Title: The Complexity and (Un)Computability of Quantum Phase Transitions

Speakers: James Watson

Date: October 26, 2022 - 11:00 AM

URL: https://pirsa.org/22100135

Abstract: The phase diagram of a material is of central importance in describing the properties and behaviour of a condensed matter system. Indeed, the study of quantum phase transitions has formed a central part of 20th and 21st Century physics. We examine the complexity and computability of determining the phase diagram of a general Hamiltonian. We show that in the worst case it is uncomputable and in more restricted cases, where the Hamiltonian is "better behaved", it remains computationally intractable even for a quantum computer. Finally, we take a look at the relations between the Renormalization Group and uncomputable Hamiltonians.

Zoom Link: https://pitp.zoom.us/j/96048987715?pwd=WGtwWk1SUnFsanNIVTZVYjNmbTh3Zz09

Computability, Complexity and Quantum Phase Transitions

James Watson
QuICS, University of Maryland

Johannes Bausch

Toby Cubitt

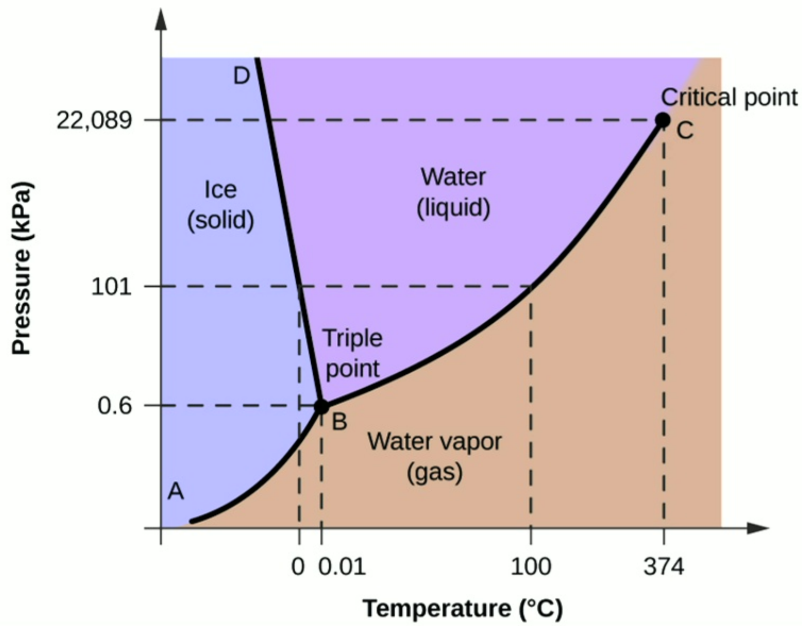
Emilio Onorati

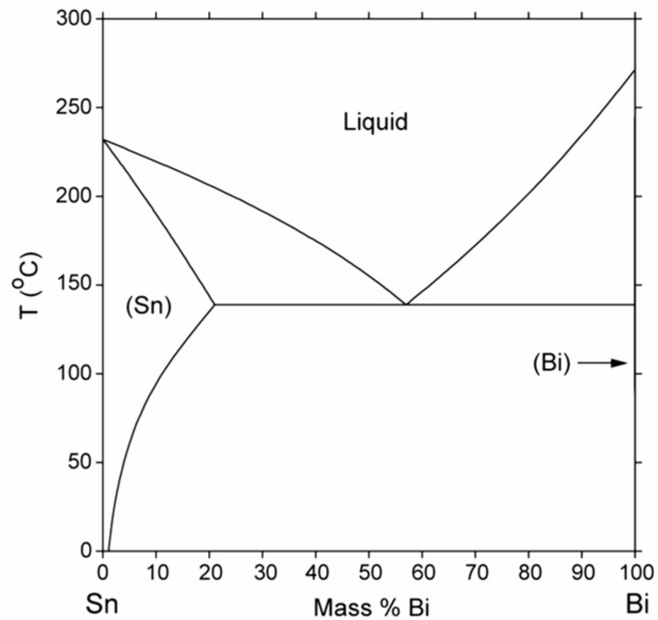
Overview

- What are quantum phase transitions, and why should you care?
- Some definitions and technical details.
- Uncomputability of Phase Diagrams
- Complexity of Phase Diagrams for “realistic” Hamiltonains
- Uncomputability and Renormalization Group Methods

Phase Transitions

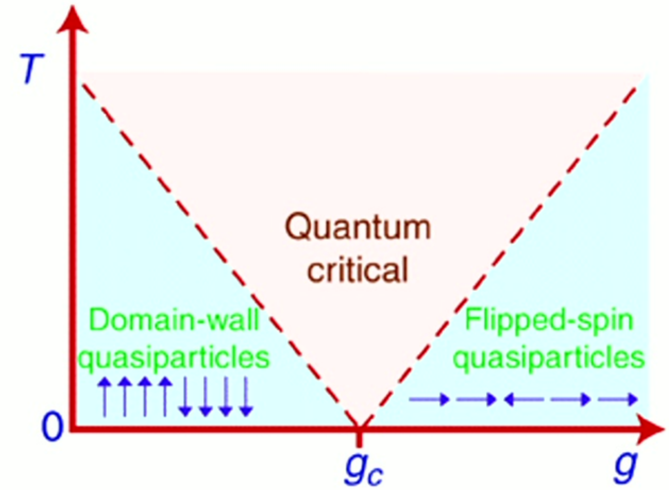
- Regular phase transitions happen at finite temperature.
- Typically driven by temperature and another non-thermal variable (e.g. pressure, magnetic field, compositions, etc).





Quantum Phase Transitions (QPTs)

- Quantum phase transitions happen at **zero temperature** and are driven by some other non-thermal variable.
- Ising model $H_{Ising} = -J \sum_{\langle i,j \rangle} Z_i Z_j - \mu \sum X_i$ has two phase depending on the ratio $g = \mu / J$
- Phase is an equilibrium property, not related to system dynamics.



Quantum Phase Transitions (QPTs)

- Superconductor-insulator phase transition.
- Quantum hall effect.
- Magnon condensation.
- Lots of other super-cool phenomena*.
- Essential for understanding material properties.

*pun intended

Question: How hard is it to compute the phase diagram of a Hamiltonian?

Definitions of Quantum Phase Transitions

Mathematical physics definition:

A Quantum Phase Transition (QPT) occurs in a Hamiltonian $H(\varphi)$ as a function of some non-thermal parameter φ where there is a non-analytic change in the ground state energy $\lambda_0(\varphi)$.

