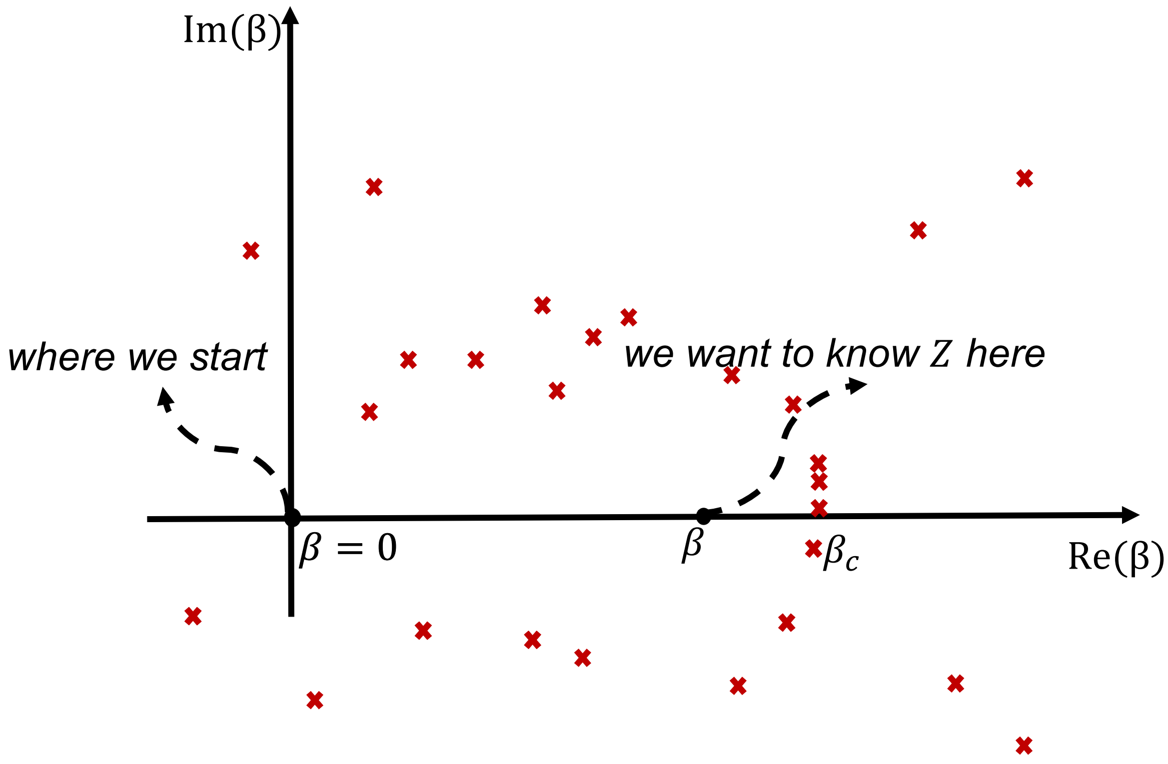
  Compared to randomized ones based on sampling

Why not go beyond the phase transition point?



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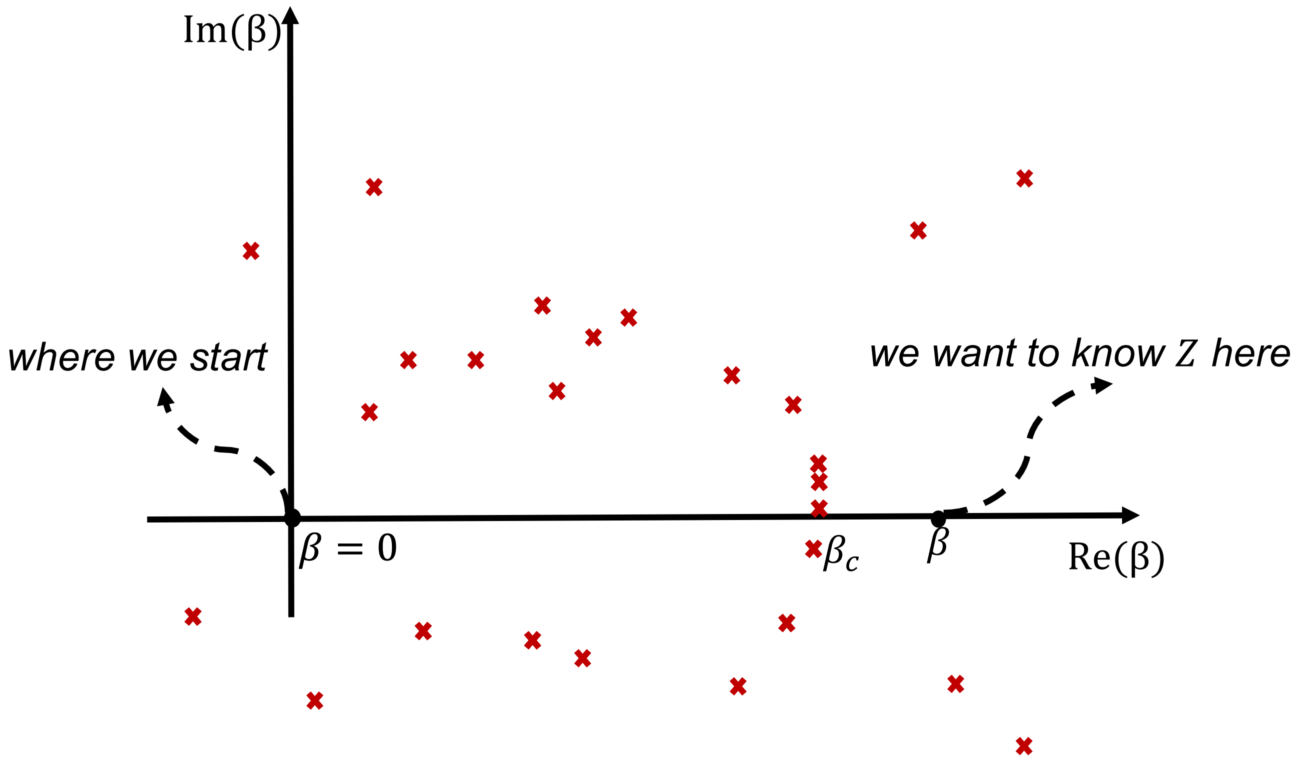

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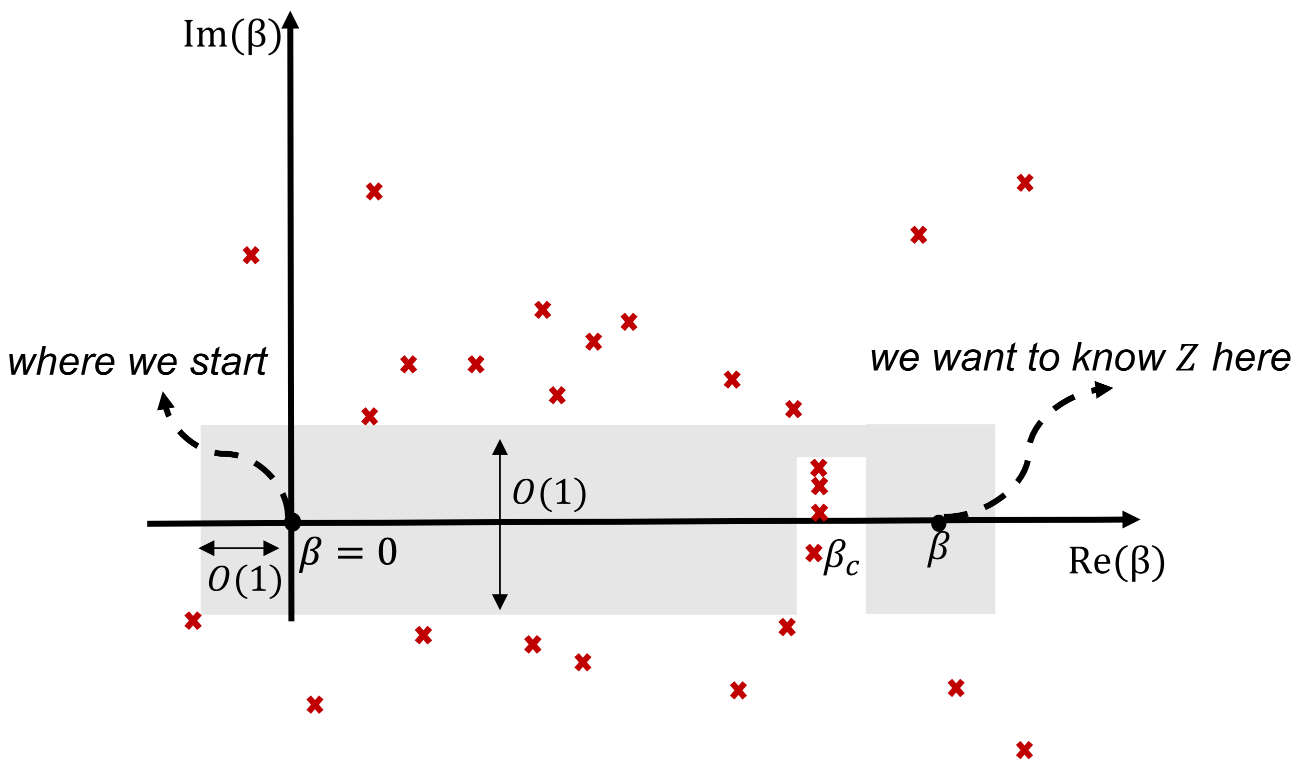

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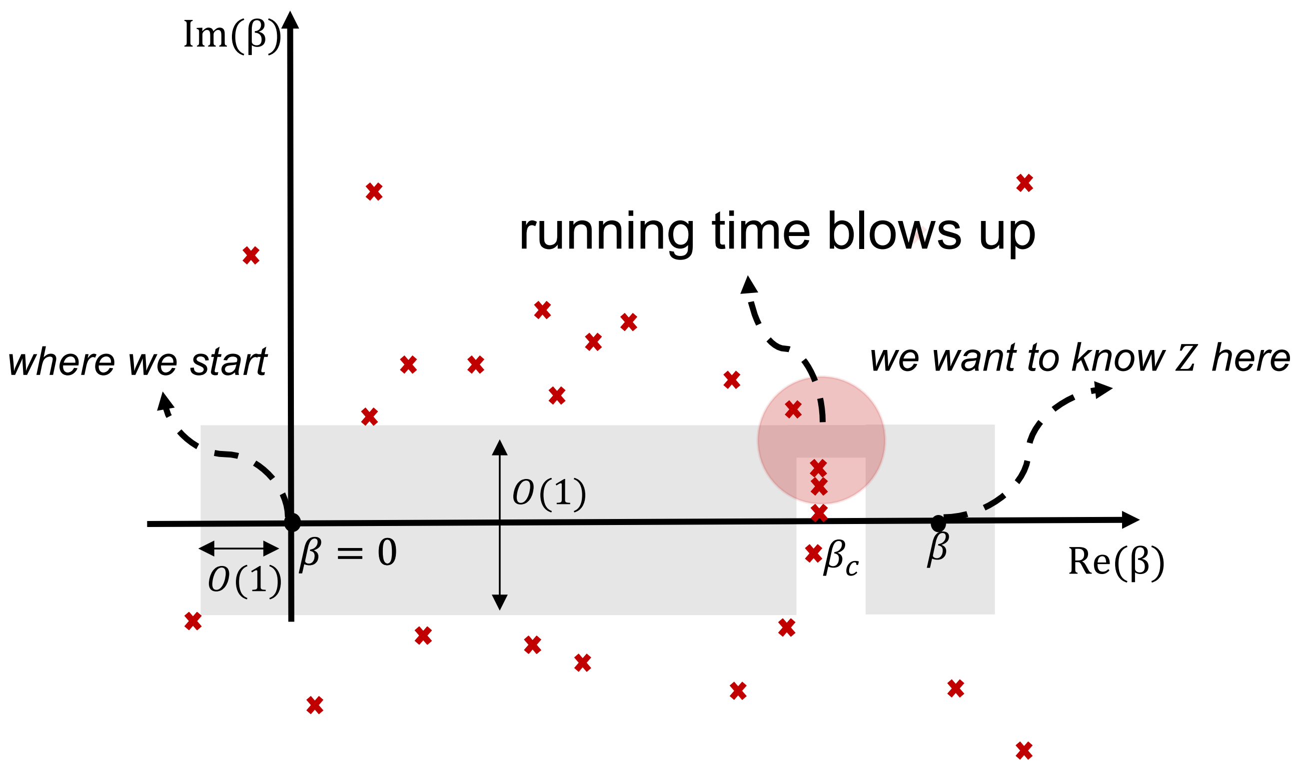

