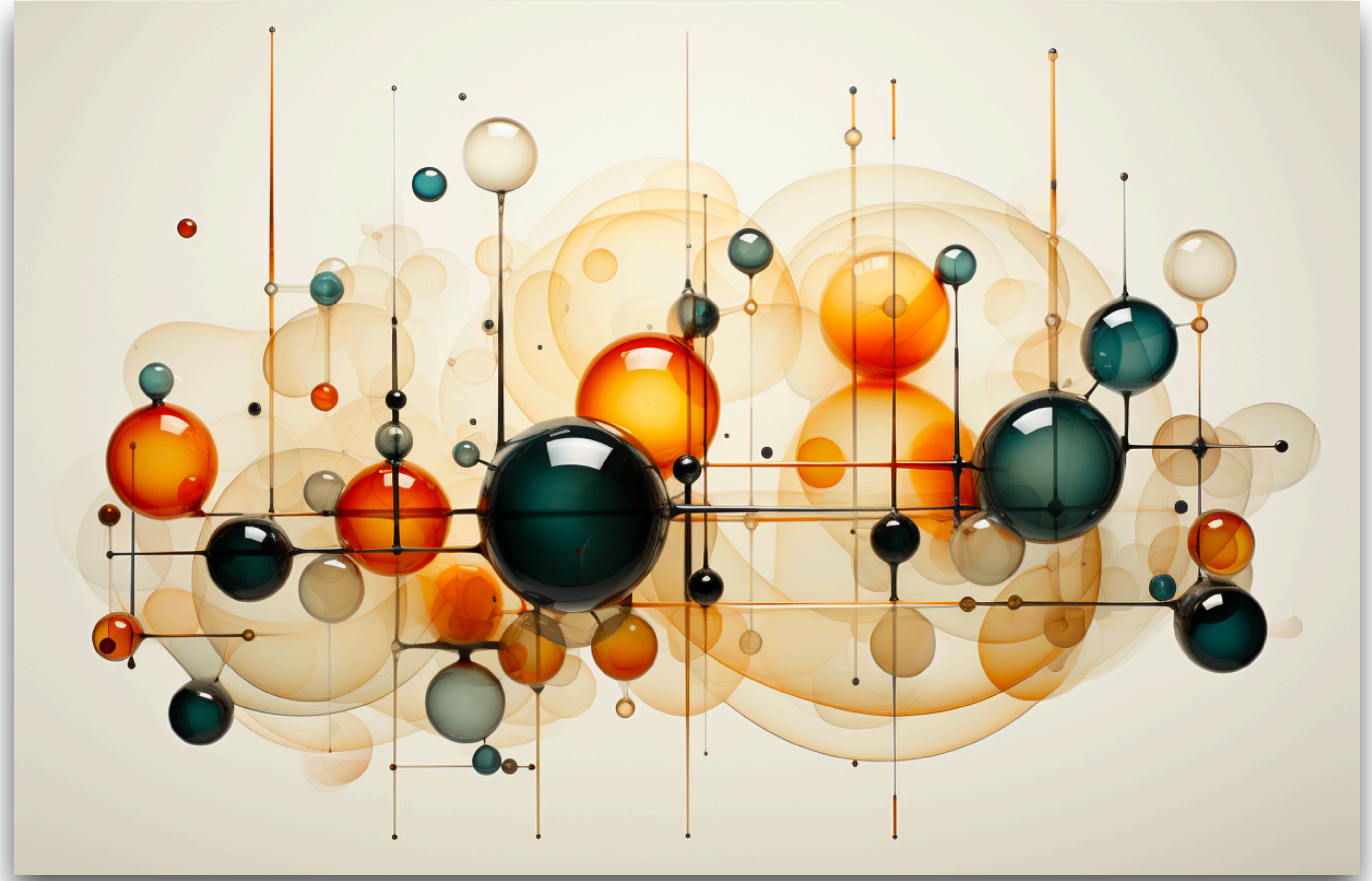
Local minima in quantum systems

Hsin-Yuan Huang (Robert)

Joint work with Chi-Fang Chen, John Preskill, Leo Zhou

Motivation

- We **hope** that quantum computing can advance physics, chemistry, material science by solving the ground states of quantum systems.