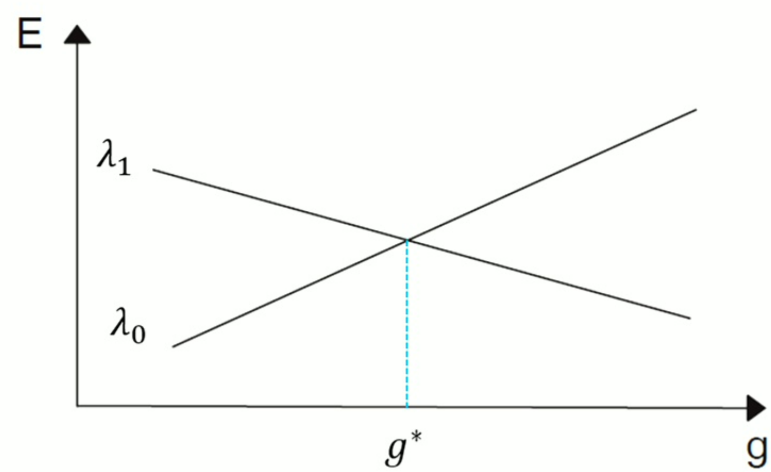
Necessary condition:

- Only way we can get a non-analytic change is if ground state and a first excited state suddenly coincide in energy ⇒ spectral gap closes

$$\Delta = \lambda_1 - \lambda_0$$

- Necessary condition for a QPT: spectral gap closes.

- May get something like:



Definitions of Quantum Phase Transitions

Physics definition

A QPT occurs where there is a non-analytic/discontinous *change in some order parameter.*

- Order parameter could be magnetisation, spin alignment, etc.

Definitions of Quantum Phase Transitions

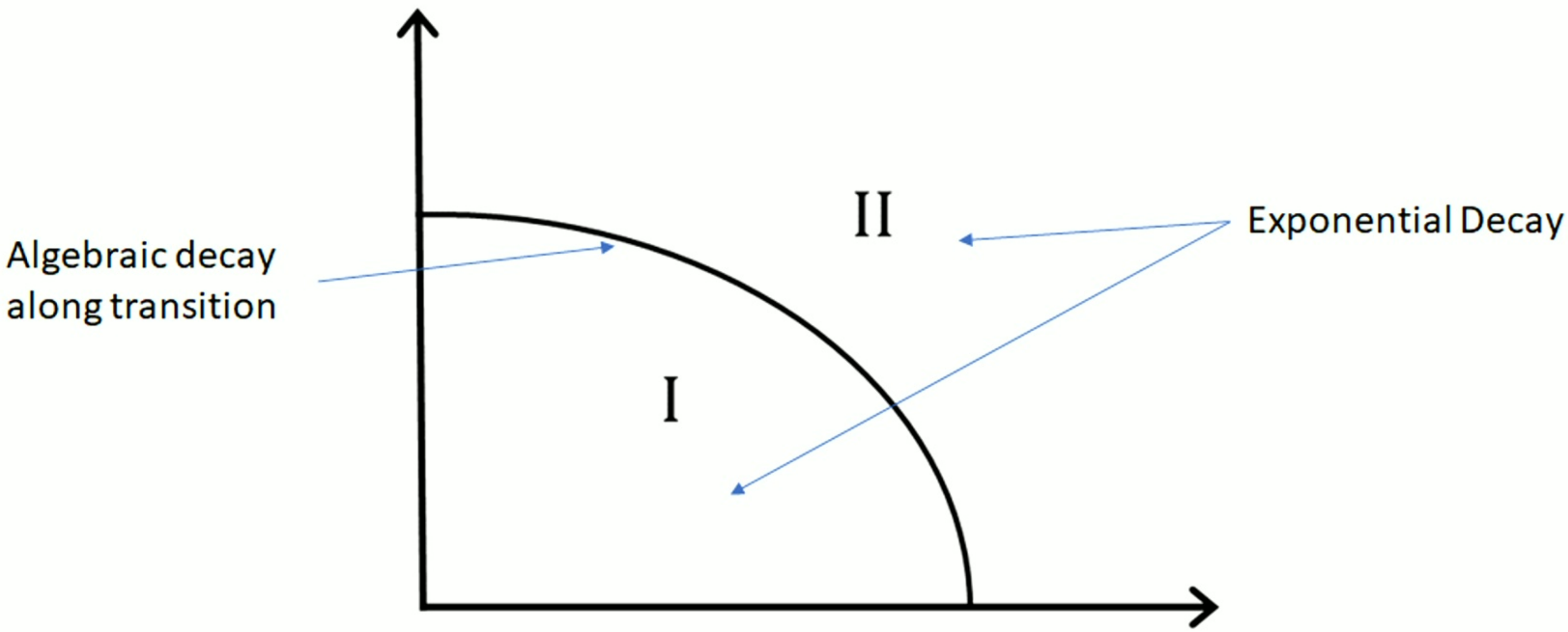
Physics definition

A QPT occurs where there is a non-analytic/discontinous *change in some order parameter.*

- Order parameter could be magnetisation, spin alignment, etc.
- Typically there is a change in the connected correlation functions at the critical point.

$$\approx \frac{1}{e^r} \quad \text{vs.} \quad \approx \frac{1}{r^k}$$

Some Examples



Uncomputability and Undecidability

What does it mean for a computational problem to be undecidable?

Given a problem, there exists no Turing Machine/algorithm running in finite time which can correctly determine the outcome of every instance of the problem.

Uncomputability and Undecidability

What does it mean for a computational problem to be undecidable?

Given a problem, there exists no Turing Machine/algorithm running in finite time which can correctly determine the outcome of every instance of the problem.

- Classical example is the Halting Problem:

  Given a TM, determine whether the TM halts or not.

- Undecidable ⇒ there is no algorithm that correctly determines whether arbitrary TMs/programs eventually halt when run.

The Phase Diagram Problem

The Phase Diagram Problem

- Phase transitions only occur in thermodynamic limit.
- Must specify with finite amount of information ⇒ define a *translationally invariant* Hamiltonian $h_{i,i+1} = h_{j,j+1} \quad \forall j$
- Each local term only has algebraic numbers as matrix elements.
- Hamiltonian's matrix elements must be an *analytic function* of the φ parameter

Input: *Description of local interaction terms,* $h_{i,i+1}(\varphi)$

Output: *The phase diagram as a function of the free parameter φ.*

Our Results

We explicitly construct a Hamiltonian $H(\phi)$ in 2D with the following properties:

- Local interactions are translationally invariant and nearest neighbour.
- Local interactions are analytic functions of φ, of the form

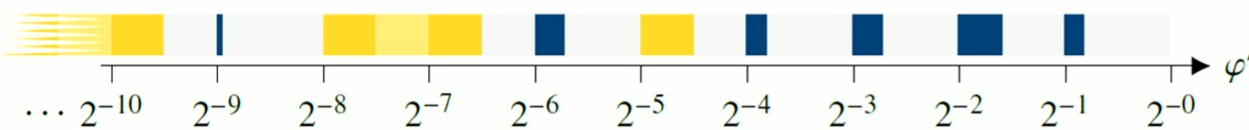
$$h_{i,i+1} = A + e^{i\pi\phi} B + h.c.$$

A, B have matrix elements 0, 1 or $1/\sqrt{2}$

- System is in one of two phases:
  - Critical phase: connected correlation functions decay algebraically.
  - Classical product : connected correlation functions are zero.