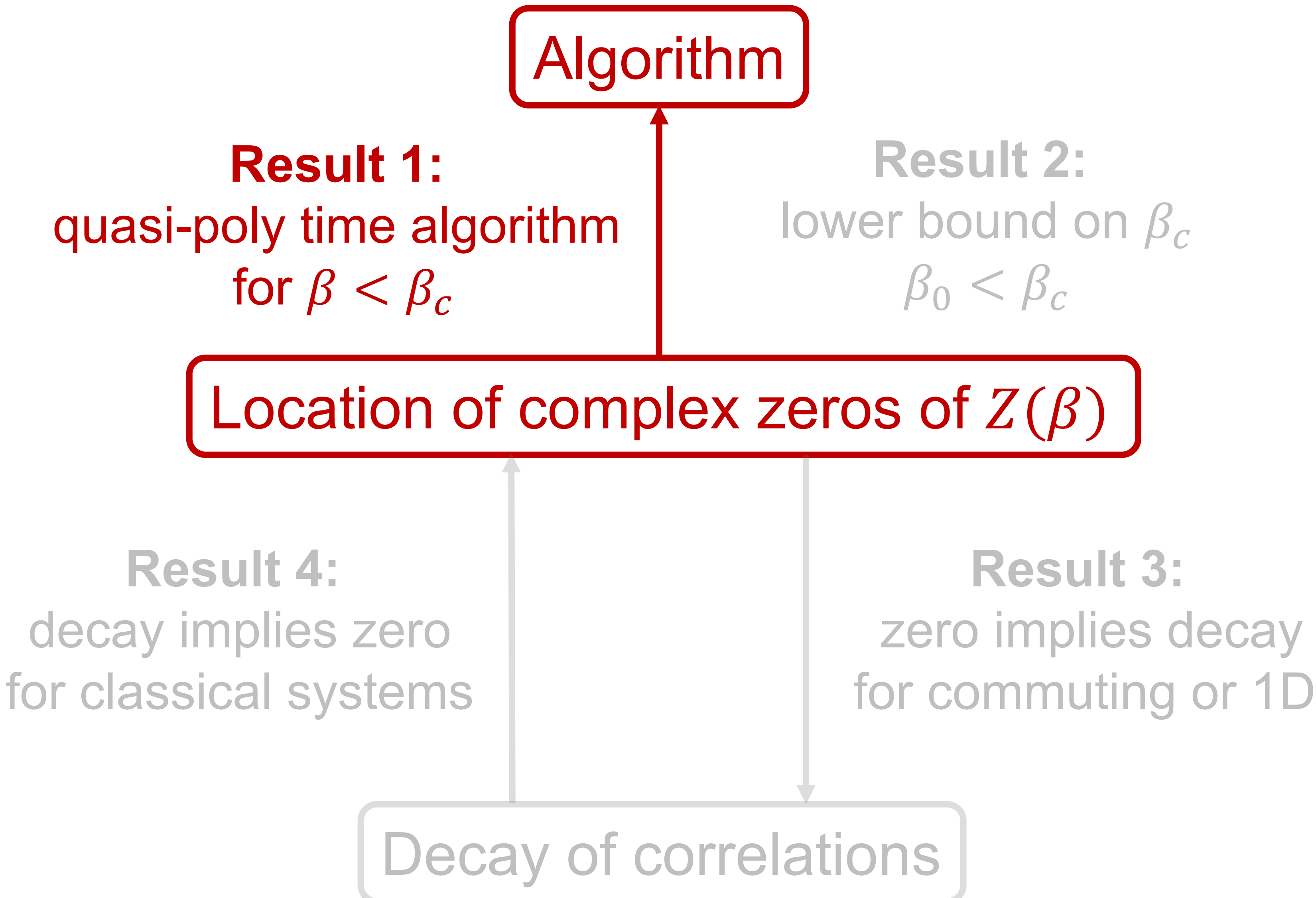

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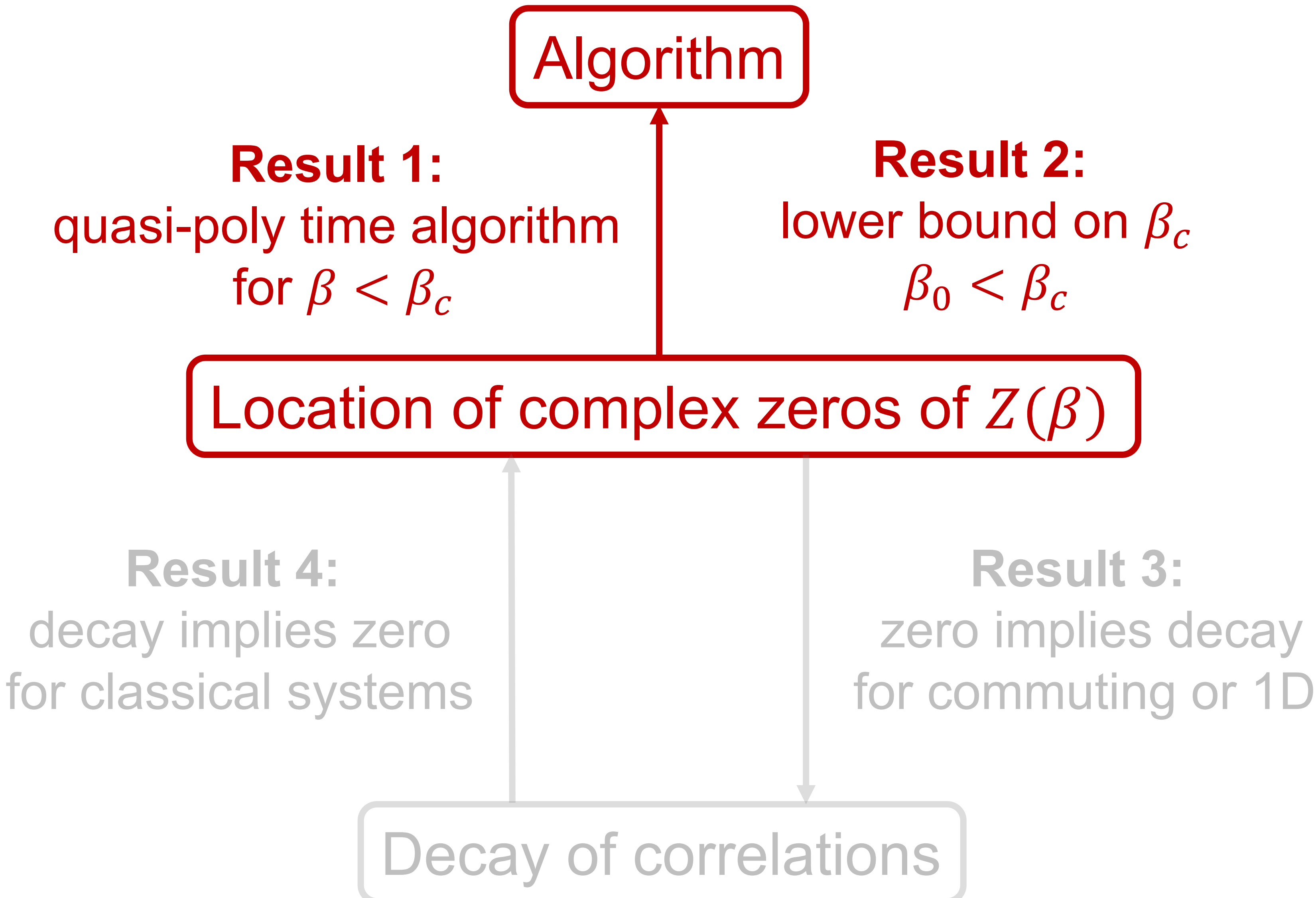

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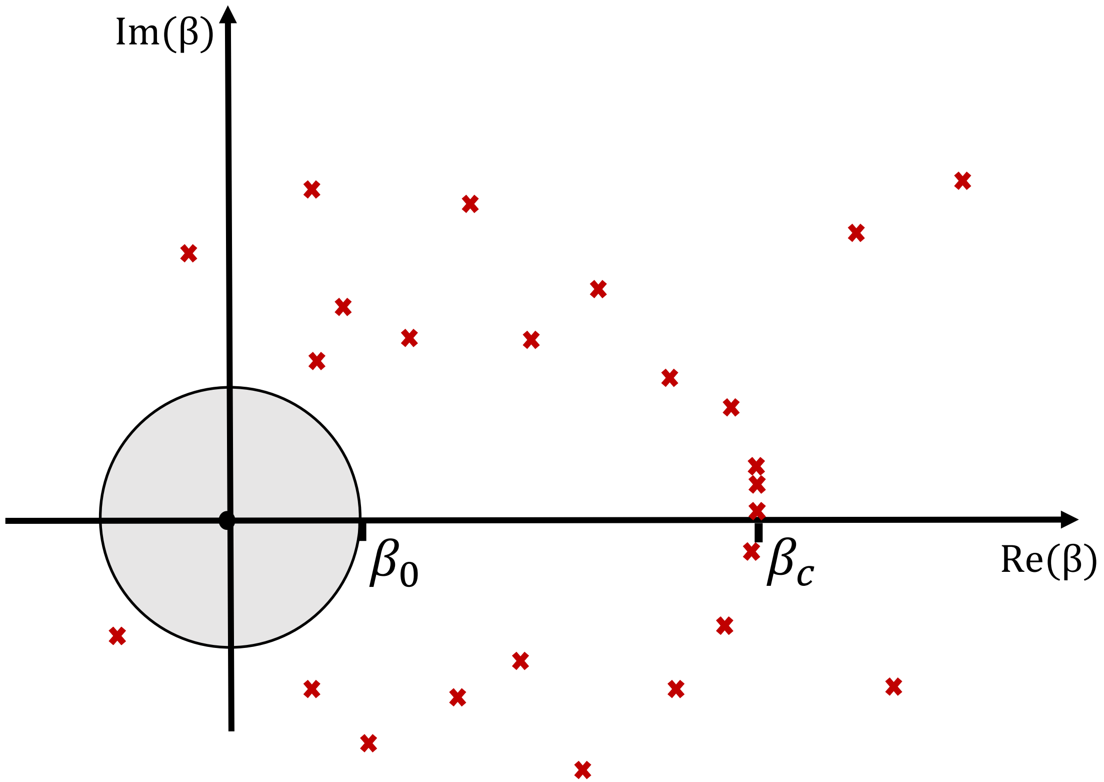

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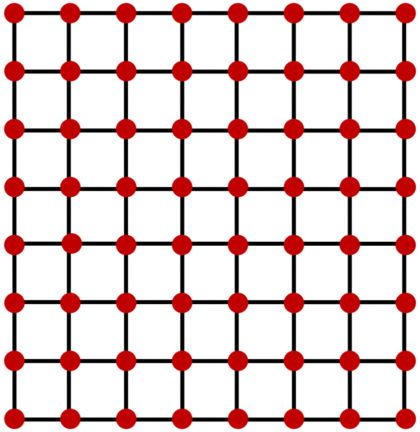

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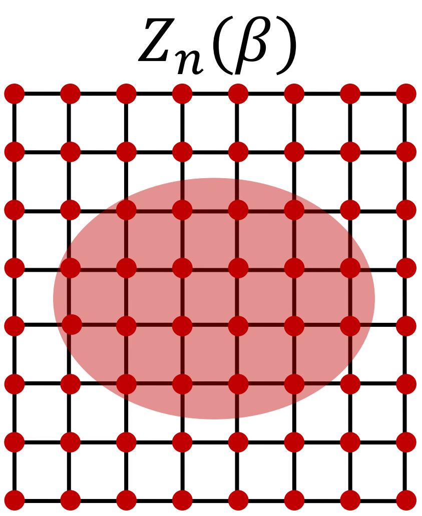

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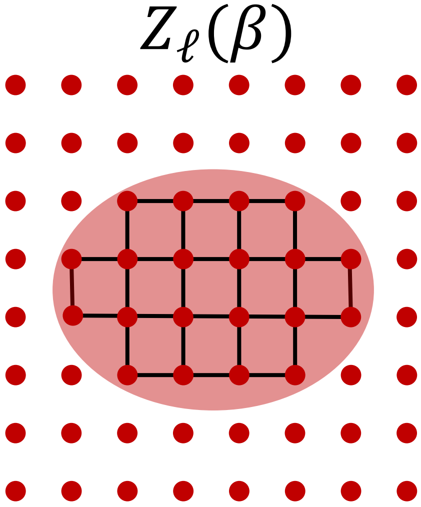

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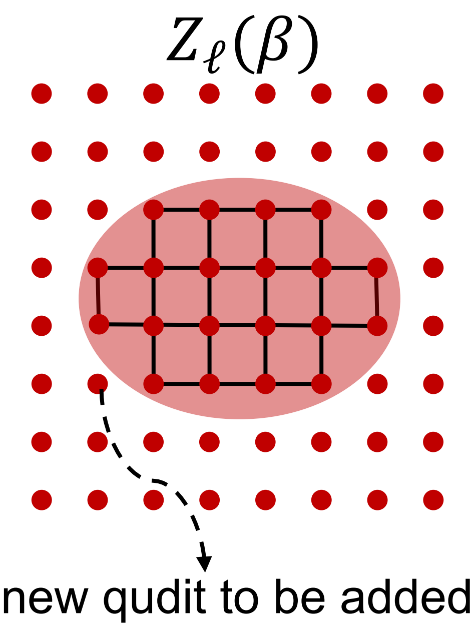

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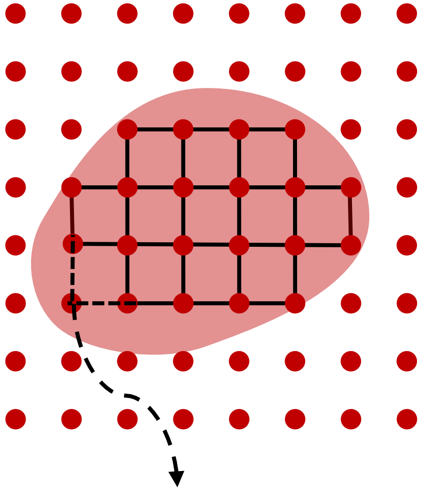

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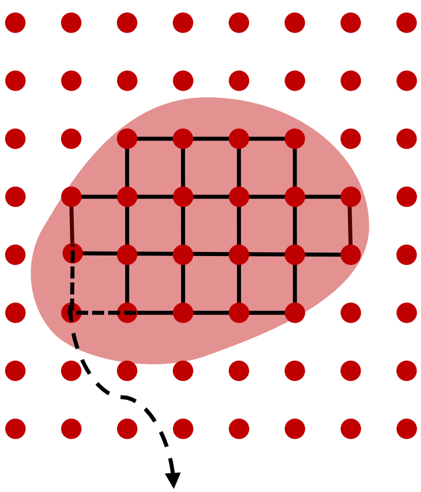

new qudit added

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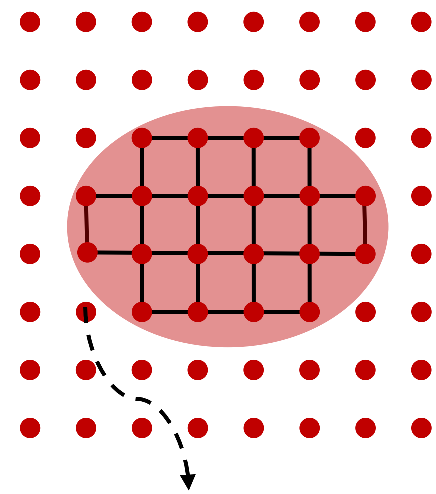

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First show

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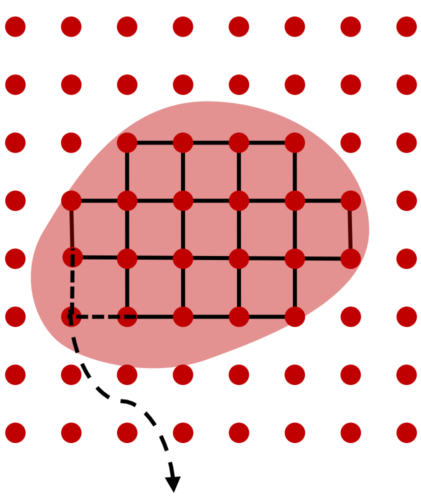

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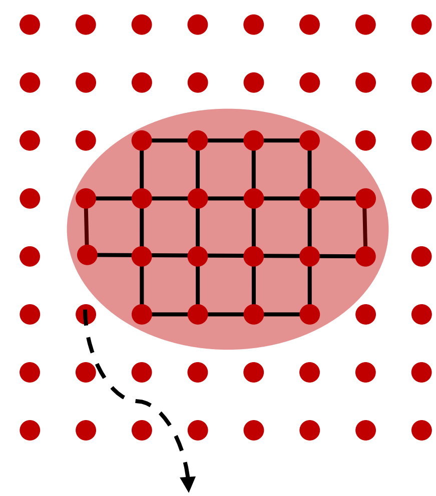

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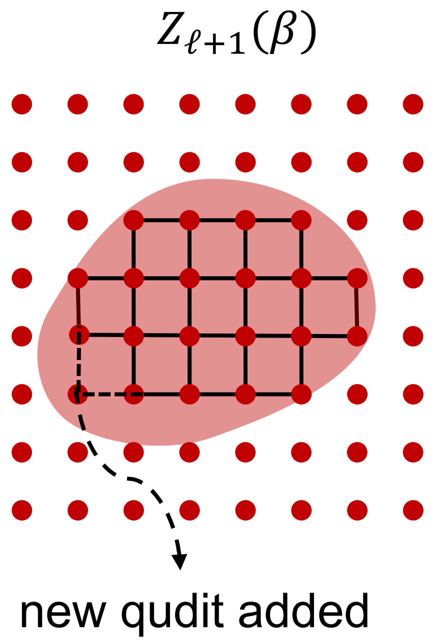

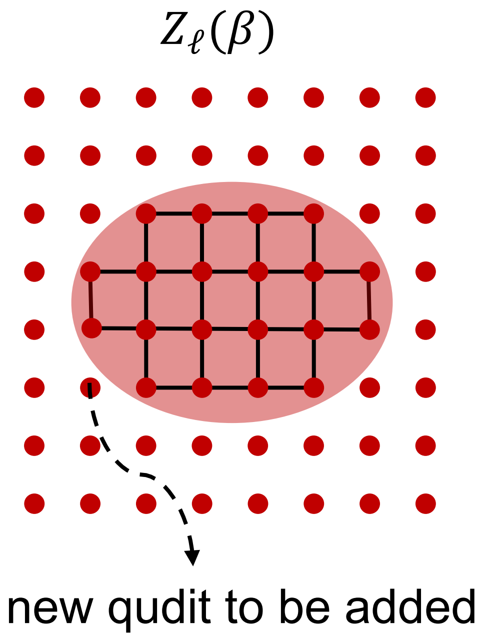

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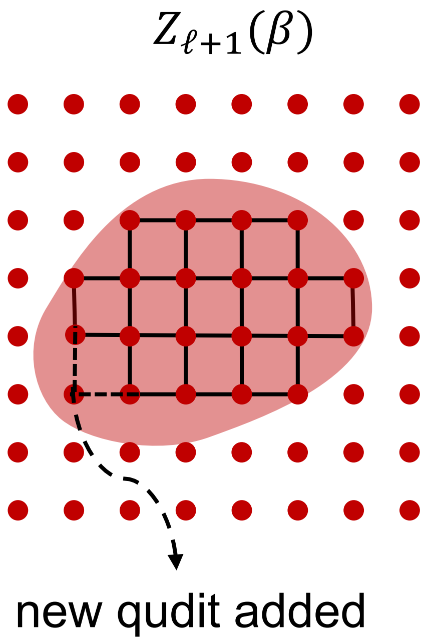

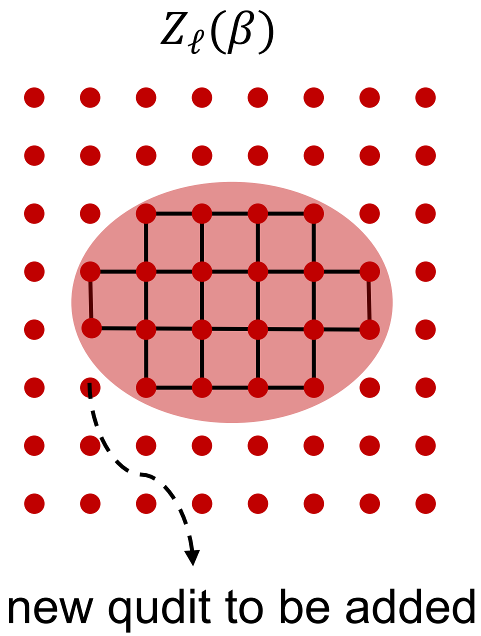

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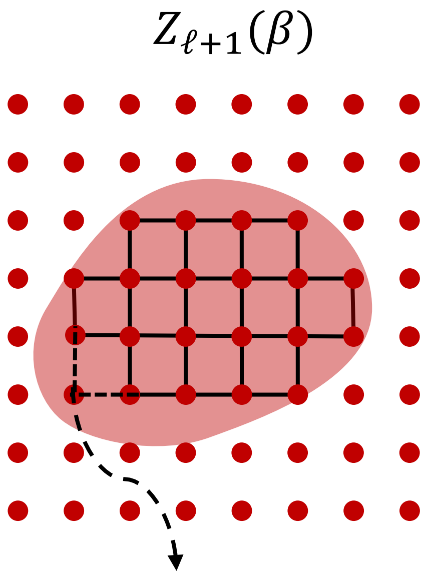