Motivation

- We **hope** that quantum computing can advance physics, chemistry, material science by solving the ground states of quantum systems.
- However, finding ground states is **QMA-hard**.
- So, ground states are both **classically & quantumly hard** to find.

Motivation

- The QMA-hardness of finding ground states implies that ground states are **not always *physical***.
- Assuming Nature cannot efficiently solve NP-hard problems, Nature **should not** always find the ground state.

Motivation

- When a quantum system is cooled in a low-temperature bath, the system finds a **local minimum** of energy.

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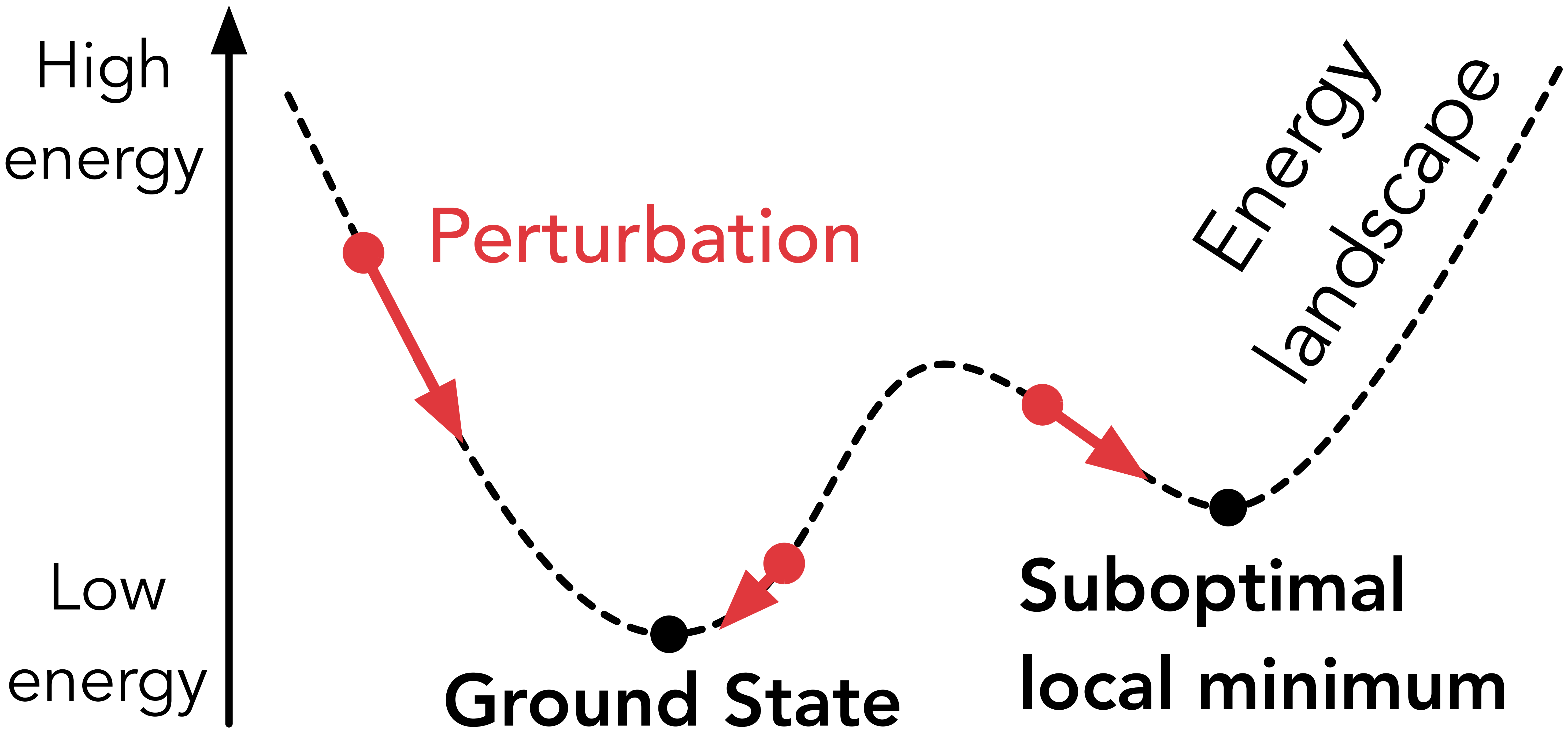
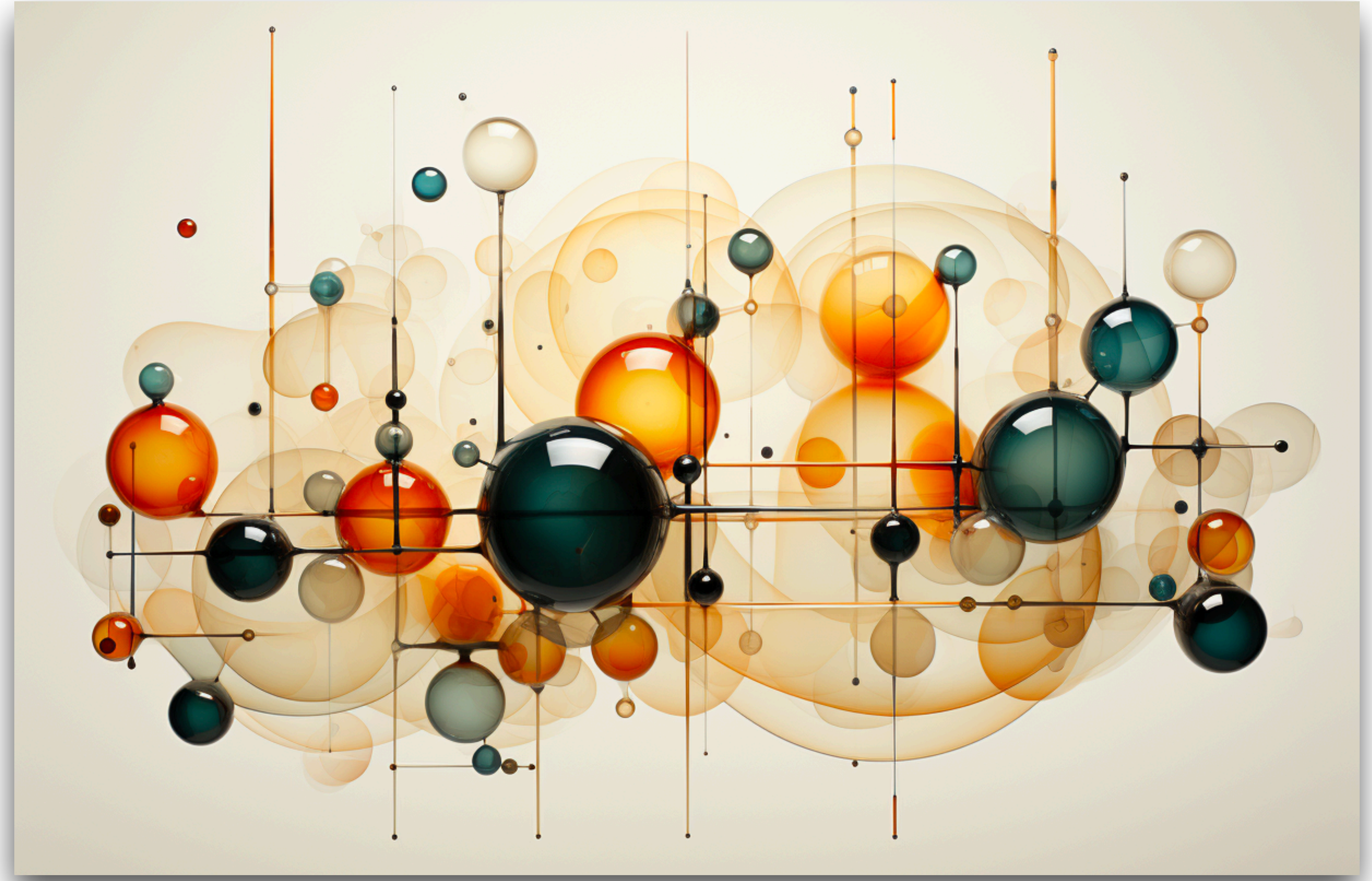


Motivation

- For some physical systems, such as **spin glasses**, the systems almost always find **suboptimal local minima**.
- In these systems, ground states are **physically irrelevant.**

Question

How tractable is the problem of finding a local minimum in quantum systems using classical vs. quantum computers?