Our Results

- System's phase is undecidable for finite measure regions of φ.



Yellow: algebraic decay of correlations.
Blue: zero correlation function.
Grey: ???

There exist Hamiltonians for which determining the phase diagram is uncomputable.

Our Results

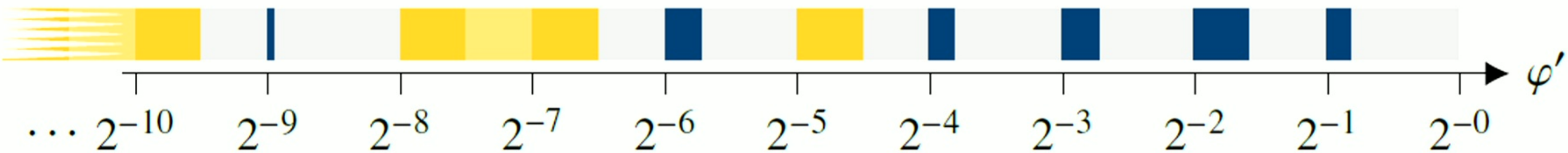
More precisely:

There exists a Hamiltonian, of the form described previously, such that in its phase diagram there is a finite measure interval around each $\varphi \in \{2^{-k}\}_{k=0}^{\infty}$ *such that the phase in this interval depends on whether a universal TM halts on input k in unary.*

Our Results: More Detail

Yellow:

- Highly entangled gs.
- Gapless, critical phase.
- Algebraic decay of correlations.

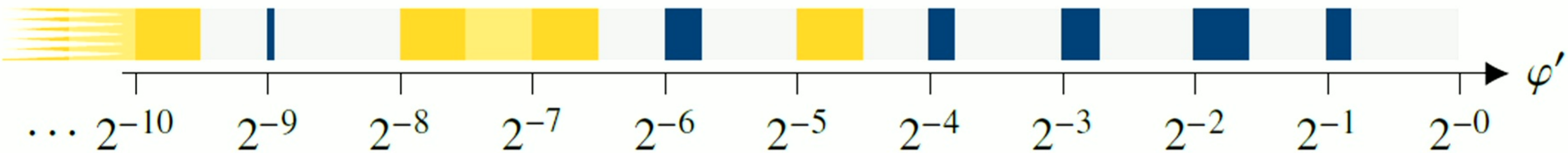


Our Results: More Detail

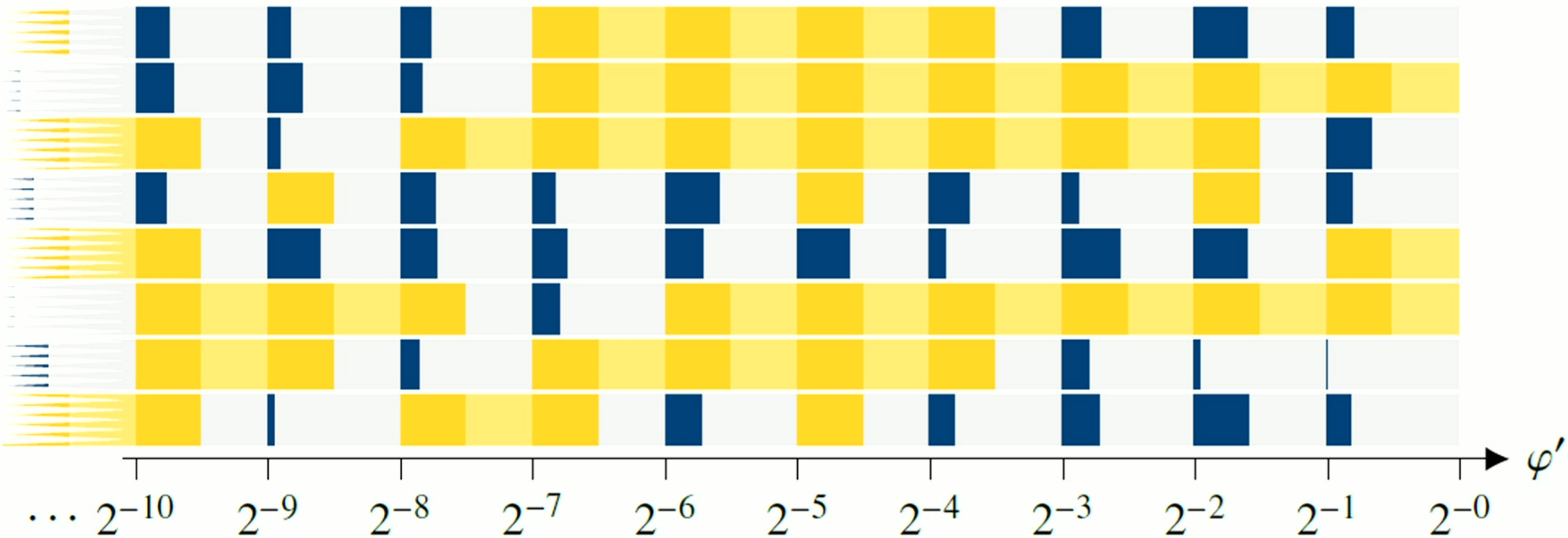
Yellow:
- Highly entangled gs.
- Gapless, critical phase.
- Algebraic decay of correlations.

Blue:
- Classical product state.
- Spectral gap >½.
- Zero correlations.

Grey:
- Unknown, but one of the others.



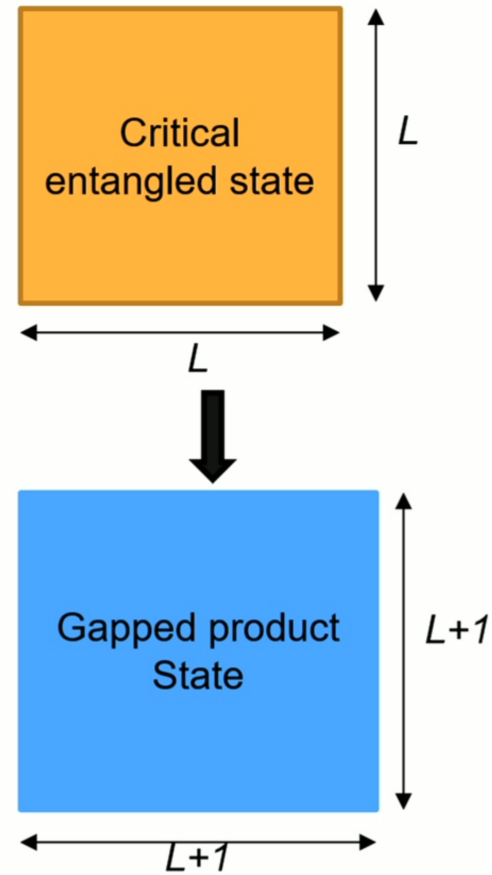
More generally, could be any of the following:



Consequences

- The phase of Hamiltonian at finite size doesn't tell us anything about the thermodynamic limit.
  - The addition of a single particle to the lattice can completely change the behaviour.
  - The size at which this change happens is uncomputable.
  - Cannot extrapolate physical properties from finite sizes.