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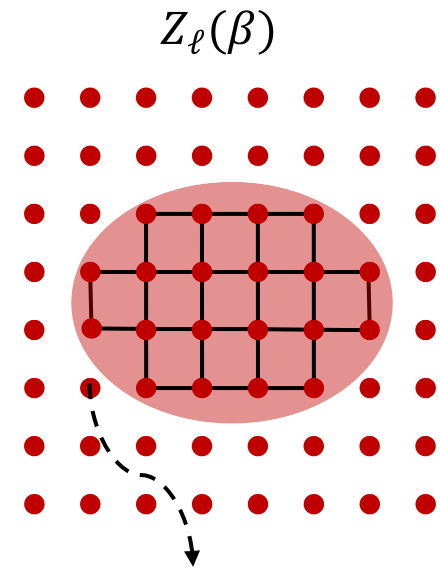
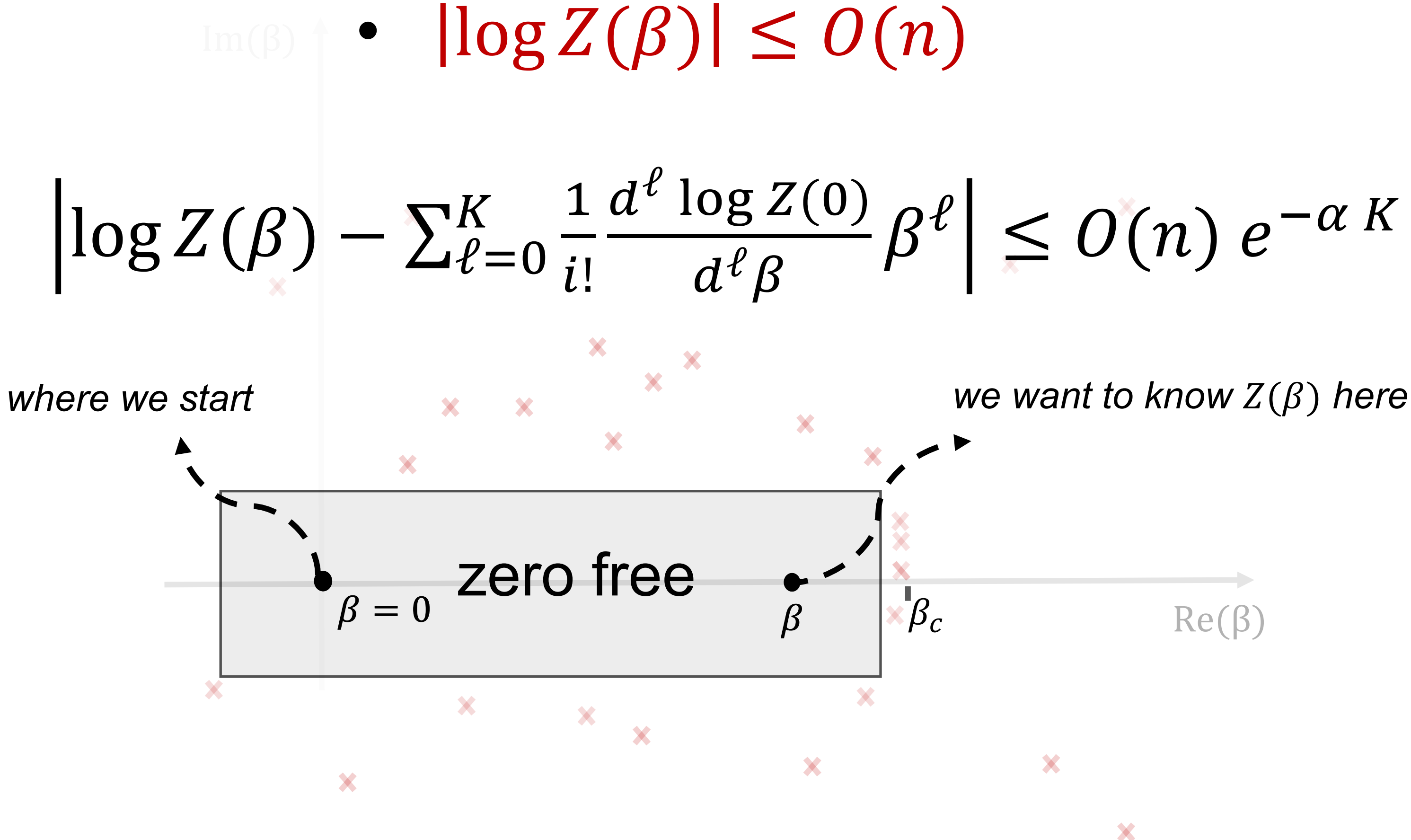


new qudit to be added

Extrapolating $\log Z(\beta)$

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

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



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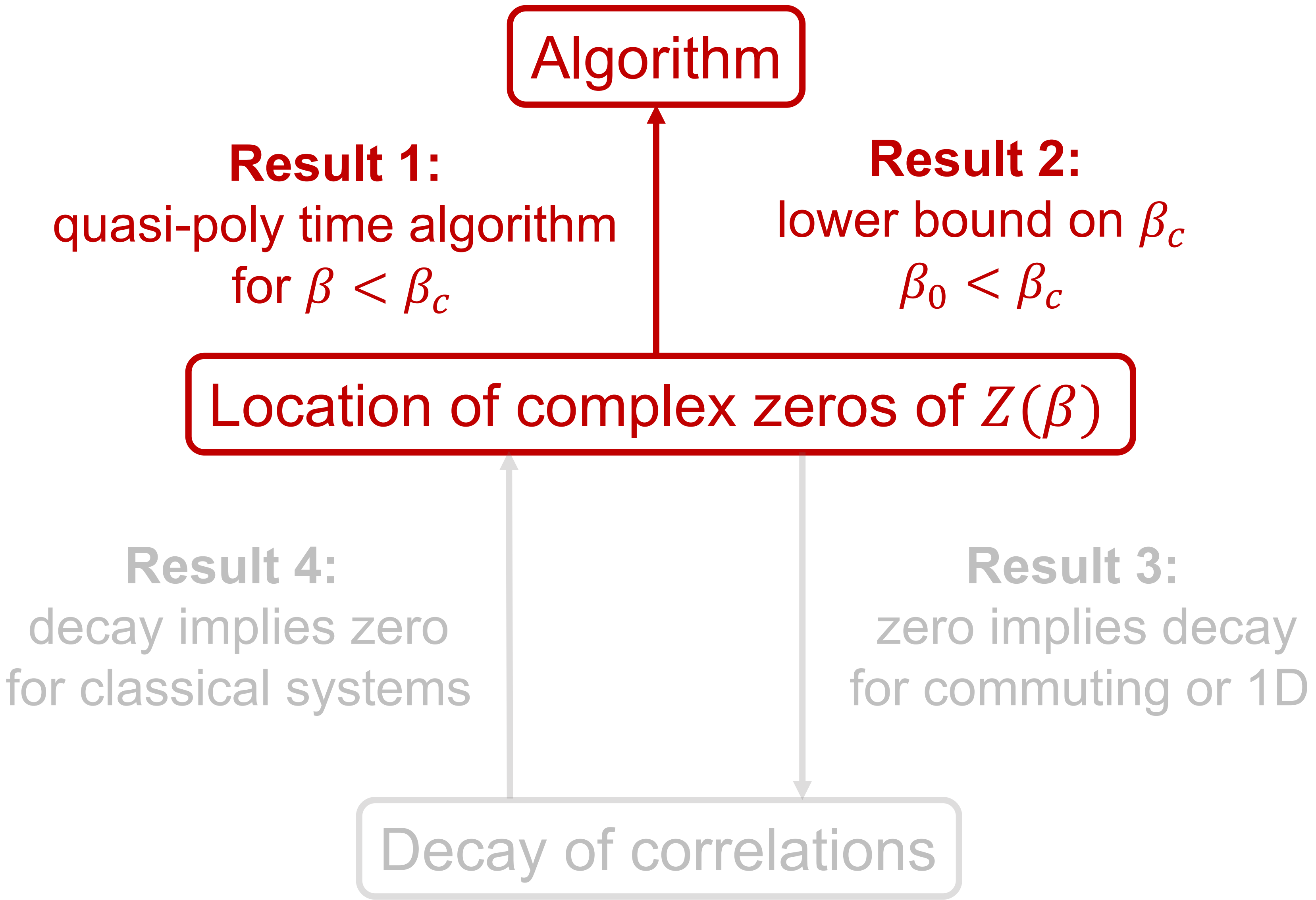
$$|\text{corrections}/Z_i(\beta)| \leq O(1)$$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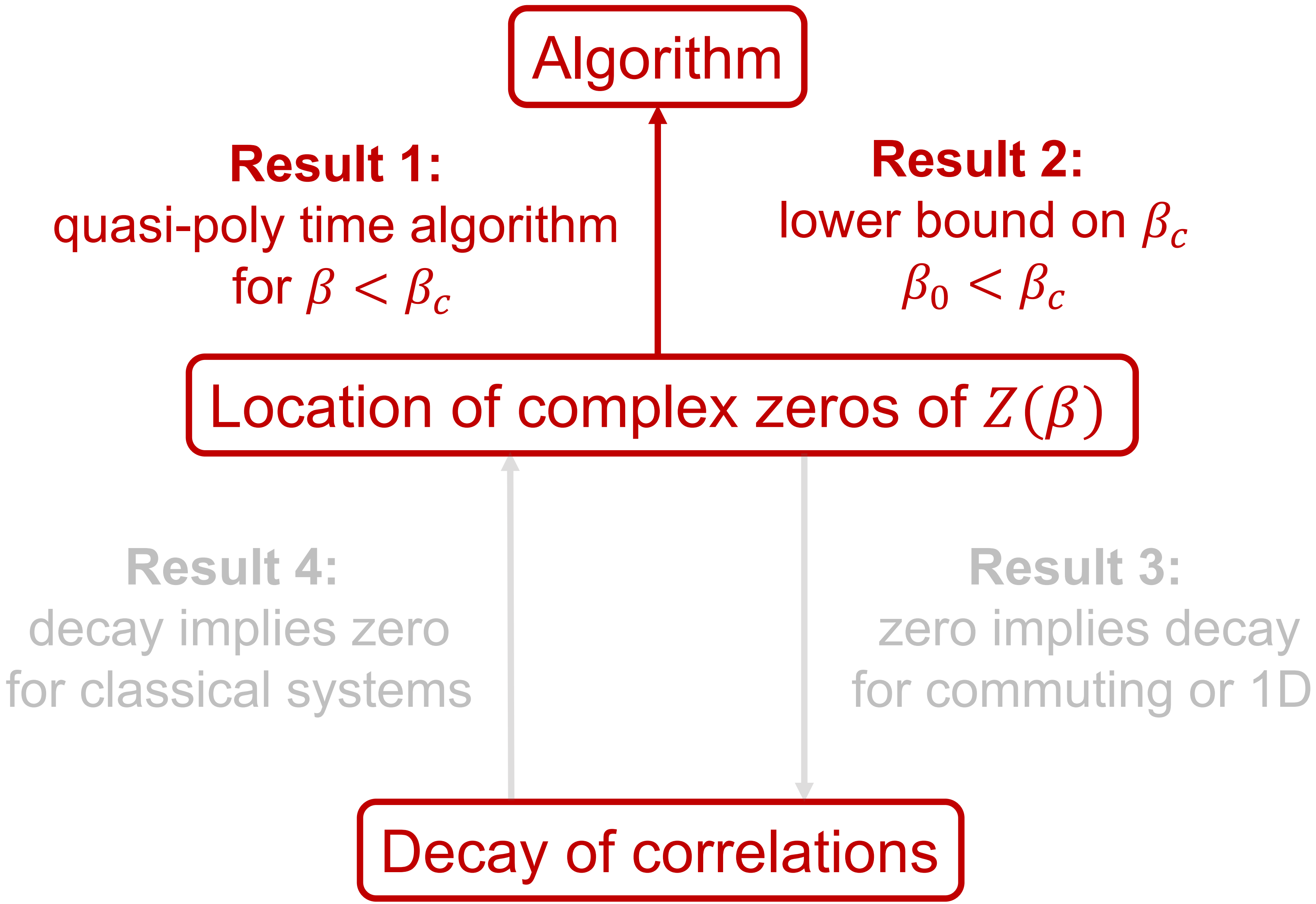

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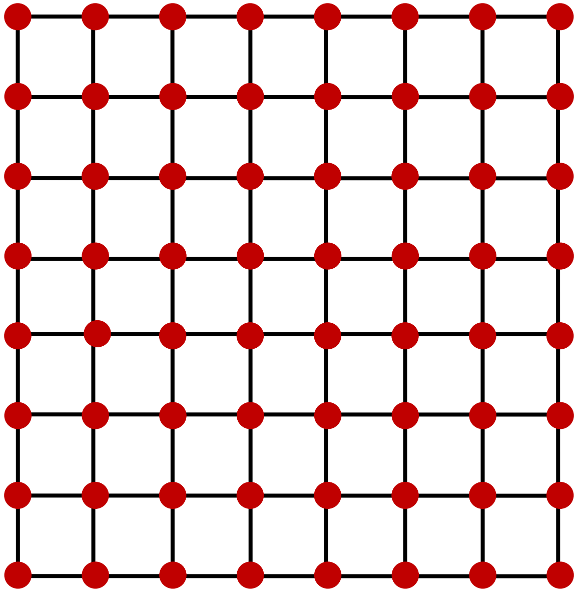
Decay of correlations vs phase transition



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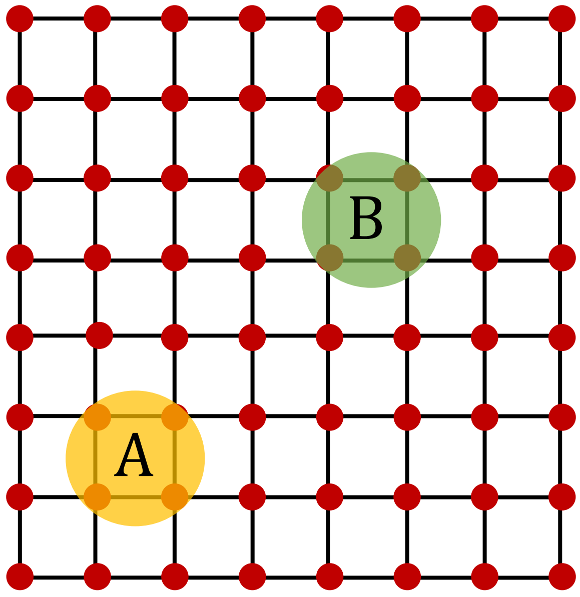

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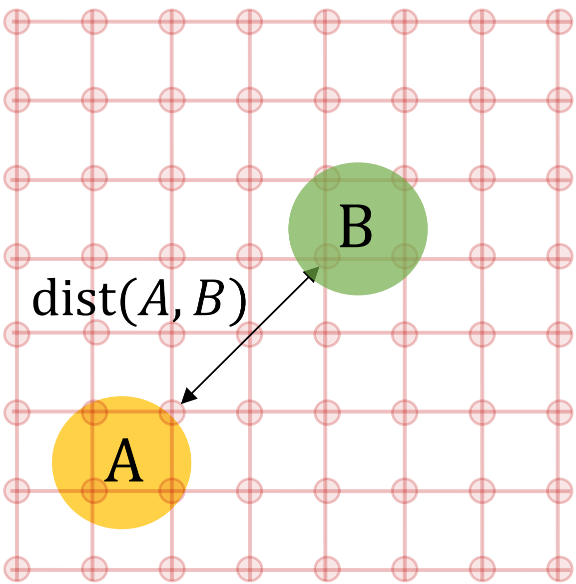

$$|\,\mathrm{Tr}[AB\rho] - \mathrm{Tr}[A\rho]\mathrm{Tr}[B\rho]| \leq c\, e^{-\mathrm{dist}(A,B)/\xi}$$

Decay of correlations vs phase transition

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

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Mixing in time $=$ Mixing in space

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(Mixing in space → exponential decay of correlations)

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↓ efficient sampling algorithm | ↓ exponential decay of correlations

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Mixing in time = Mixing in space

Mixing in time ↓ efficient sampling algorithm

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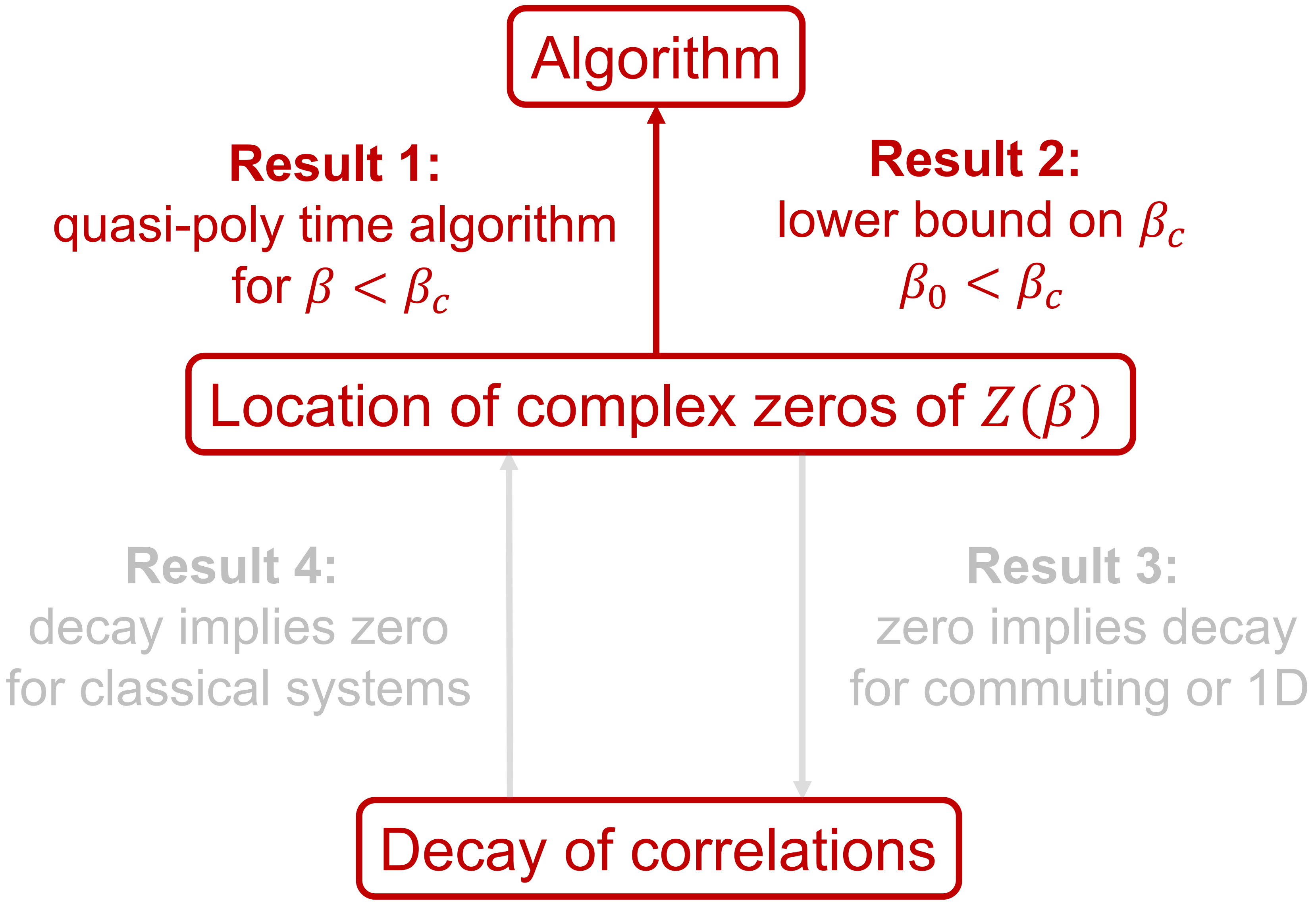
Mixing in time ← Mixing in space + Decay of quantum CMI "Markov property"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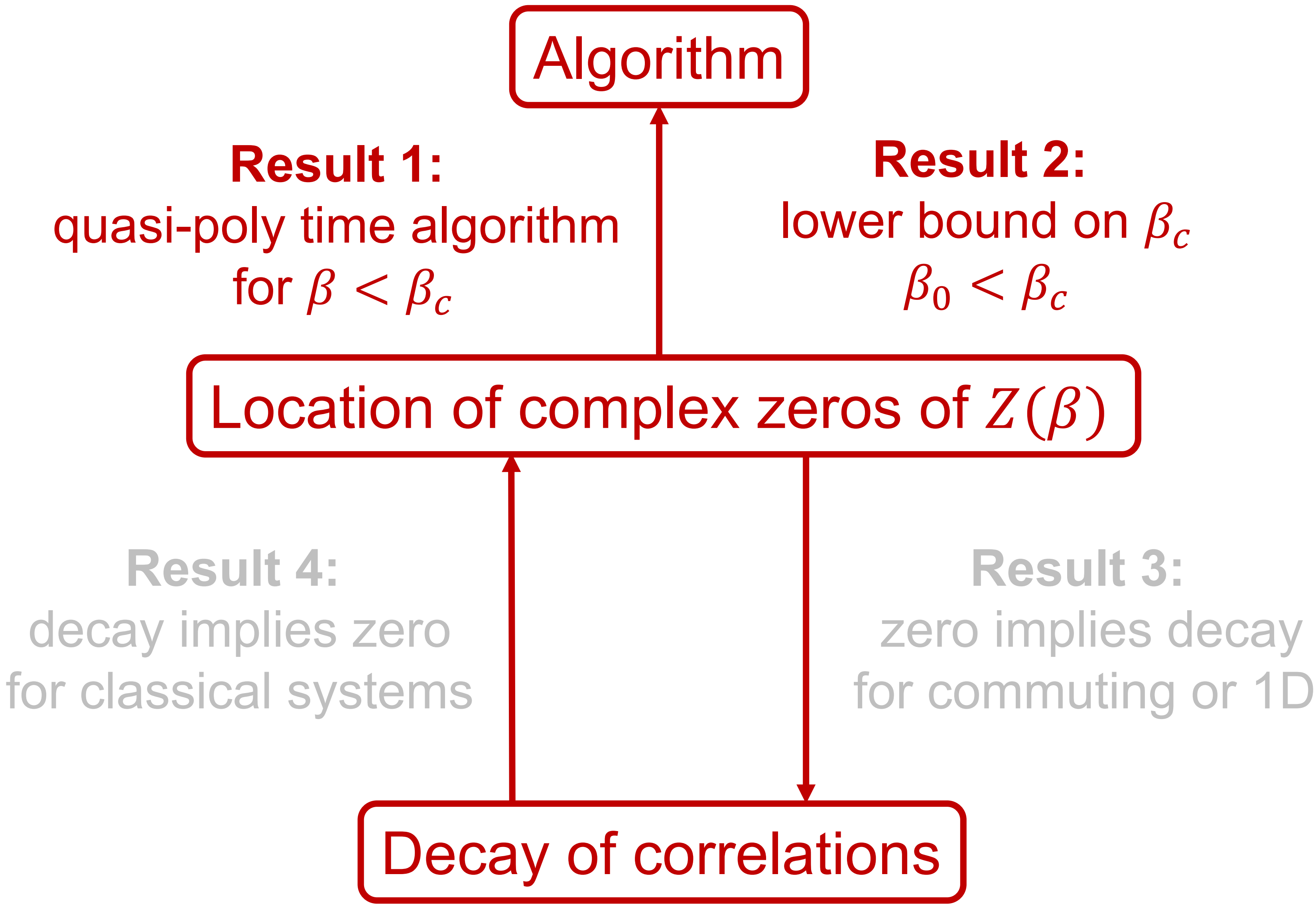
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What is the relation between zeros of $Z(\beta)$ and decay of correlations?

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

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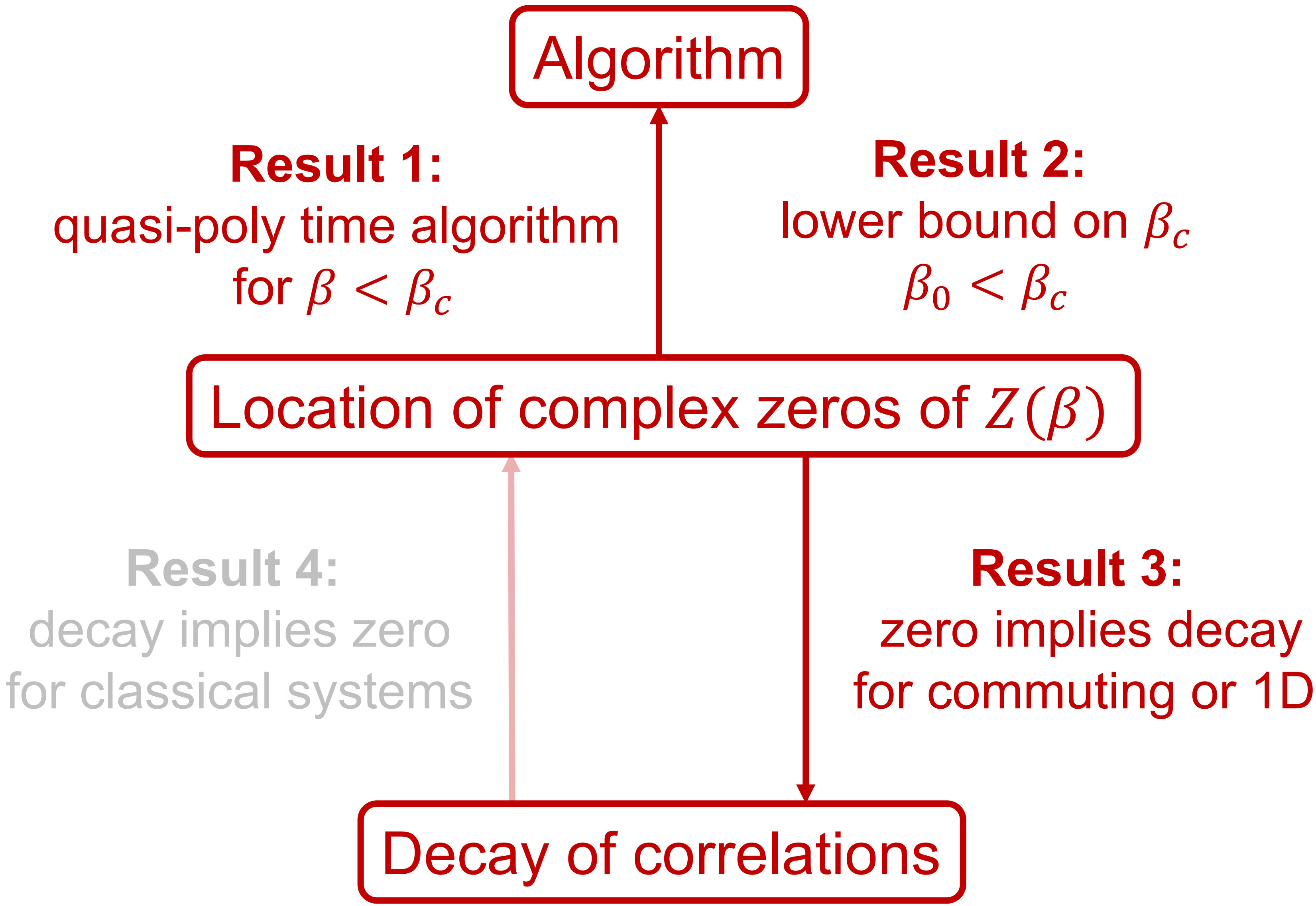
How about quantum systems?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Result 3

We show absence of zeros near real axis

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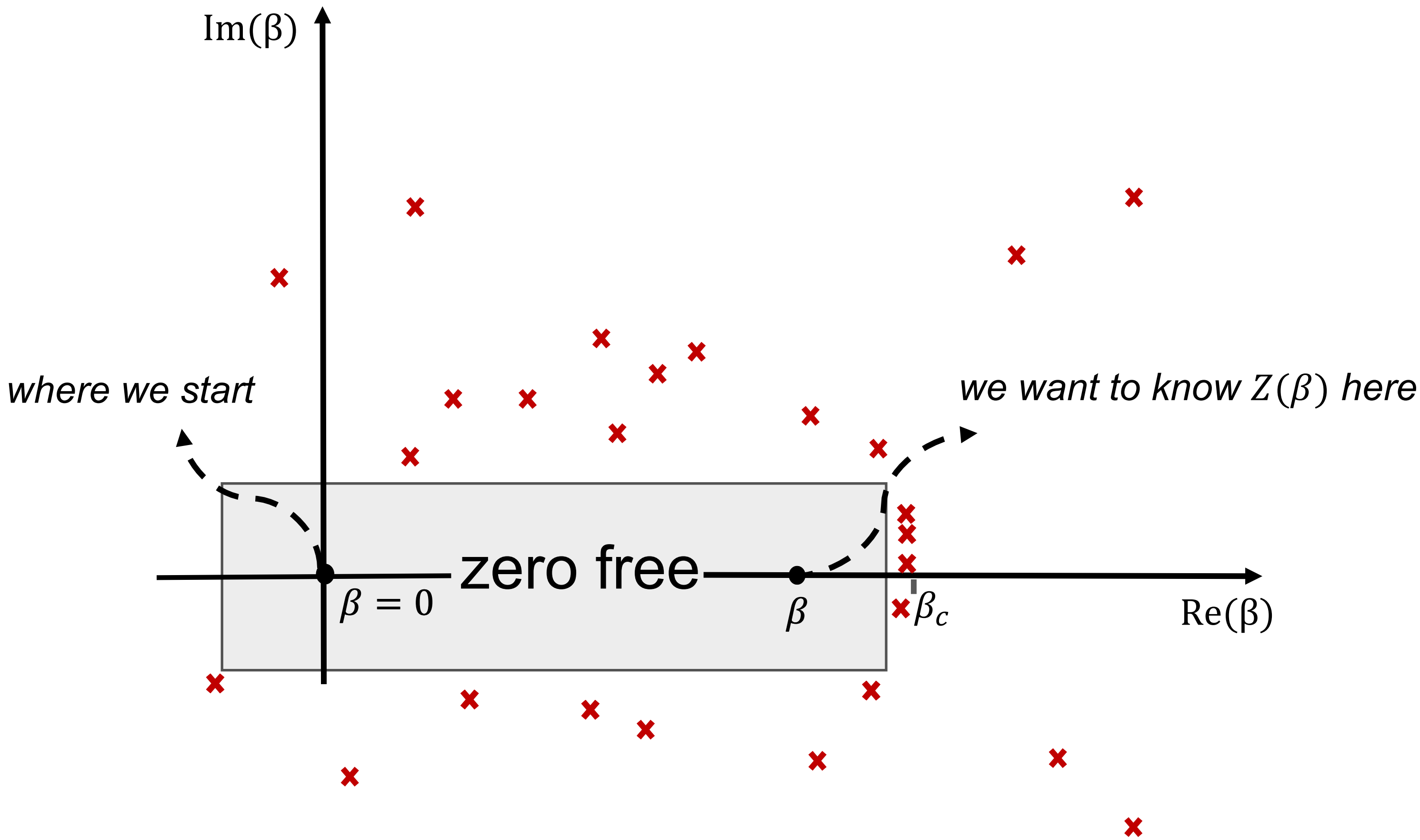

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When

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When

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Result 3

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- General H on a one-dimensional chain

Result 3

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

When

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

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

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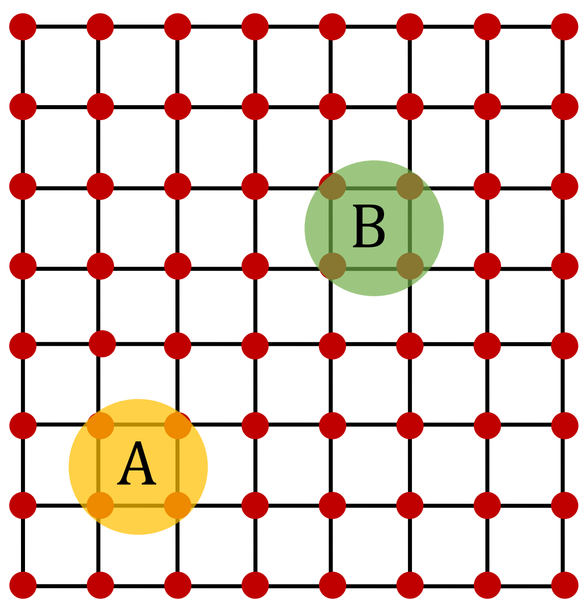
- Define a function that measures correlations btw A, B

$$f(A, B)$$



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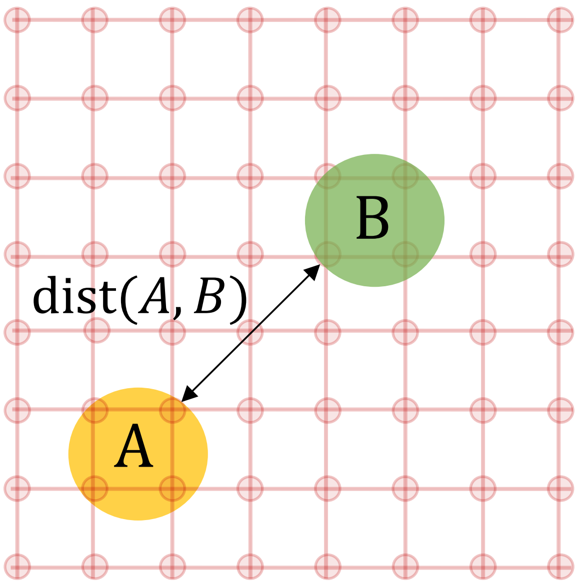

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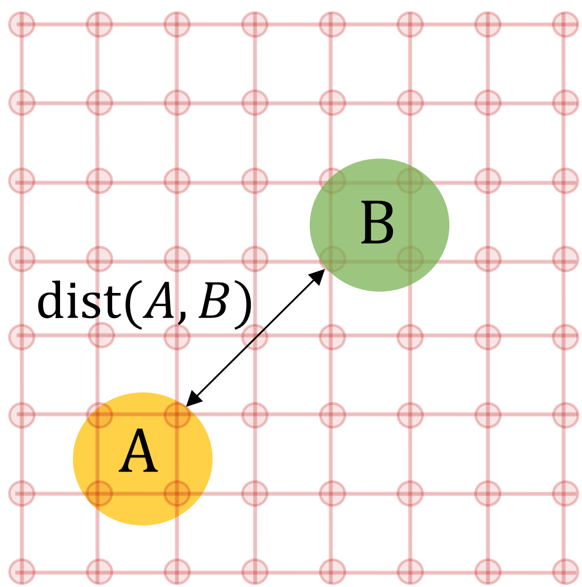