- This means that, in general, phase diagrams at finite size may not be reflective of the "true'' properties of the Hamiltonian for larger sizes.



Consequences

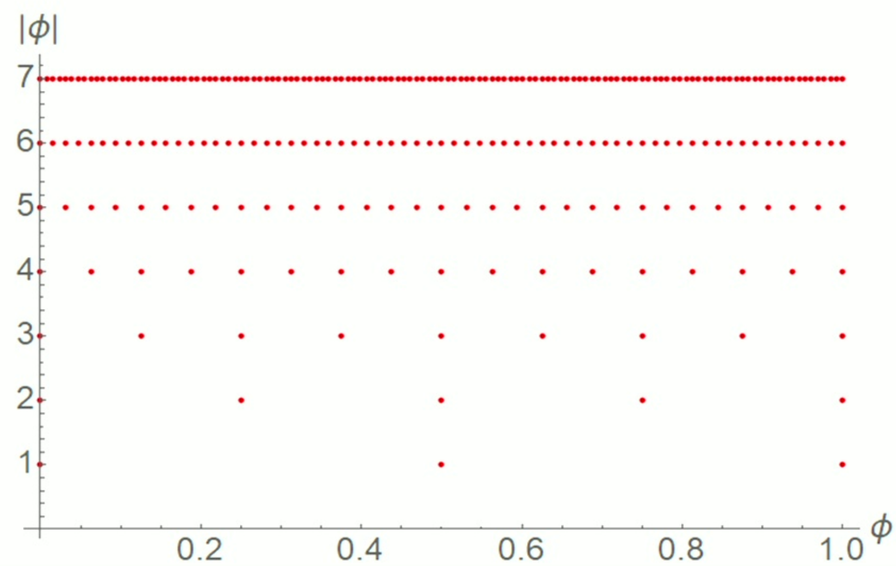
- But does this mean that we can’t ever rigorously calculate phase diagrams for any materials ever?

NO

- But it does mean that there are systems for which you can’t.

Related Results

- Our work builds off "Undecidability of the Spectral Gap"*, who showed there exists a Hamiltonian $H(\varphi, |\varphi|)$ with the following properties:
  - Nearest neighbour and translationally invariant.
  - Determining the spectral gap is undecidable in terms of $\varphi, |\varphi|$
- Hamiltonian is a discontinuous function of φ, so we cannot draw a meaningful phase diagram.
- Hamiltonian's matrix elements are not analytic functions of φ, so the ground state energy cannot be.



T. Cubitt, D. Perez-Garcia, M. Wolf, arXiv: 1502.04135

Definitions of Quantum Phase Transitions

Mathematical physics definition:

A Quantum Phase Transition (QPT) occurs in a Hamiltonian $H(\varphi)$ as a function of some non-thermal parameter φ where there is a ***non-analytic change in the ground state energy $\lambda_0(\varphi)$.***

What is a phase of the Hamiltonian:

$$H(\varphi) = \varphi \sum_i Z_i Z_{i+1} + |\varphi| \sum_i X_i \qquad ?$$

For those familiar

- Use Feynman-Kitaev Hamiltonian to encode Turing Machine in ground state.

$$|\Psi\rangle = \frac{1}{\sqrt{T}} \sum_{t=1}^{T} |t\rangle \otimes \; U_t \dots U_1 |\psi_0\rangle$$

where U_t is the unitary for the t^{th} step of the computation.

- Make Turing Machine run phase estimation to extract parameter φ from matrix elements.

- Run Turing Machine on input φ, and apply energy penalty when it halts.

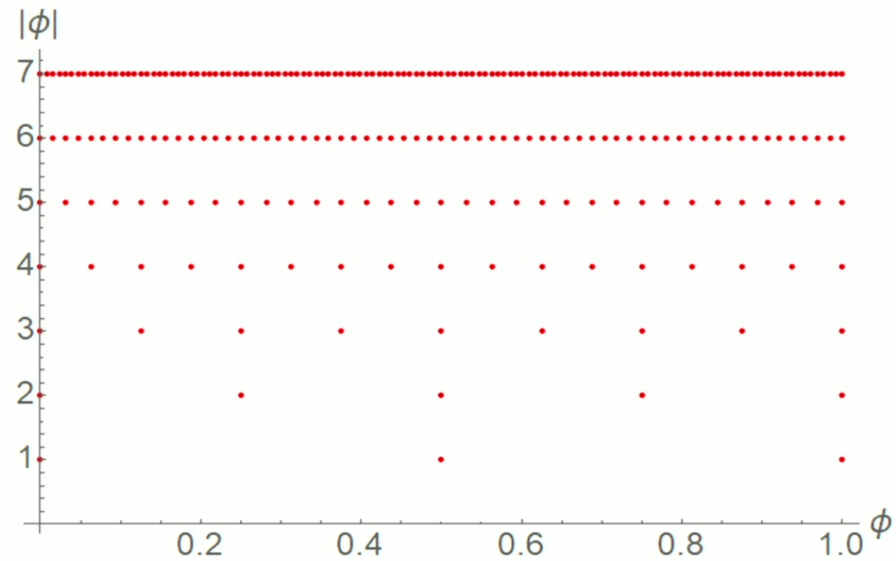
- Energy penalty opens up the spectral gap in the halting case, remains gapless in non-halting case.

For those familiar

- Phase estimation is made approximate, so introduces error.
- To mitigate the approximation error we couple each history state Hamiltonian a negative energy Hamiltonian.
- This splits the energy of each pair to be positive in the non-halting case, and negative in the halting case.
- Then apply a similar construction to [CPW15] by combining with tiles.

Related Results

- Our work builds off “Undecidability of the Spectral Gap”*, who showed there exists a Hamiltonian $H(\varphi, |\varphi|)$ with the following properties:
  - Nearest neighbour and translationally invariant.
  - Determining the spectral gap is undecidable in terms of $\varphi, |\varphi|$
- Hamiltonian is a discontinuous function of φ, so we cannot draw a meaningful phase diagram.



*T. Cubitt, D. Perez-Garcia, M. Wolf, arXiv: 1502.04135

For those familiar

- Use Feynman-Kitaev Hamiltonian to encode Turing Machine in ground state.

$$|\Psi\rangle = \frac{1}{\sqrt{T}} \sum_{t=1}^{T} |t\rangle \otimes \, U_t \ldots U_1 |\psi_0\rangle$$

where U_t is the unitary for the t^{th} step of the computation.

- Make Turing Machine run phase estimation to extract parameter φ from matrix elements.

- Run Turing Machine on input φ, and apply energy penalty when it halts.

- Energy penalty opens up the spectral gap in the halting case, remains gapless in non-halting case.

Summary so far…

- Quantum Phase Transitions (QPTs) are phase transitions a T=0 associated with a non-analyticity in the ground state.