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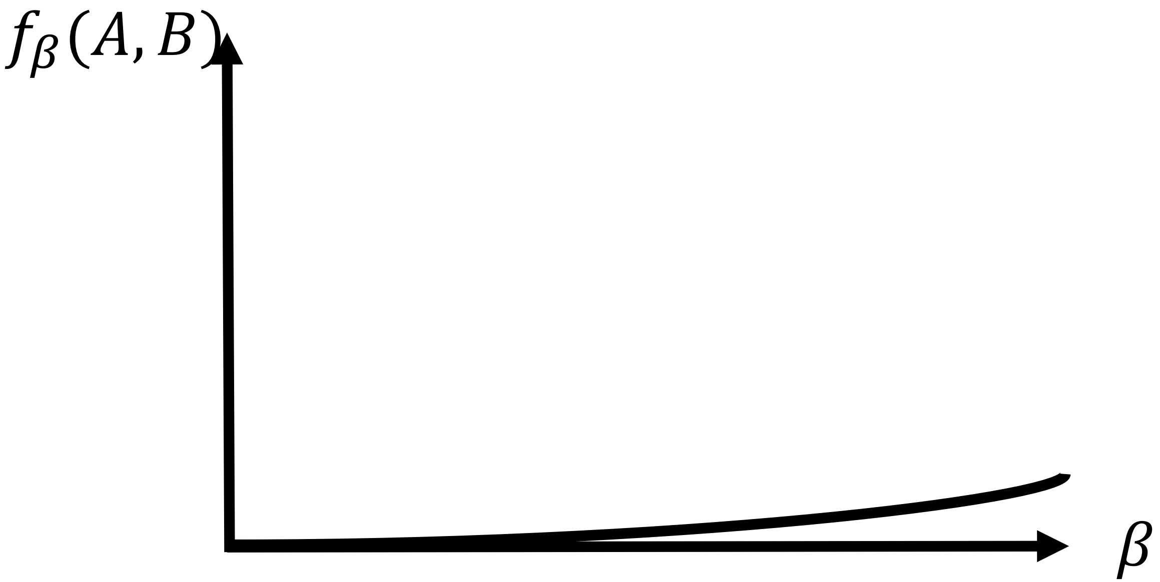

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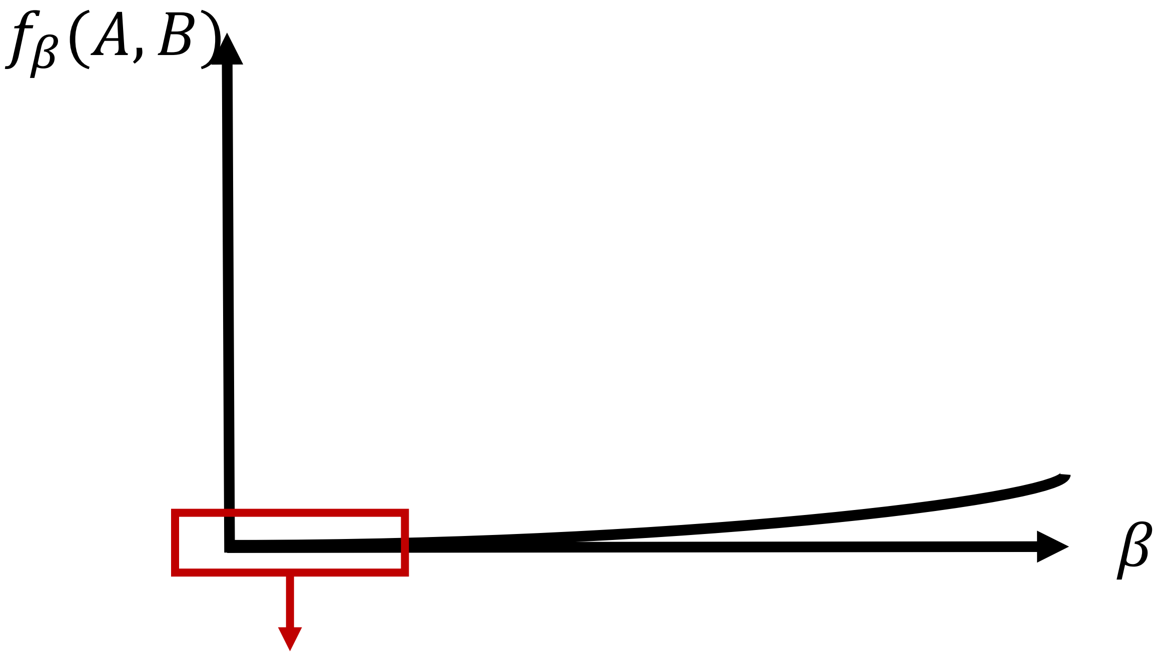

$f_\beta(A, B) = 0$ at $\beta = 0$

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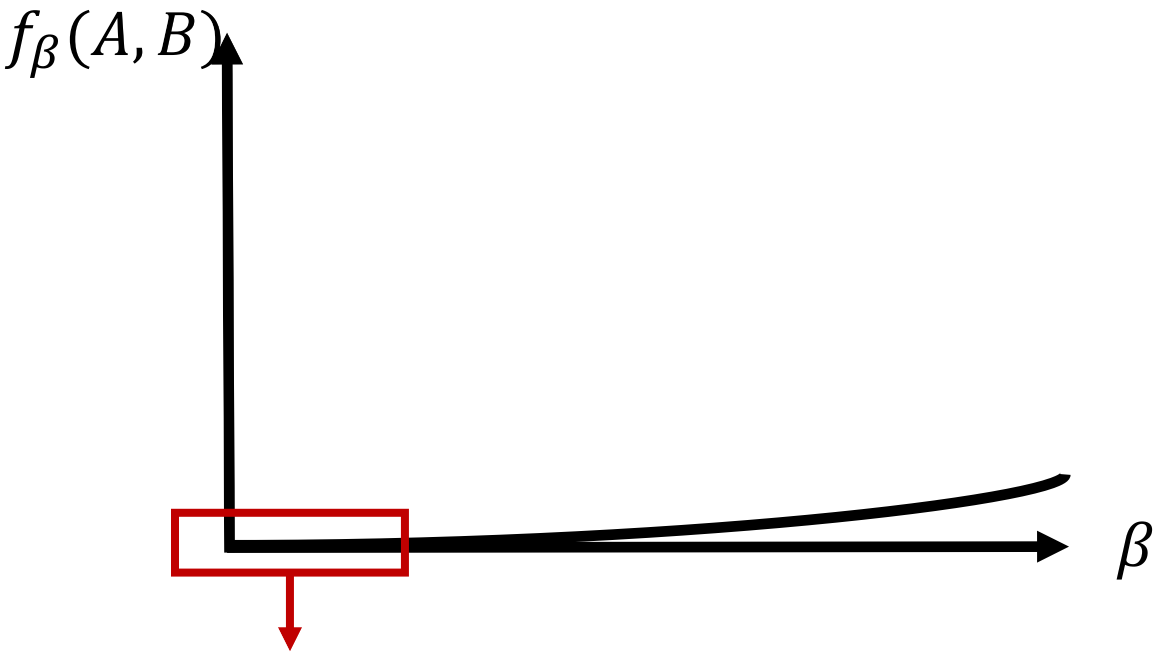

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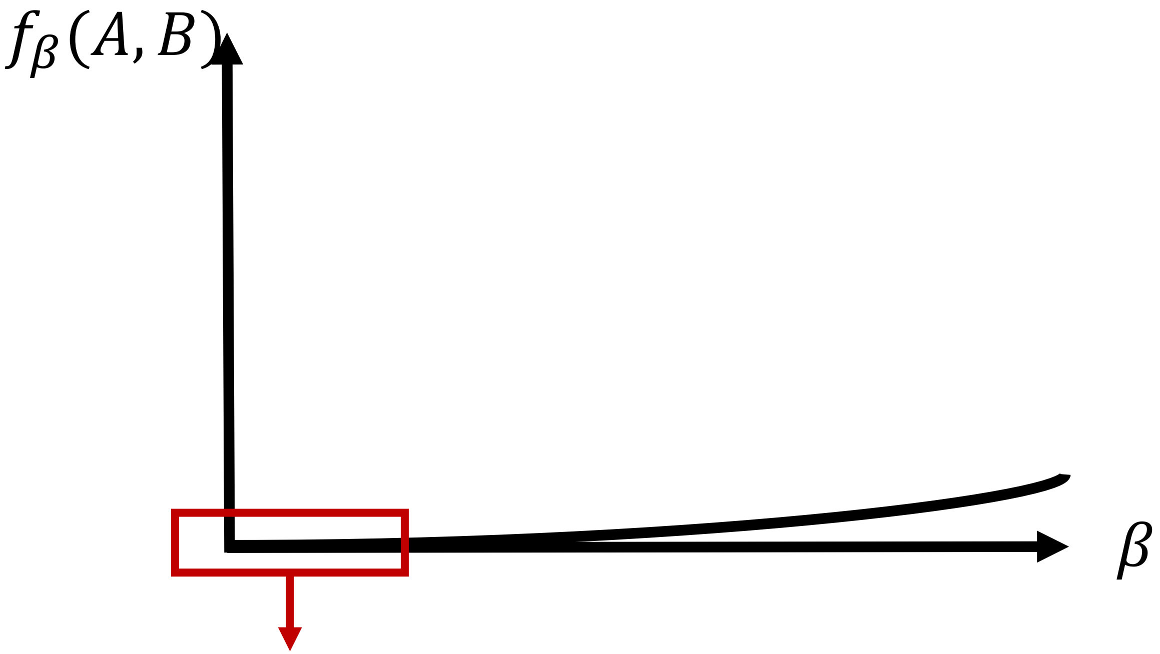

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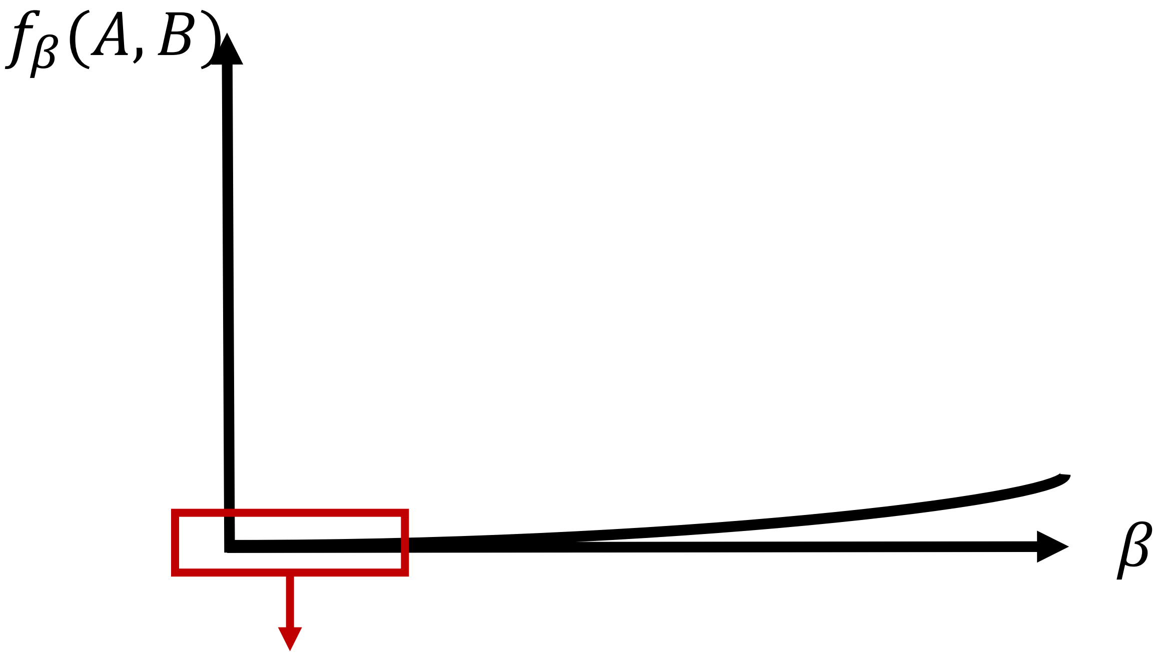

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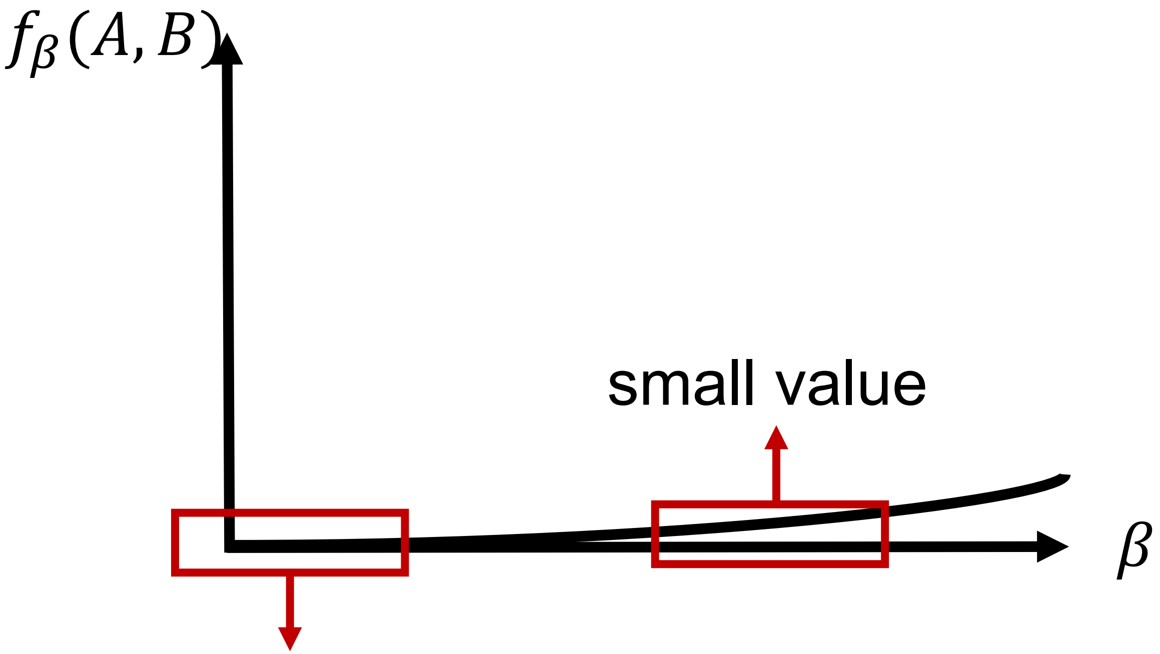

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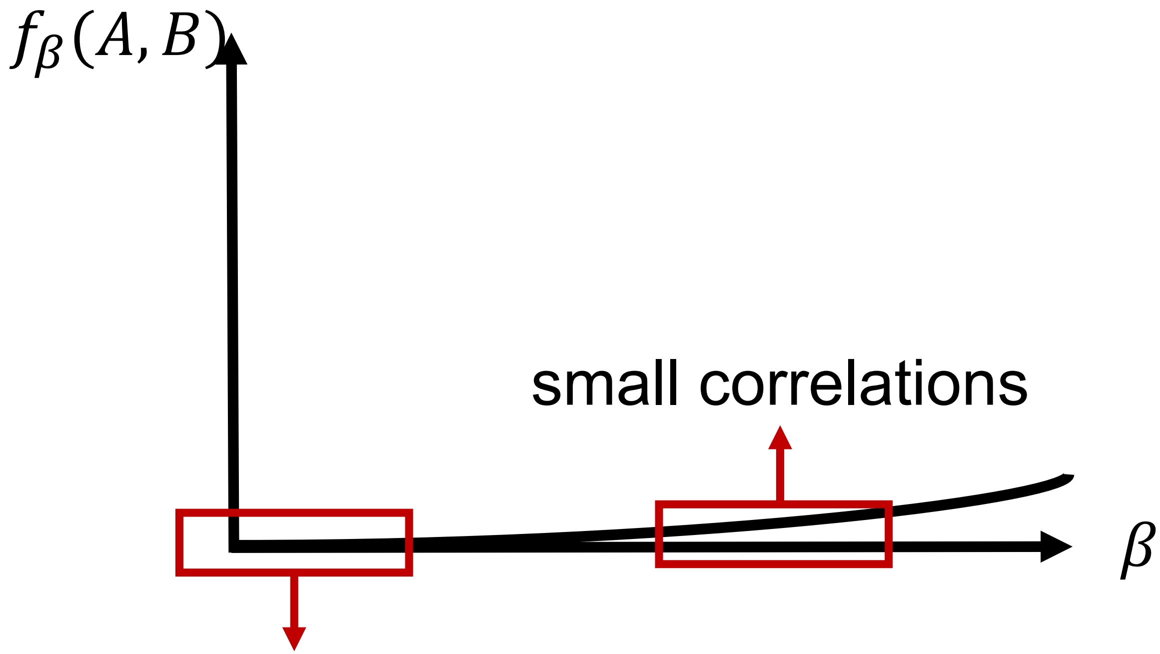