The Construction

- This Hamiltonian then either has energy >0 or $-\infty$ depending on the halting of a universal TM on input φ.
- Combine with other Hamiltonians to get different phases depending on which energy occurs.

For those familiar

- Use Feynman-Kitaev Hamiltonian to encode Turing Machine in ground state.

$$|\Psi\rangle = \frac{1}{\sqrt{T}} \sum_{t=1}^{T} |t\rangle \otimes\ U_t \ldots U_1 |\psi_0\rangle$$

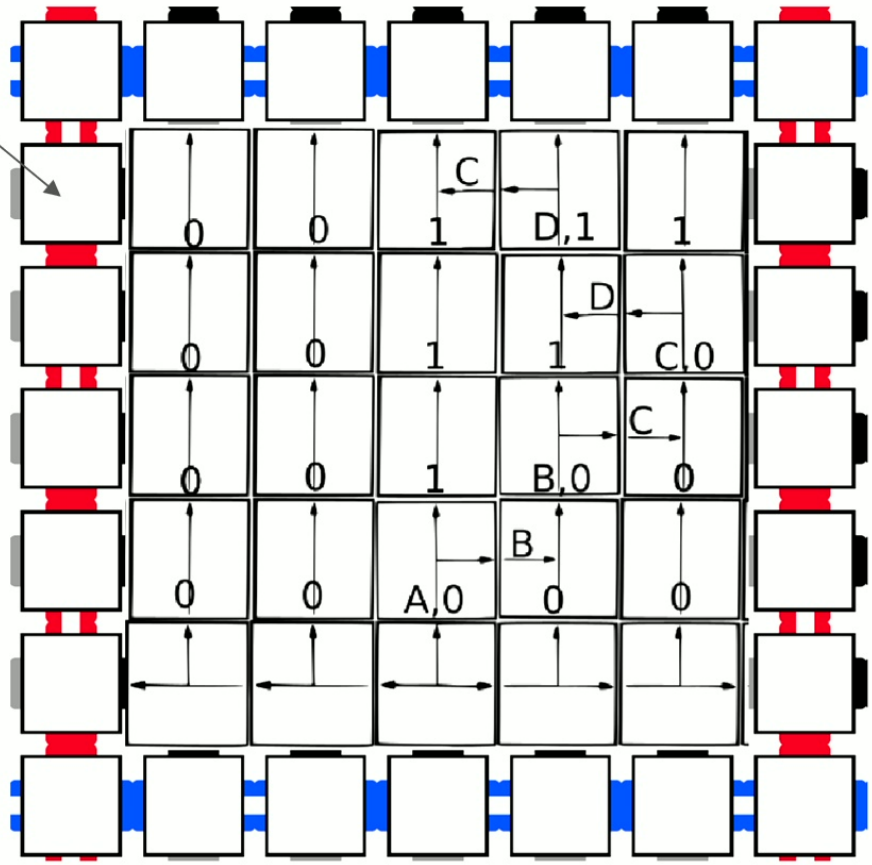
  where U_t is the unitary for the t^{th} step of the computation.

- Make Turing Machine run phase estimation to extract parameter φ from matrix elements.

- Run Turing Machine on input φ, and apply energy penalty when it halts.

- Energy penalty opens up the spectral gap in the halting case, remains gapless in non-halting case.

$\mathcal{H} \cong \mathcal{H}_{tile} \otimes \mathcal{H}_{quantum}$



Map tiles to a classical Hamiltonian:

$$H_{tiling} = \sum_{\langle i,j \rangle} |t_i t_j\rangle\langle t_i t_j|$$

Penalise pairs that don't satisfy tiling rules.

Summary so far…

- Quantum Phase Transitions (QPTs) are phase transitions a T=0 associated with a non-analyticity in the ground state.

Summary so far…

- Quantum Phase Transitions (QPTs) are phase transitions a T=0 associated with a non-analyticity in the ground state.
- We explicitly construct a 2D Hamiltonian with a single free parameter φ with the following properties:
  - translationally invariant,
  - nearest neighbour,
  - fixed local Hilbert space dimension,
  - **determining phase diagram is uncomputable.**

⇒ *determining phase diagrams in general is uncomputable.*

More Realistic Hamiltonians

- Uncomputable Hamiltonians don't act like the Hamiltonians we expect to see in nature:
    - Properties change at large, uncomputable sizes.
    - Infinite number of phase transitions.
- We expect most materials to act as if they were in the thermodynamic limit once we have a "sufficiently big" chunk of the material.
- We expect the phase diagram to be independent of size.

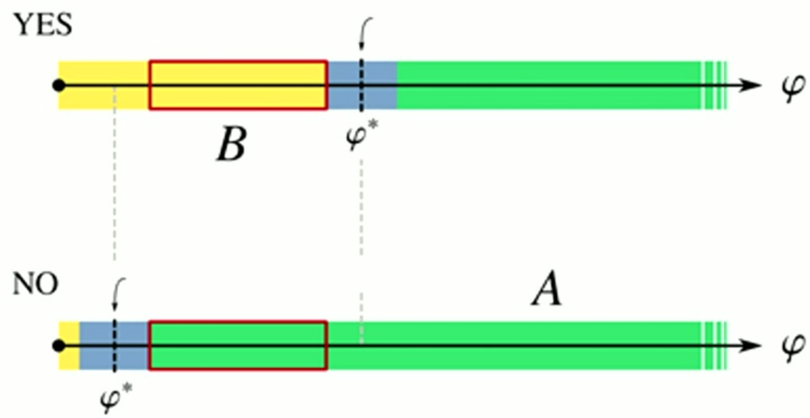
More Realistic Hamiltonians

- How hard is it to compute the phase diagram of Hamiltonians which:
  - are in the same phase for a fixed set of parameters for all lattice sizes $L > L_0,\, L_0 = O\big(poly(n)\big)$,
  - and only have a single phase transitions?
- First condition characterizes the set of Hamiltonians for which we can do numerics on finite sized systems.
- Systems which do not satisfy the first property cannot be studied via small-scale numerics.

Estimating Critical Parameters

- Formalise determining where a phase transition takes place as a promise problem:

CRT-PRM: *Given a translationally invariant Hamiltonian terms* $h_{i,i+1}(\varphi)$ *satisfying the conditions given previously, and promise it has a single phase transition at* φ^*. *Is* $\varphi^* < \alpha$ *or* $\varphi^* > \beta$ *for* $\beta - \alpha = \Omega(1)$.