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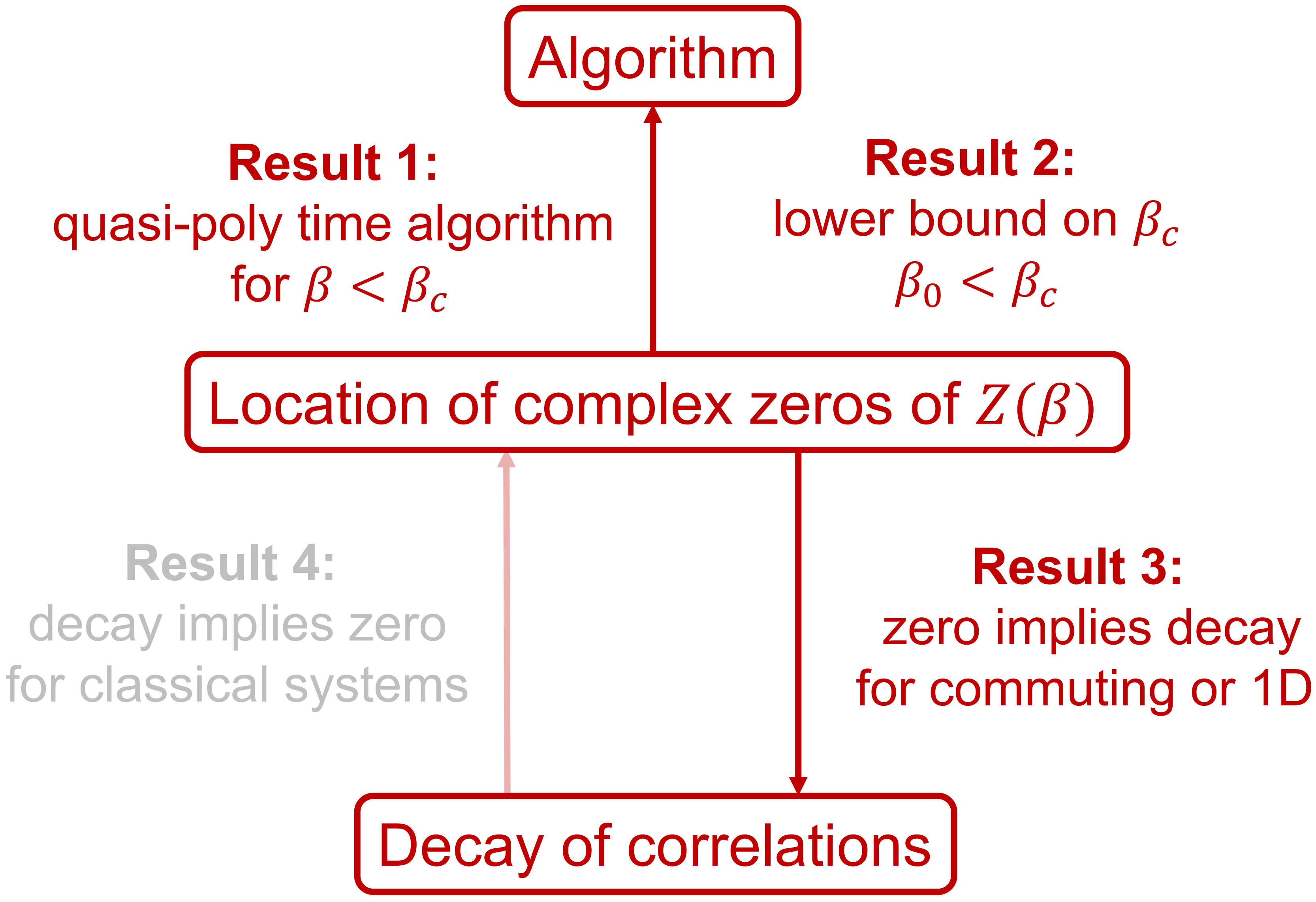

Algorithm
Result 1:
quasi-poly time algorithm
for $\beta < \beta_c$
Result 2:
lower bound on β_c
$\beta_0 < \beta_c$
Location of complex zeros of $Z(\beta)$
Result 4:
decay implies zero
for classical systems
Result 3:
zero implies decay
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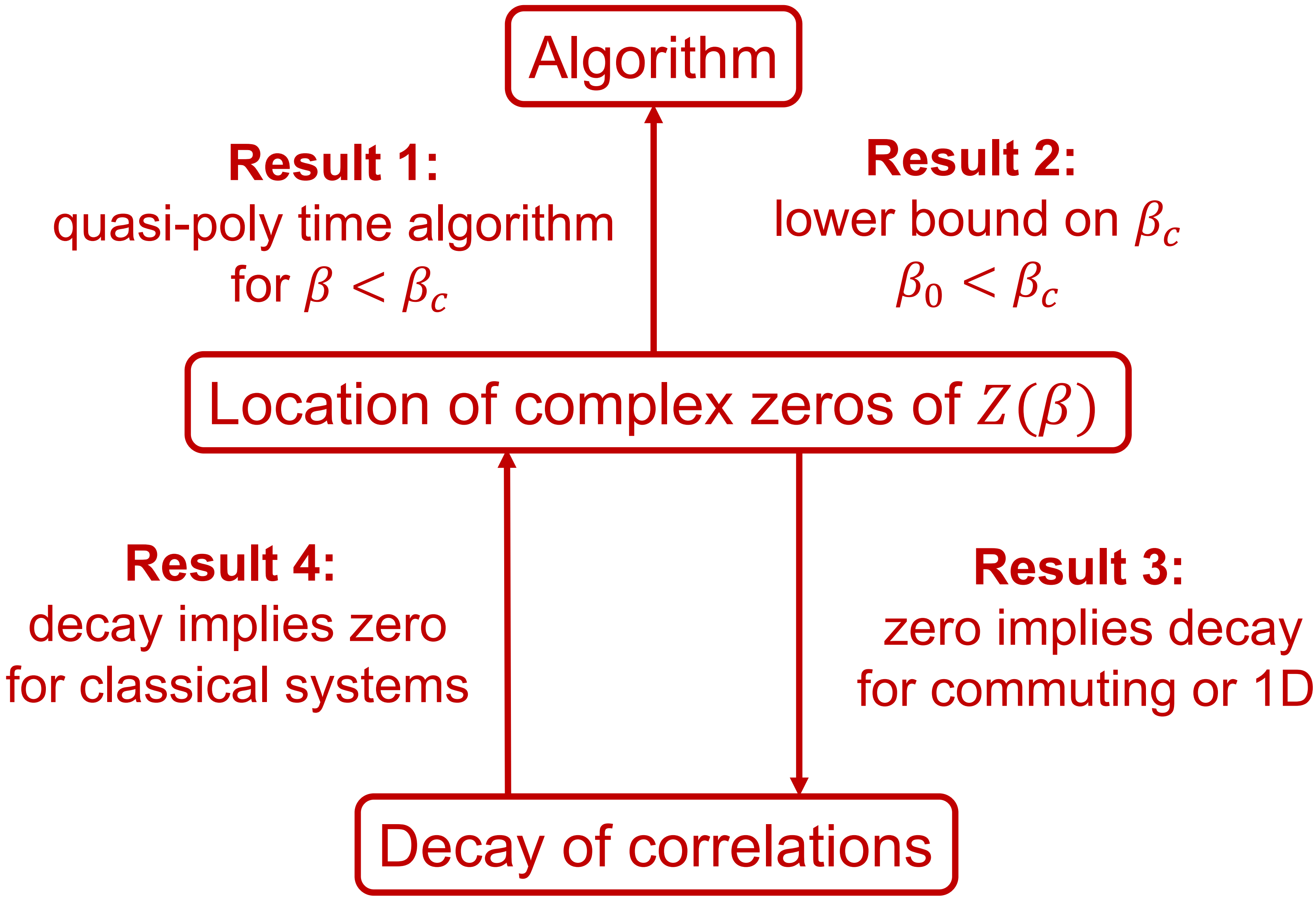
Decay of correlations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- Proved for translationally-invariant classical systems [DS'85]

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

Rough high level idea

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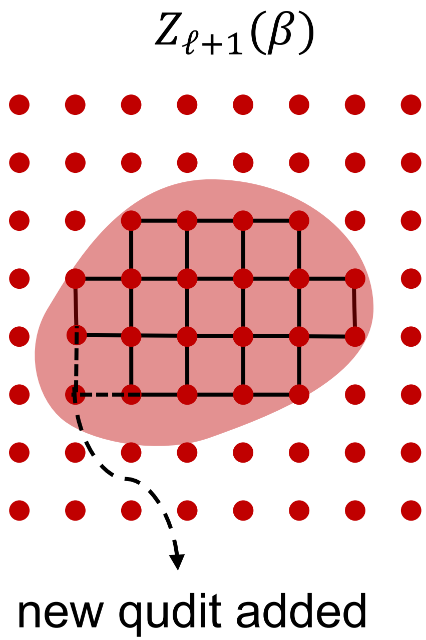
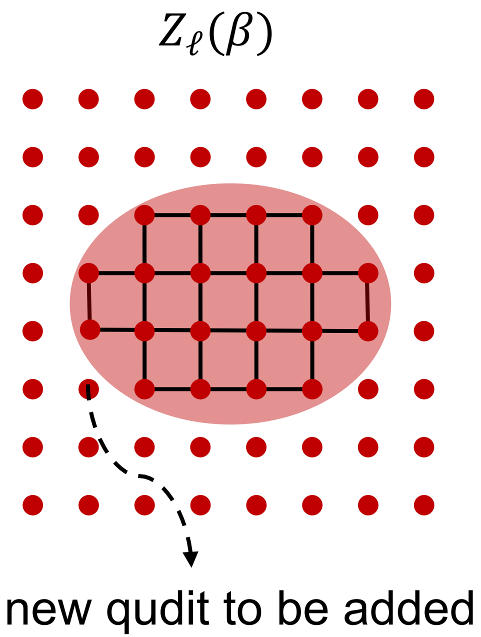
Similar to **Result 2**





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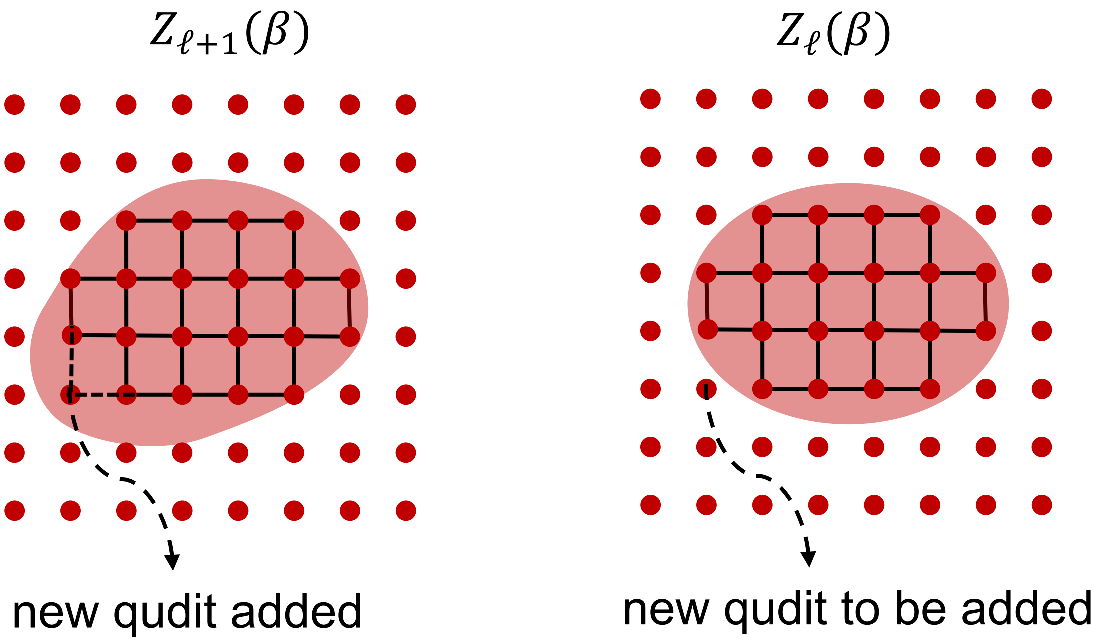
Instead of cluster expansions use decay of correlations



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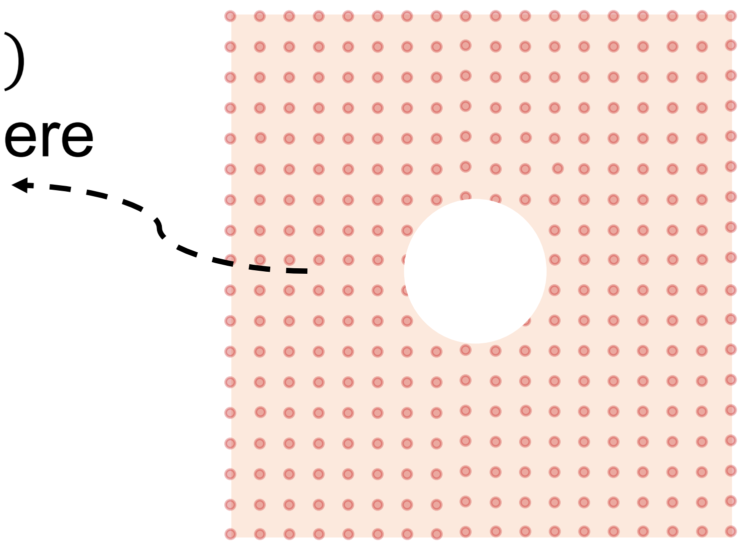

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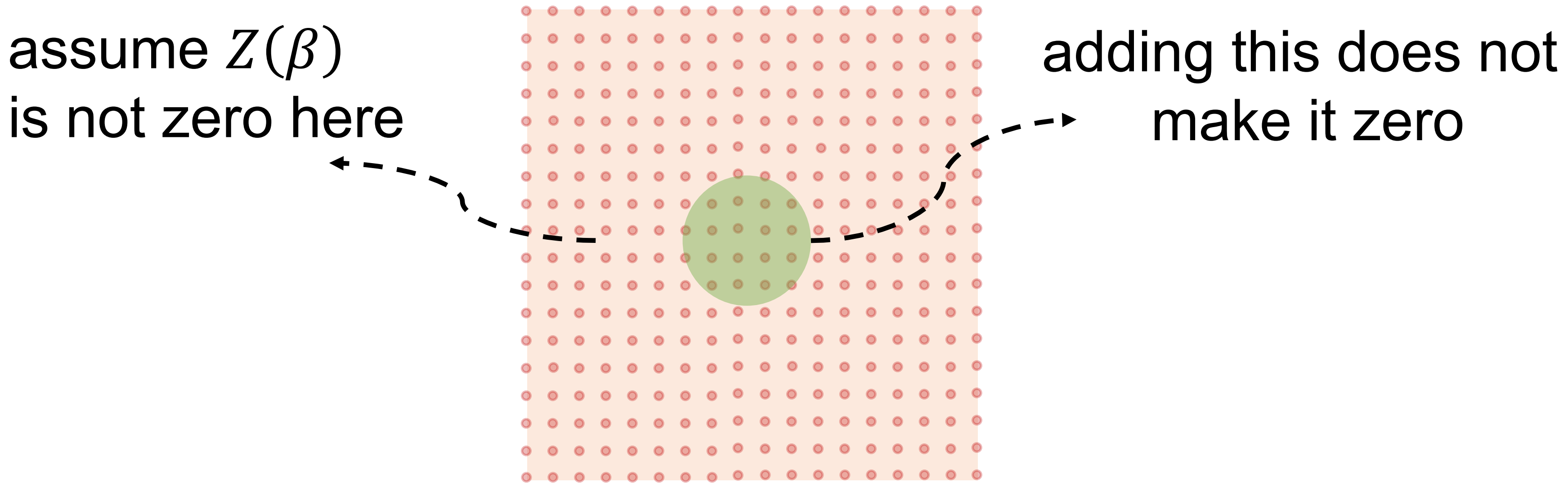

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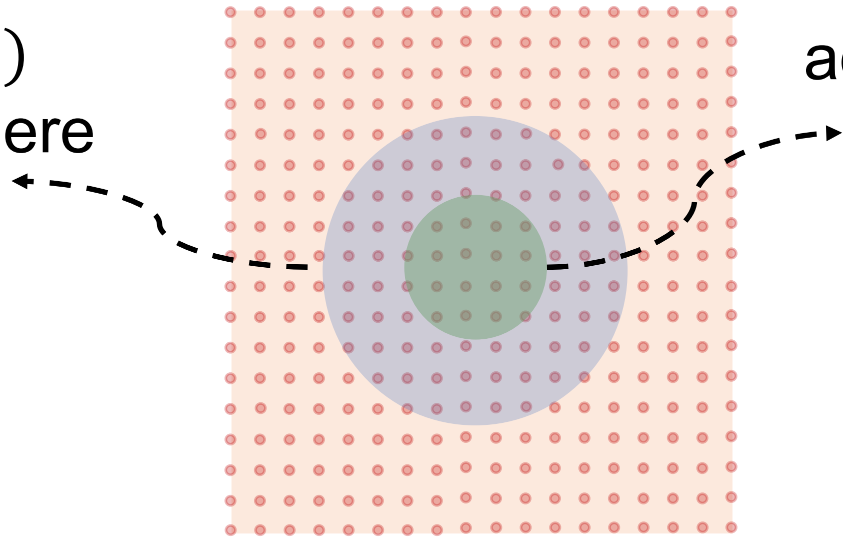

adding this does not make it zero

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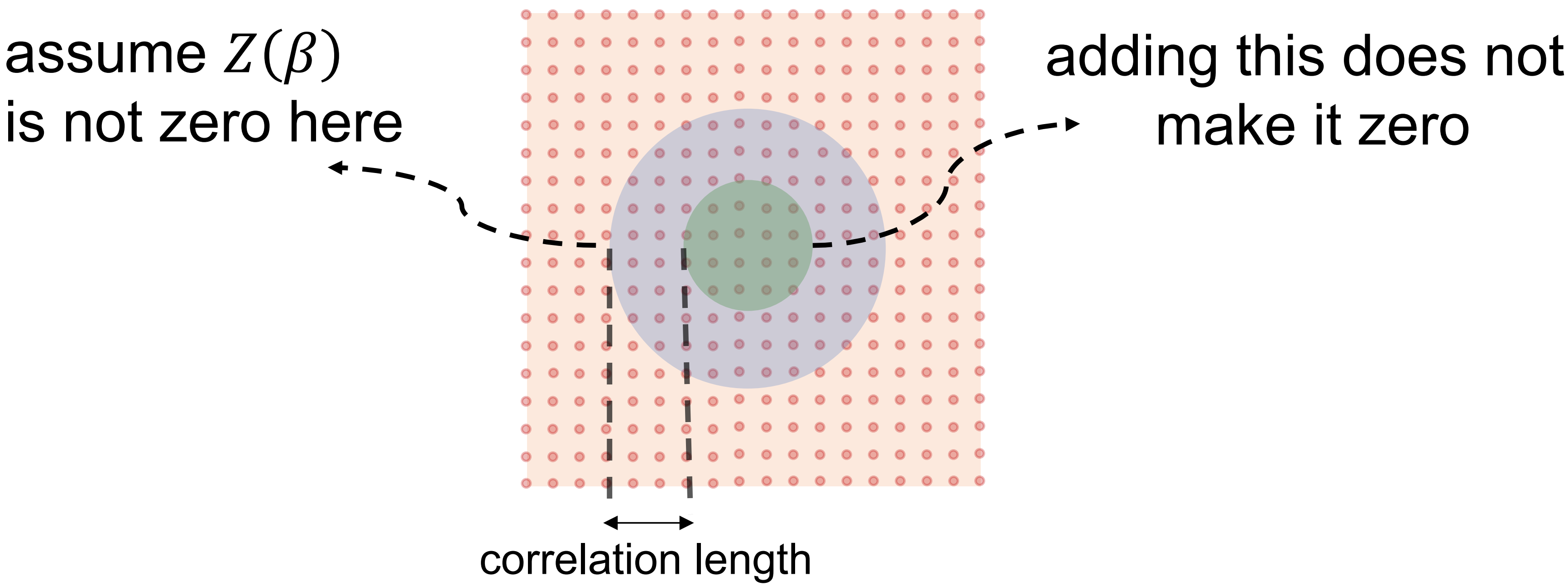

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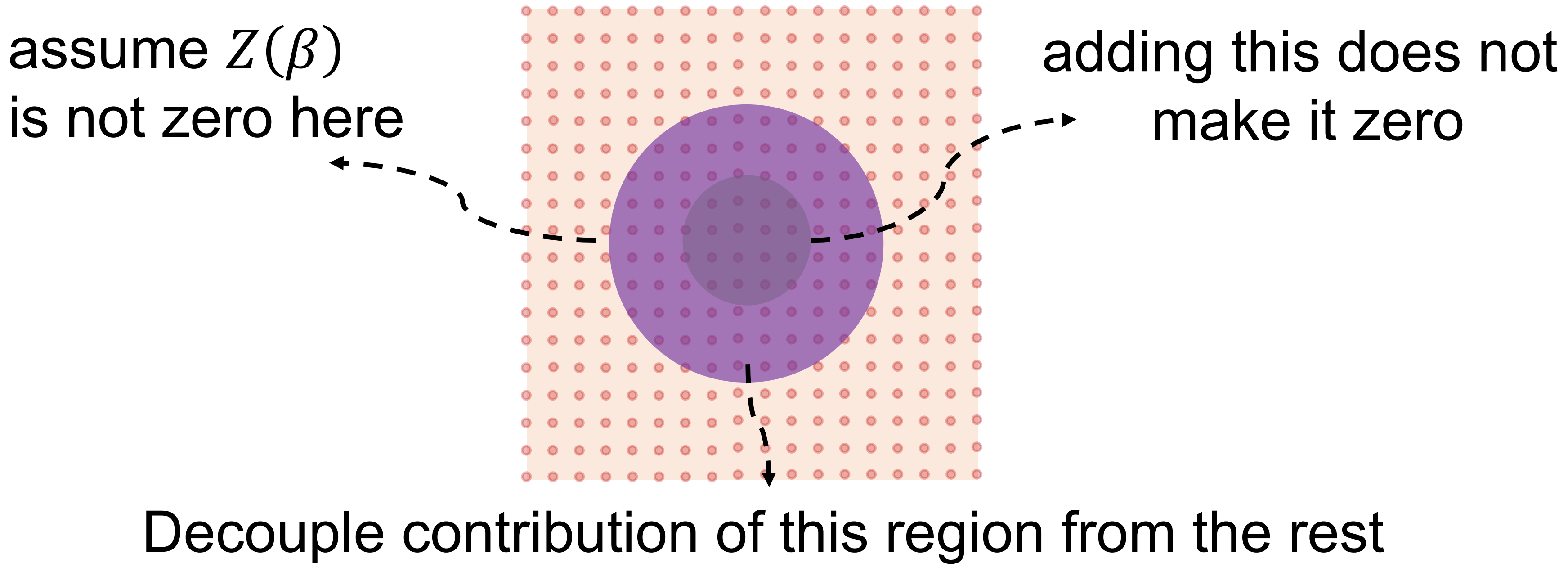

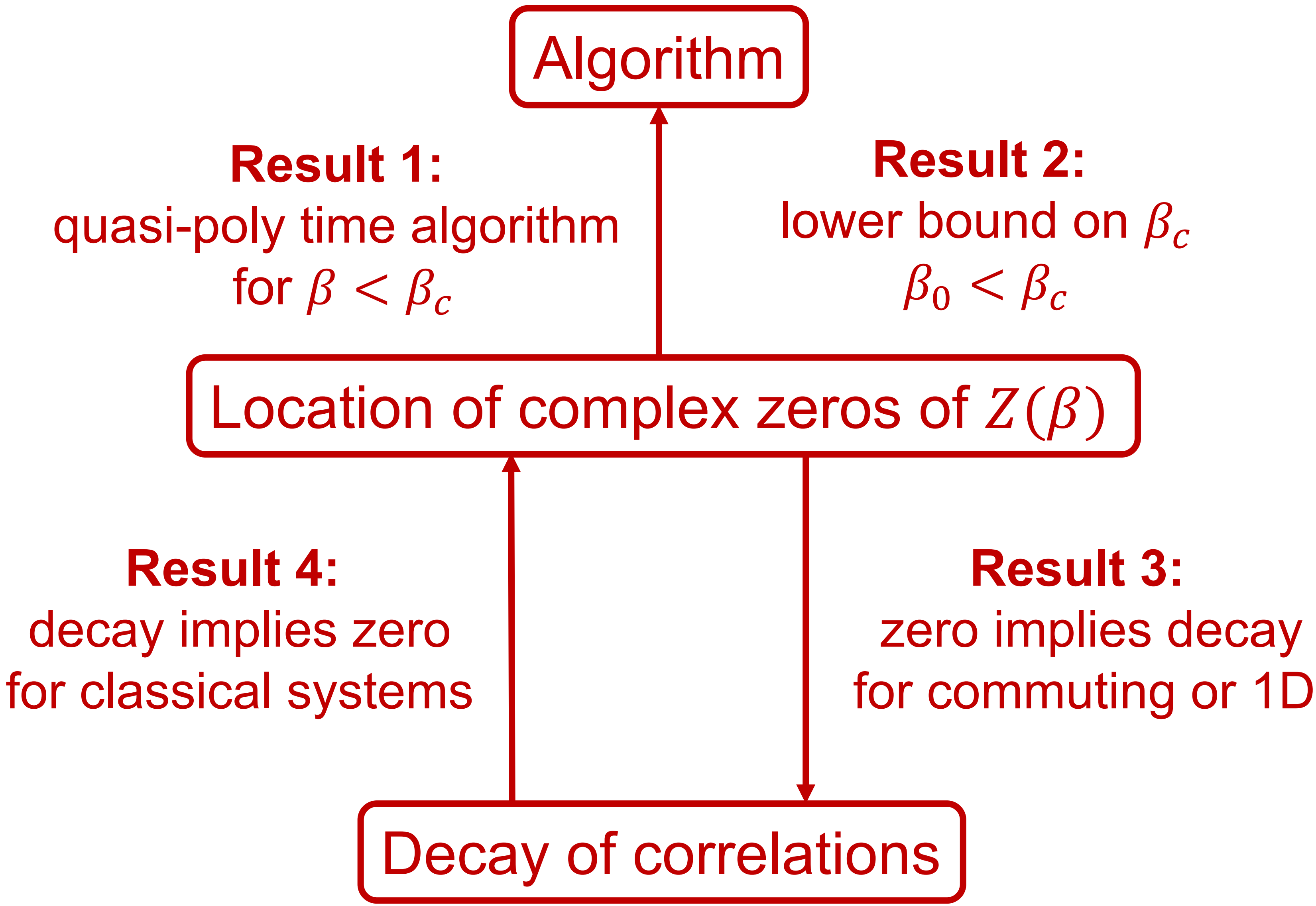
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Extrapolation in other parameters

Extrapolating in external field

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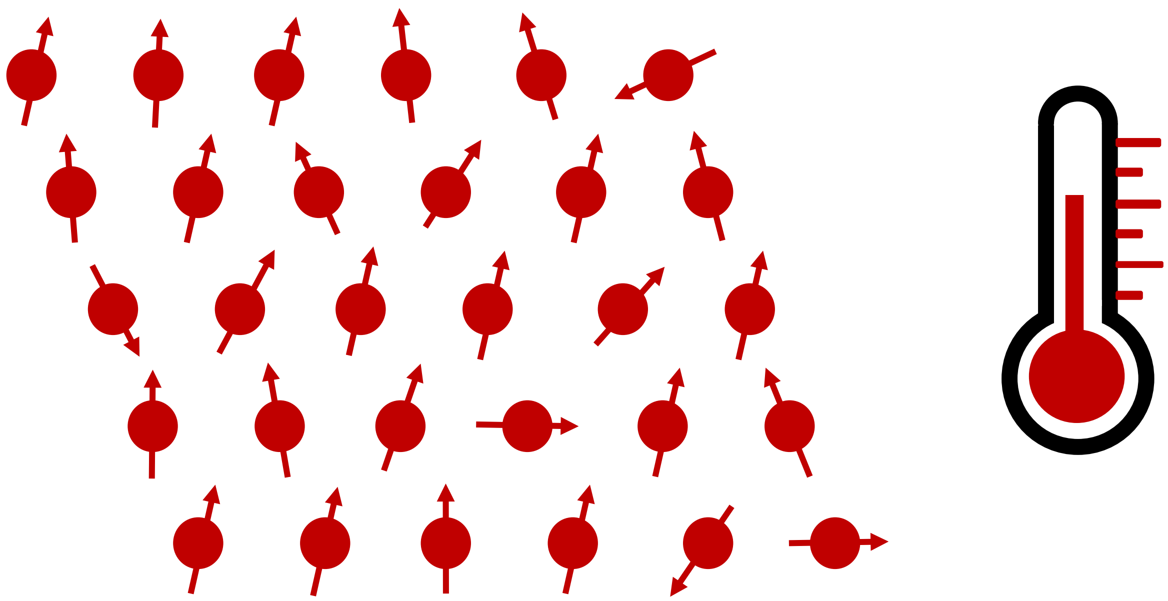

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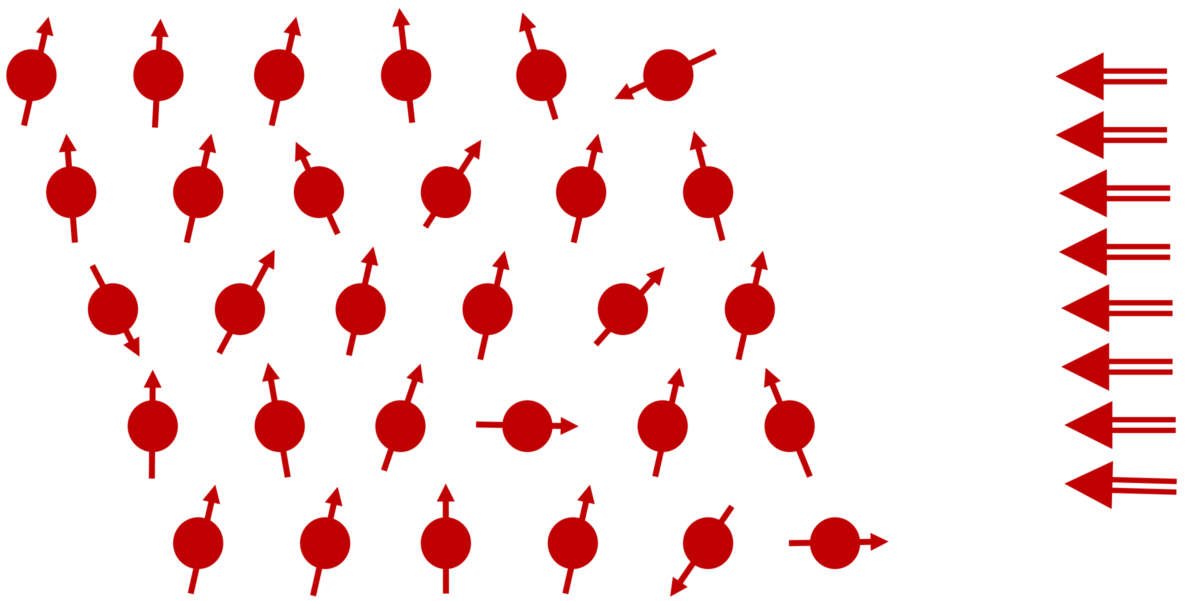

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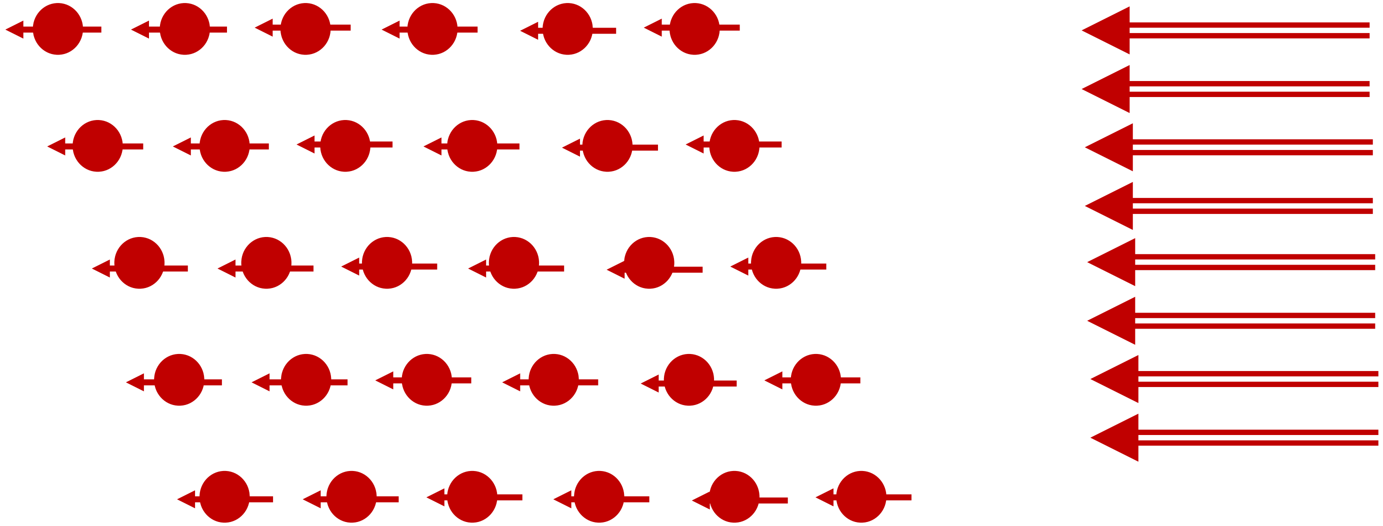