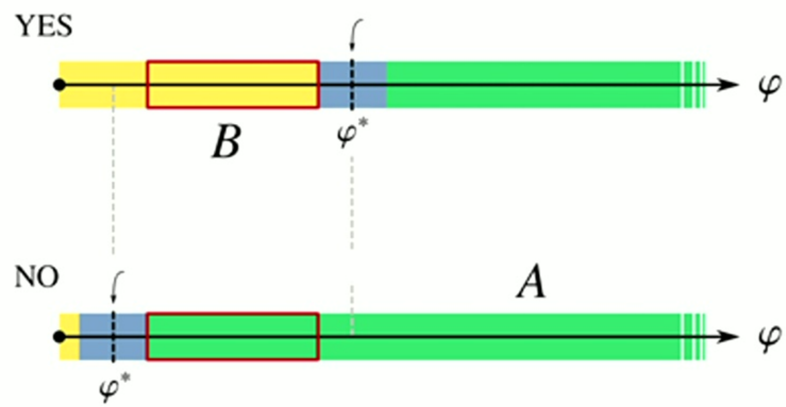
Estimating Critical Parameters

- Formalise determining where a phase transition takes place as a promise problem:

CRT-PRM: *Given a translationally invariant Hamiltonian terms $h_{i,i+1}(\varphi)$ satisfying the conditions given previously, and promise it has a single phase transition at φ^*. Is $\varphi^* < \alpha$ or $\varphi^* > \beta$ for $\beta - \alpha = \Omega(1)$.*

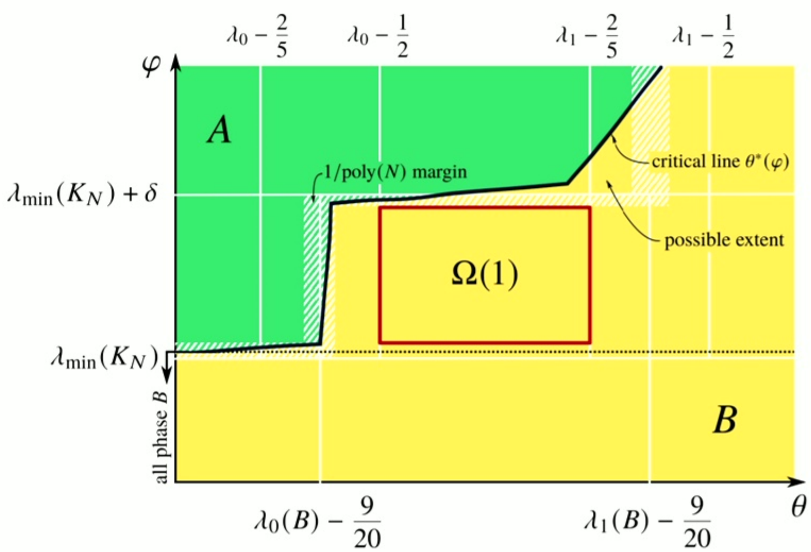
Theorem: CRT-PRM is QMA_{EXP}-hard and contained in $P^{QMA_{EXP}}$.

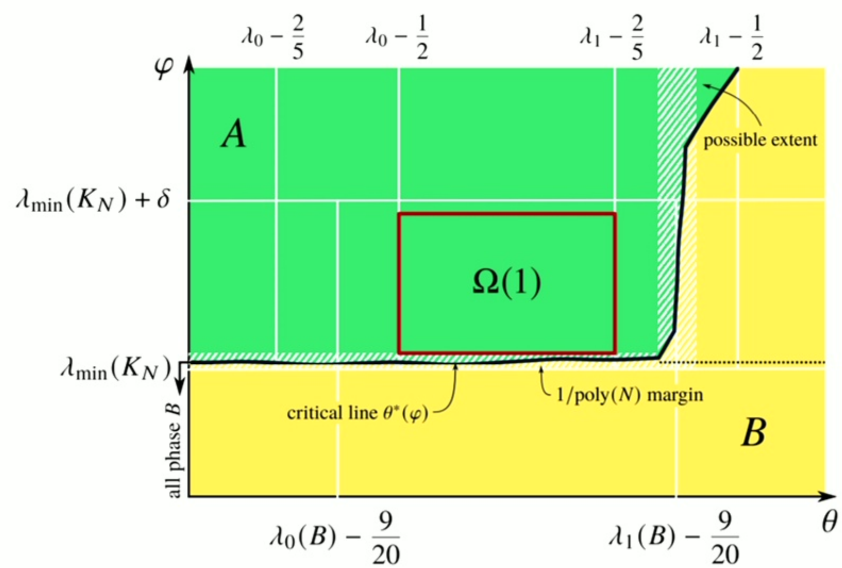
Proof is by a reduction to the local Hamiltonian problem.



Estimating Critical Parameters

- Or for a 2 parameter case for a Hamiltonian $H(\theta, \varphi)$:





Theorem: *CRT-PRM is* $P^{QMA_{EXP}}$*–complete in the 2-parameter case*

Containment Proof

- To prove the problem isn't undecidable, make use of the property that the phase at finite size $L_0 = O(poly(n))$ reflects the phase for all larger sizes.
- For an $L_0 \times L_0$ sized lattice, use algorithm from [Ambainis 2013]* to get estimate of spectral gap (or order parameter) using $poly(n)$ queries to a QMA_{EXP} oracle.
- Do a binary search in parameter space φ to determine where the critical point is.
- Algorithm requires $poly(n)$ queries to QMA_{EXP} oracle, hence contained in $P^{QMA_{EXP}}$.

*"On Physical Problems that are slightly more difficult than QMA", Ambainis, 2013

Consequences

Even for translationally invariant, nearest neighbour Hamiltonians which:

- are in the same phase for a fixed set of parameters for all lattice sizes $L > L_0$, $L_0 = O(poly(n))$.
- and only have a single phase transitions,

determining the phase diagram and critical points to $O(1)$ precision remains an intractable task!

Uncomputable Hamiltonians and The Renormalization Group

(or why doesn't the renormalization group work?)

arXiv:2102.05145

The Renormalization Group

- Renormalization Group methods are widely used family of methods to determine phase diagrams (and other properties) from the microscopic description of Hamiltonian.

- Have been enormously influential in 20^{th} Century physics.

- Basic idea:
  - Apply an iterative process which removes degrees of freedom from the Hamiltonian, but preserves macroscopic properties.
  - This generates a flow in the parameter space of Hamiltonians.
  - The flow tells us about the physics of the system.

Initial Hamiltonian
H

→ RG →

Simpler Hamiltonian
H'

→ RG →

Even Simpler Hamiltonian
H''

→ RG →

Apply RG lots of times

→ RG →

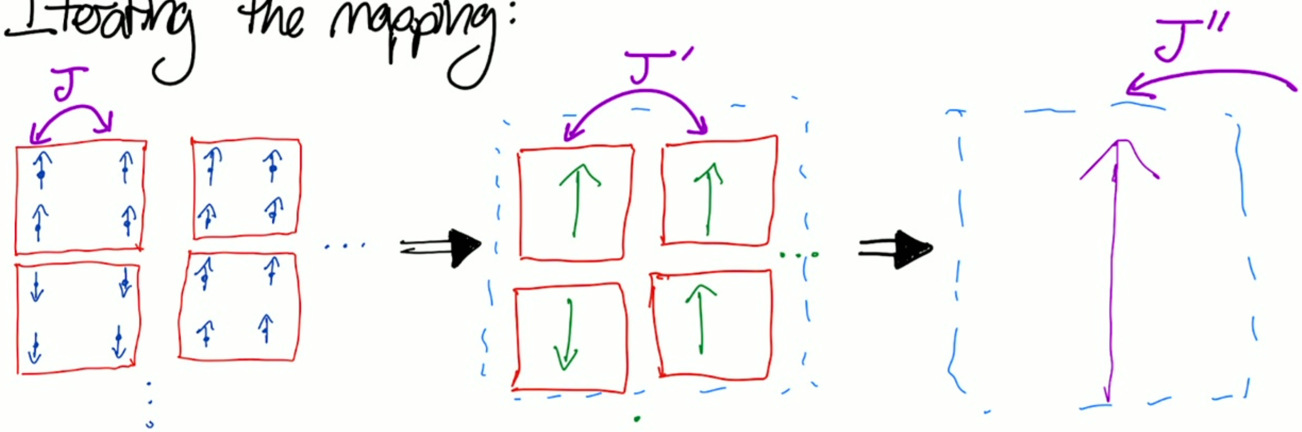
Converges to fixed point Hamiltonian
H^*

Ideally H^* is simple enough that we can straightforwardly extract its physical properties.

An Example

2D Ising Model: $H = J \sum_{\langle i,j \rangle} Z_i Z_j + B \sum_i Z_i$

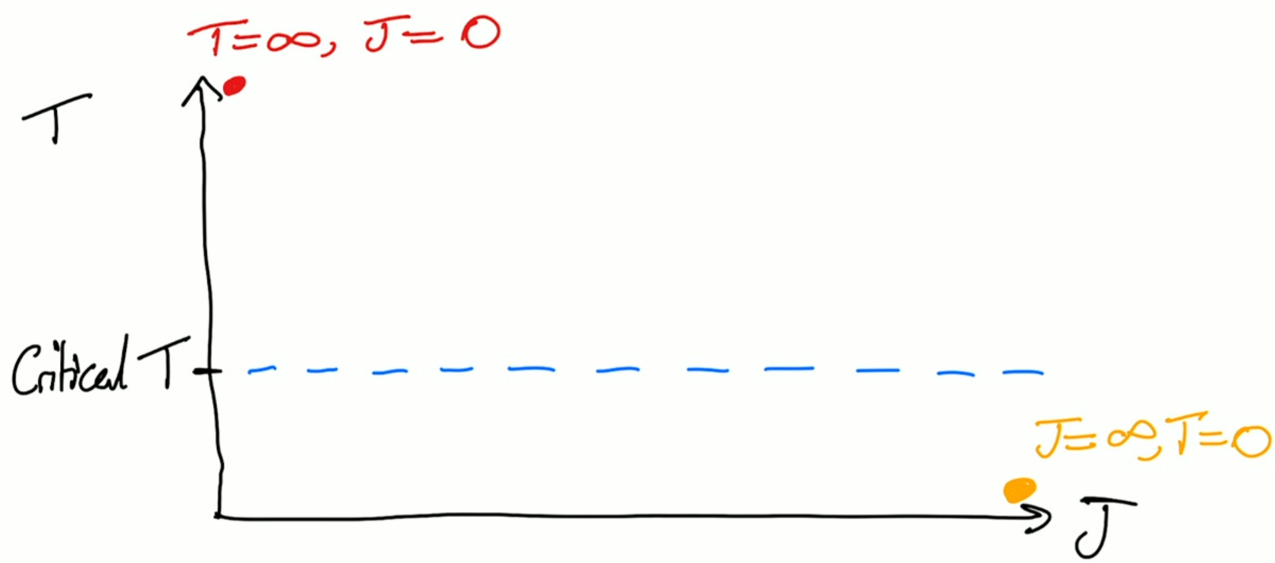
- Iterating the mapping:



$$Z(\beta, J, B) = Z(\beta', J', B') = Z(\beta'', J'', B'') = \dots$$

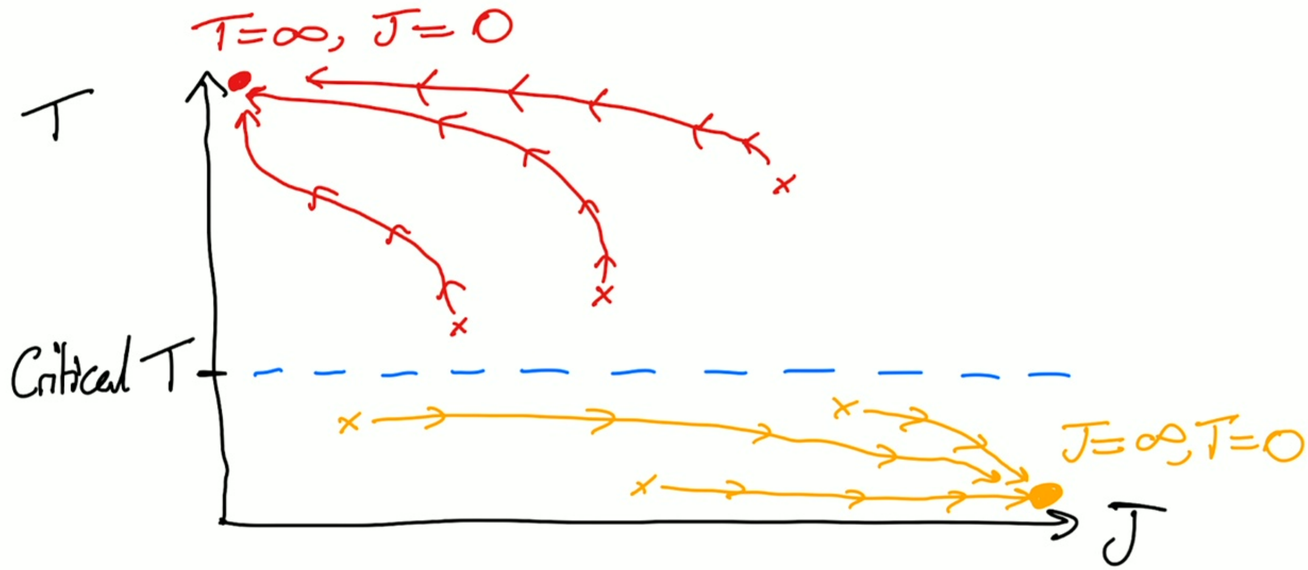
$$Z(\beta, J, B) = Z(\beta', J', B') = Z(\beta'', J'', B'') = \ldots$$

- Iterating the map generates a "flow" in parameter space:



$$Z(\beta, J, B) = Z(\beta', J', B') = Z(\beta'', J'', B'') = \ldots$$

- Iterating the map generates a "flow" in parameter space:



Failure of RG Techniques

- Uncomputability of the phase diagram means that RG methods necessarily can't solve the phase diagram.

- We expect fundamental theories to be renormalizable – if no "legitimate" renormalization methods exist for uncomputable systems, it might suggest renormalizable theories cannot be uncomputable!