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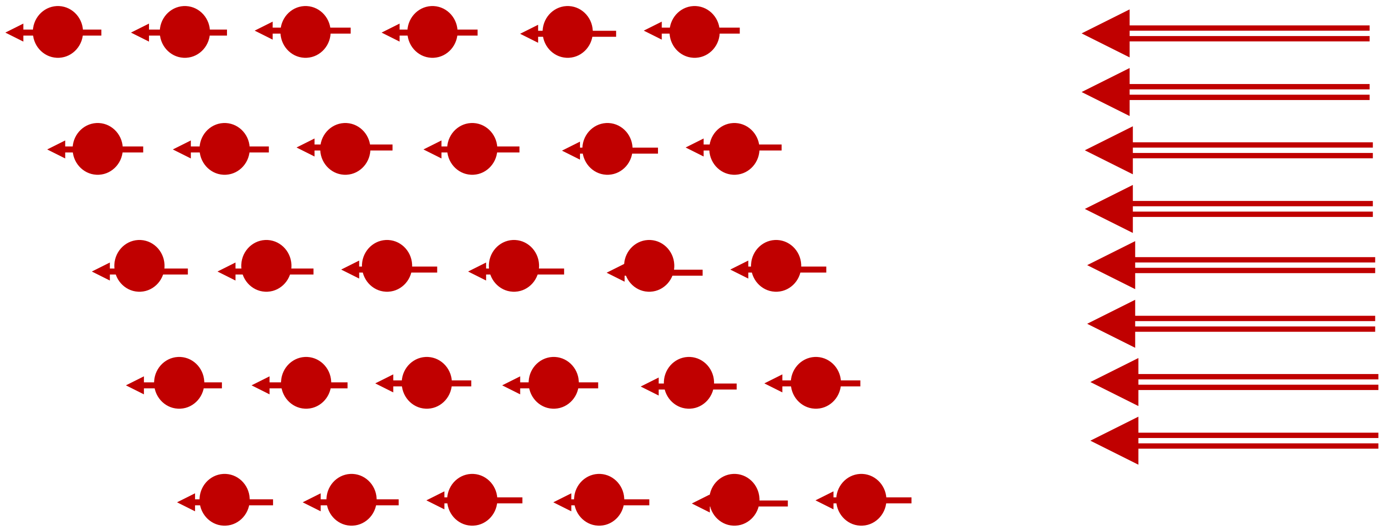
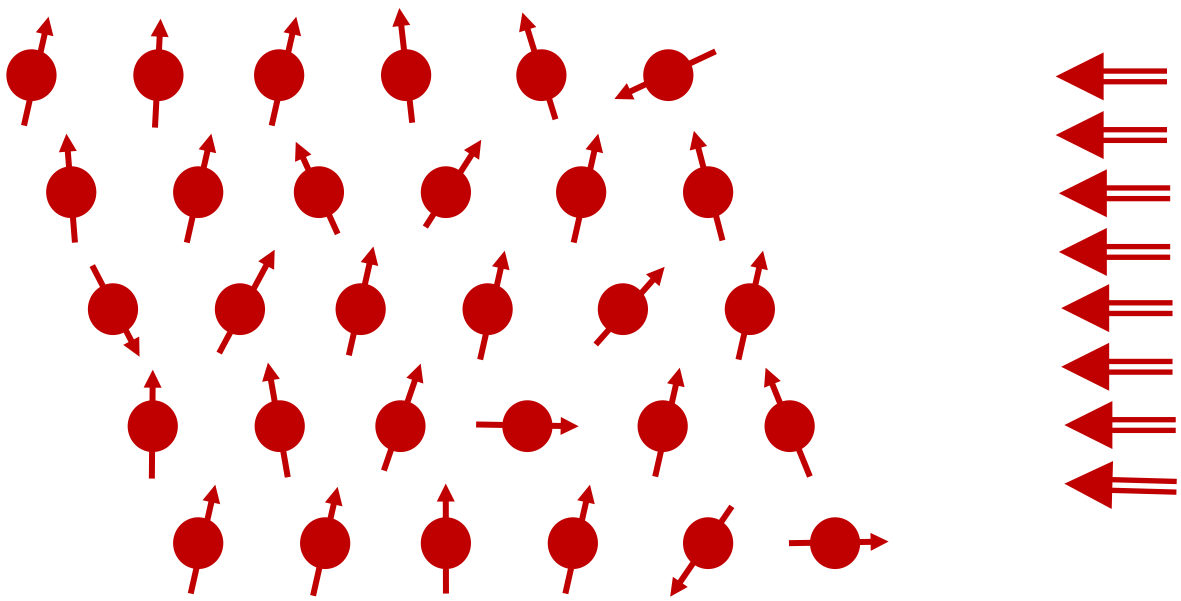


Easy regime

Extrapolating in external field



Hard regime

Result 5:

Ferromagnetic Heisenberg model

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

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

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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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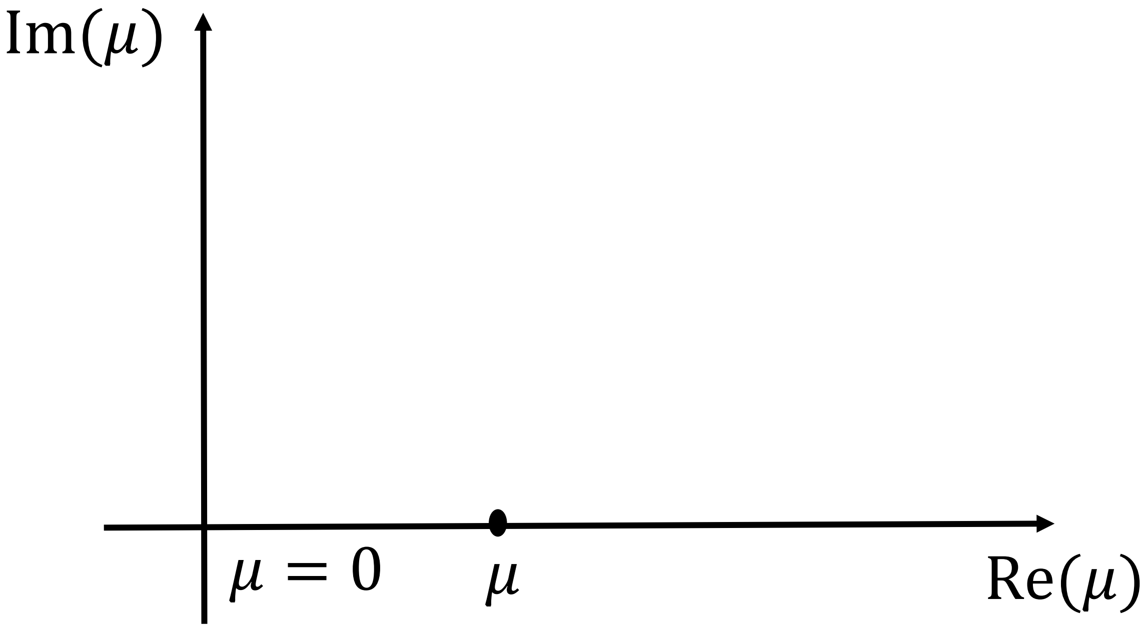

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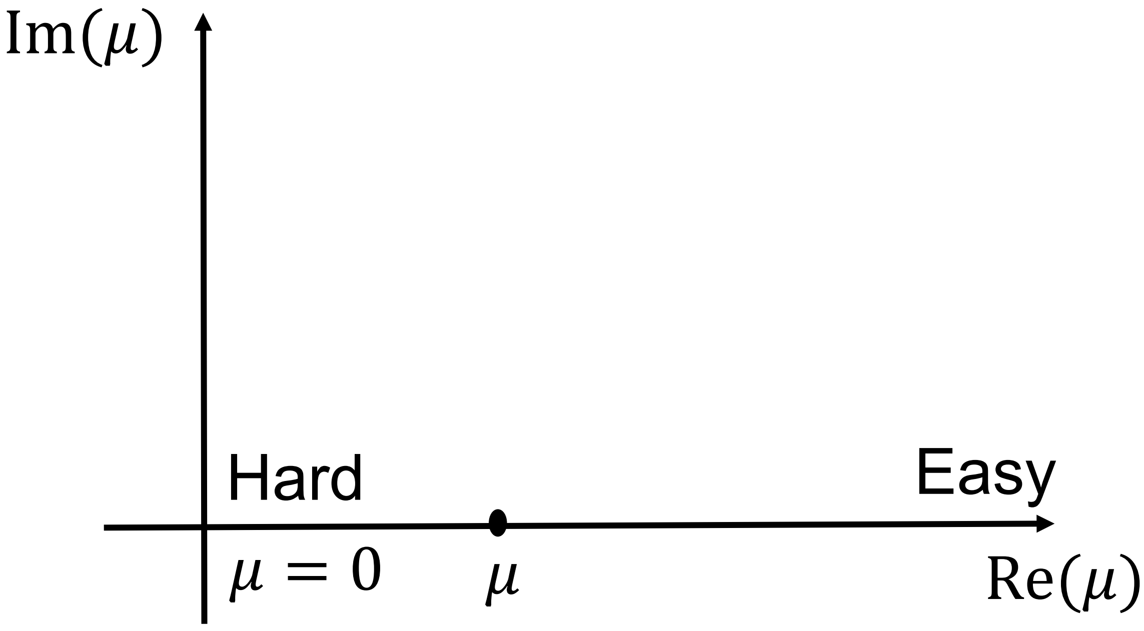

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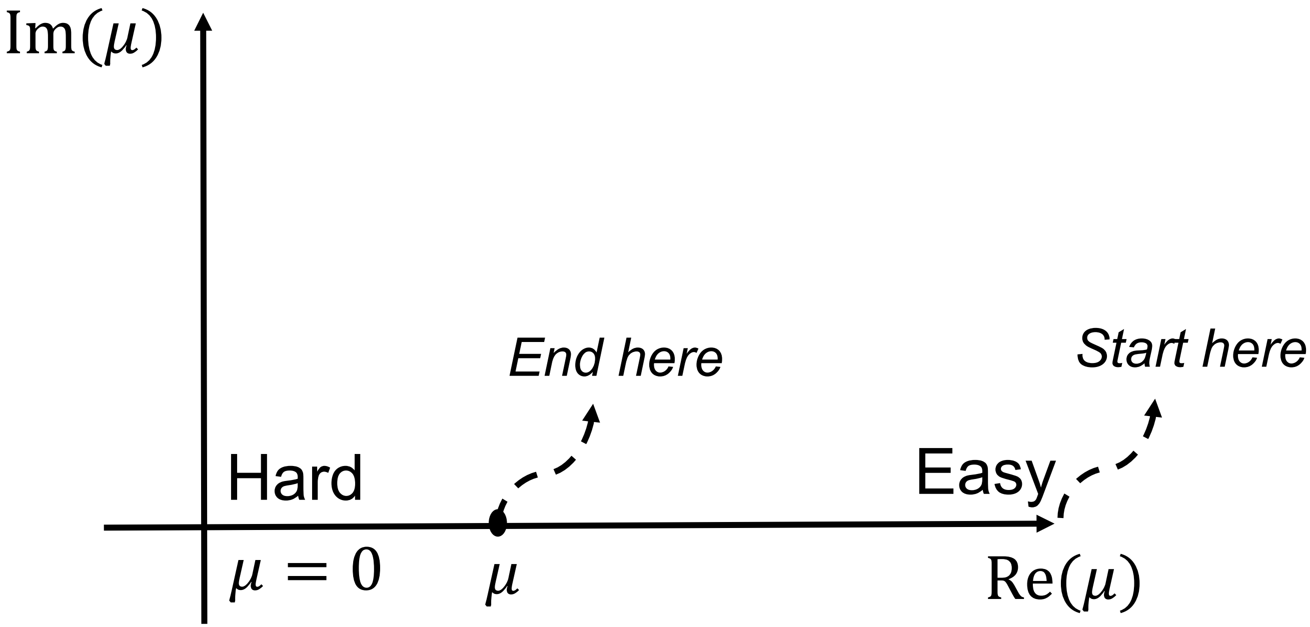

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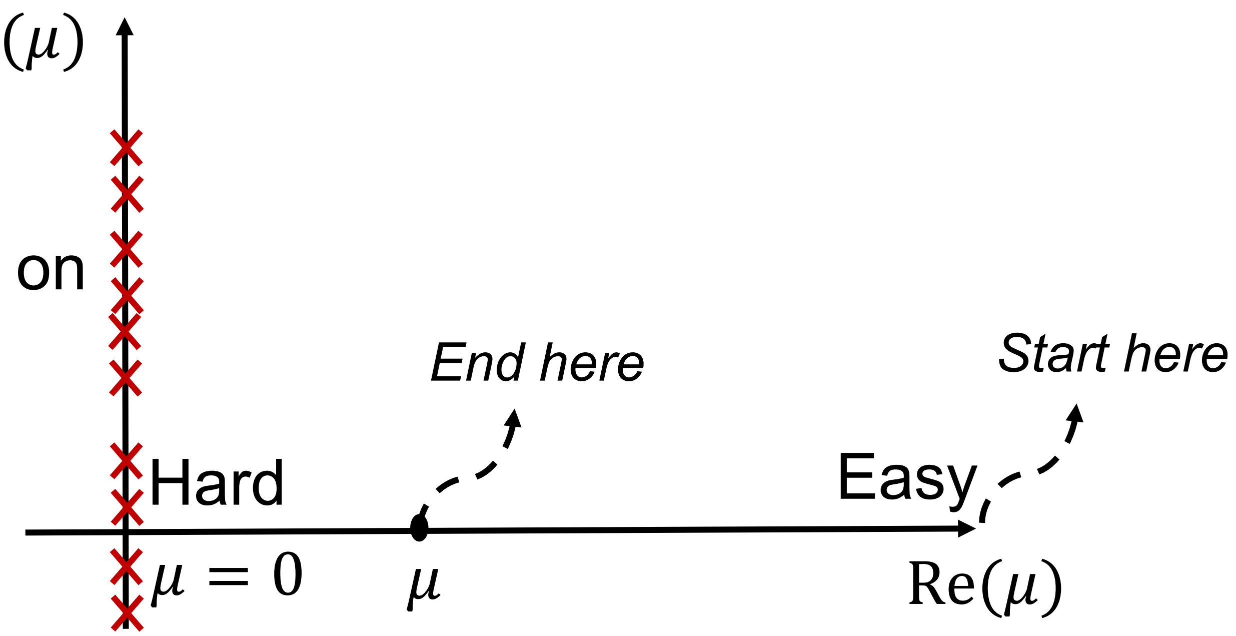
Lee-Yang zeros on imaginary μ [SF'71]



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Solved by reducing to counting perfect matchings

Open questions

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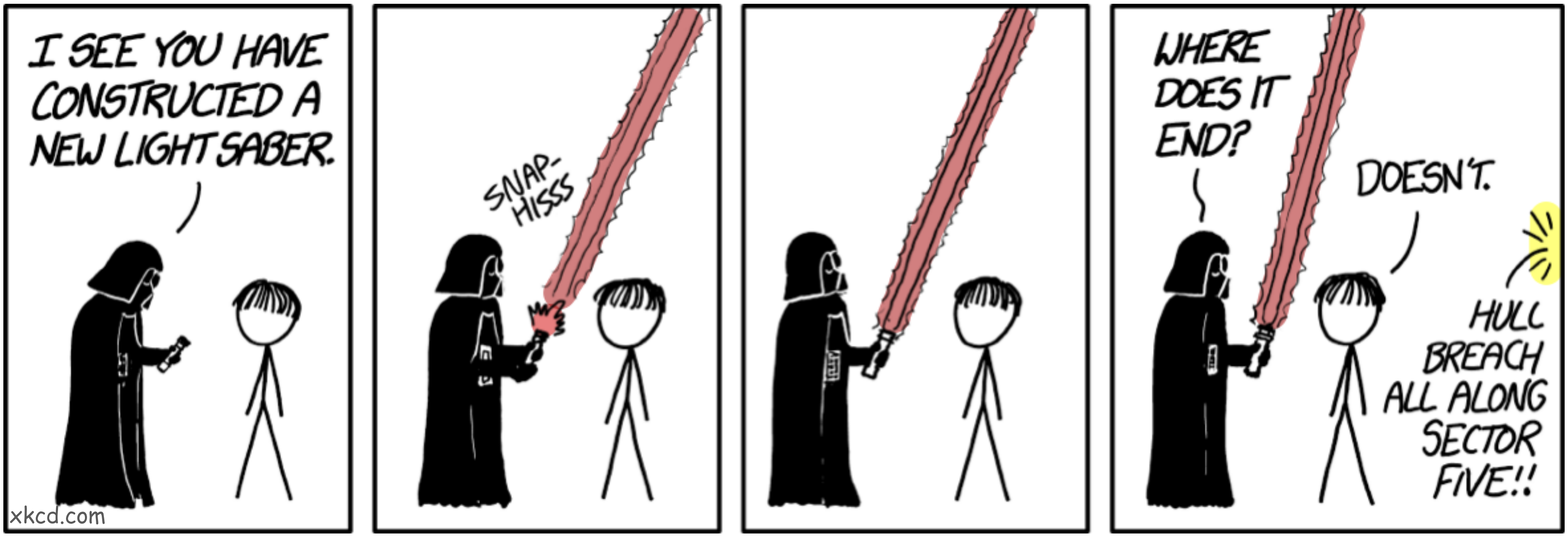
- Other algorithms for $Z(\beta)$ like convex relaxations?

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