Failure of RG Techniques

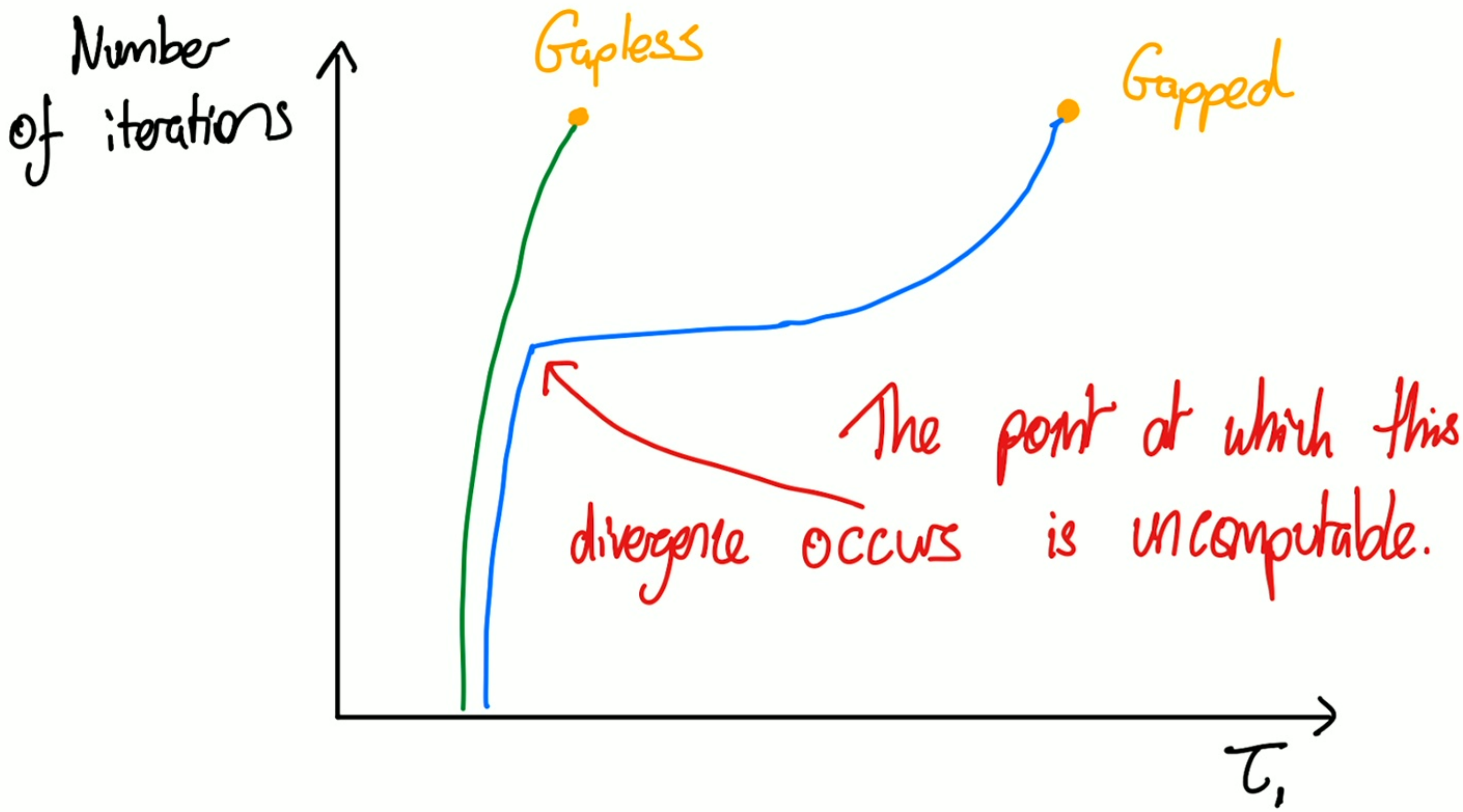
- Uncomputability of the phase diagram means that RG methods necessarily can't solve the phase diagram.
- We expect fundamental theories to be renormalizable – if no "legitimate" renormalization methods exist for uncomputable systems, it might suggest renormalizable theories cannot be uncomputable!
- Why do RG methods fail on the uncomputable Hamiltonians seen earlier?
    - Potentially no way of constructing an RG procedure for these Hamiltonians?
    - Perhaps the RG procedures fail to preserve key properties such as the spectral gap?

Failure of RG Techniques

Theorem
It is possible to explicitly construct an RG scheme for the uncomputable Hamiltonian seen previously such that:

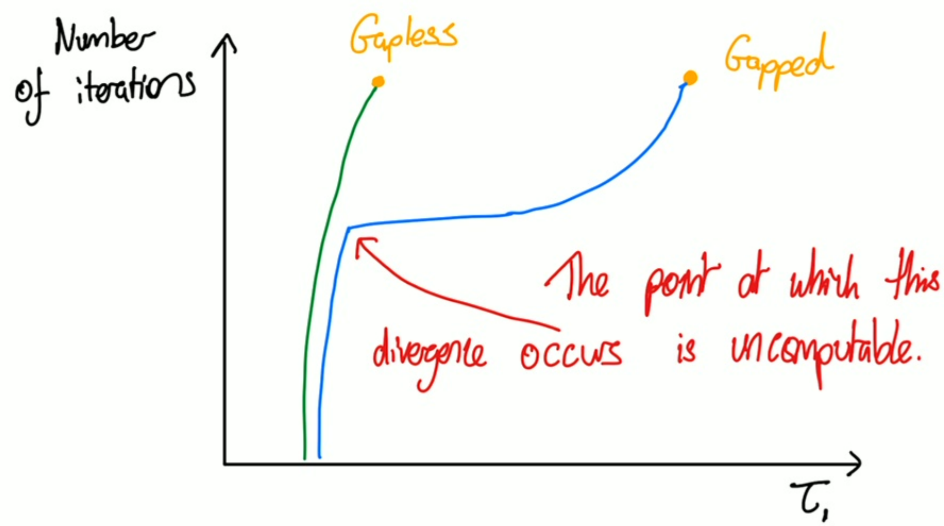
- *Each step of the RG scheme is efficiently computable.*
- *All properties reflecting the phase of matter are preserved (e.g. spectral gap, order parameters).*
- *The Hamiltonian flows to one of two fixed points.*
- *The overall RG flow is uncomputable, and determining which fixed point it flows to is undecidable.*

Failure of RG Techniques



Failure of RG Techniques

- Good, well formed RG schemes do exist for uncomputable Hamiltonians.
- But they have to flow in an uncomputable manner.
- Demonstrates new and previously unseen behavior.
- Expect this behavior to be generic for "good" RG schemes applied to uncomputable Hamiltonains.



Overall Summary

- Determining phase diagrams is an uncomputable task!
- Even for Hamiltonians with “natural properties”, it is computationally intractable.
- RG methods fail, and in the process show novel and unseen behavior.

Further Questions

- Can determining phase diagrams be harder than "uncomputable"?
- Uncomputability of finite temperature phase transitions?
- Robustness of these results to perturbations in Hamiltonian?