Question

How tractable is the problem of finding a local minimum in quantum systems using classical vs. quantum computers?

To answer this, we need

(1) a formal definition of local minima,

(2) a characterization of these local minima.

Outline

- Define local minima in quantum systems
- Complexity of finding local minima
- Future directions

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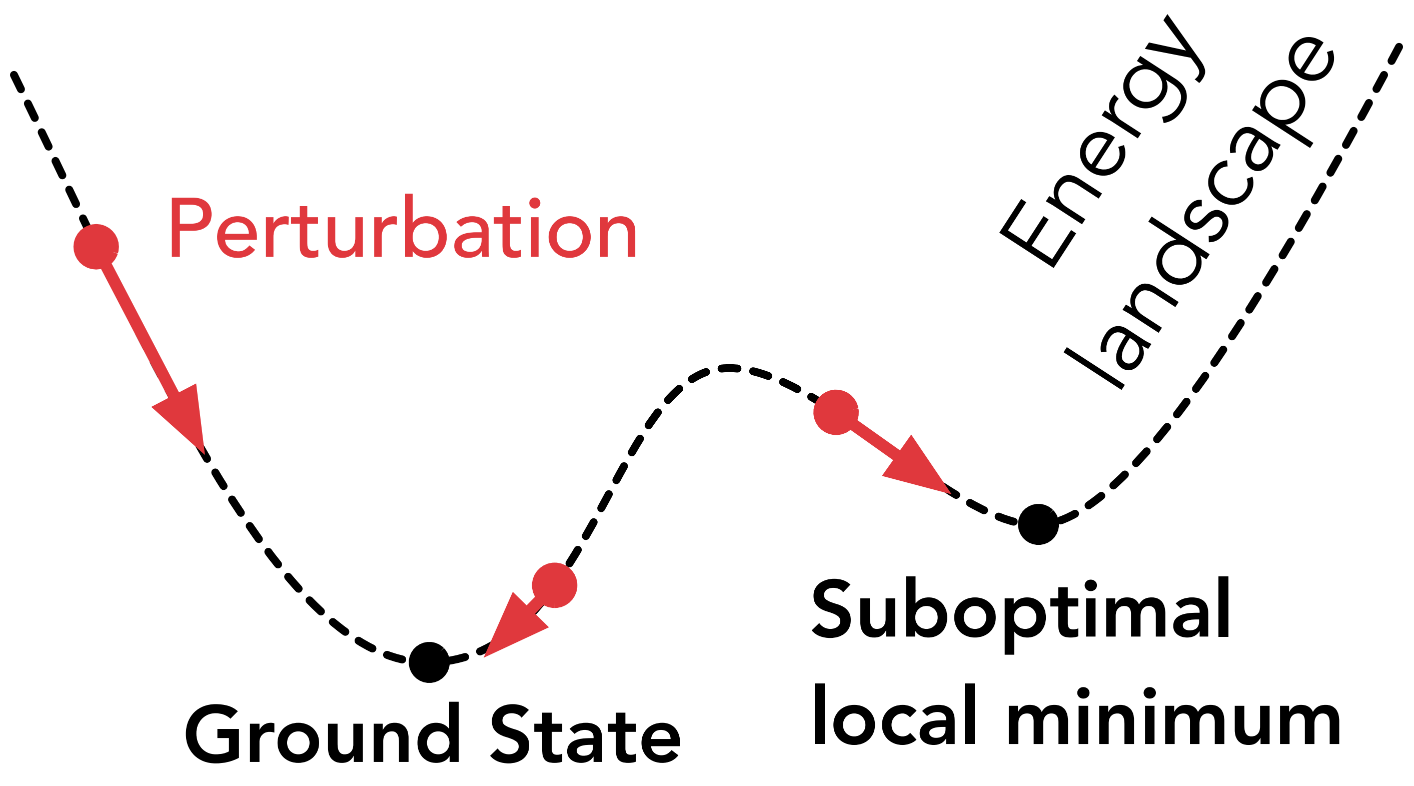
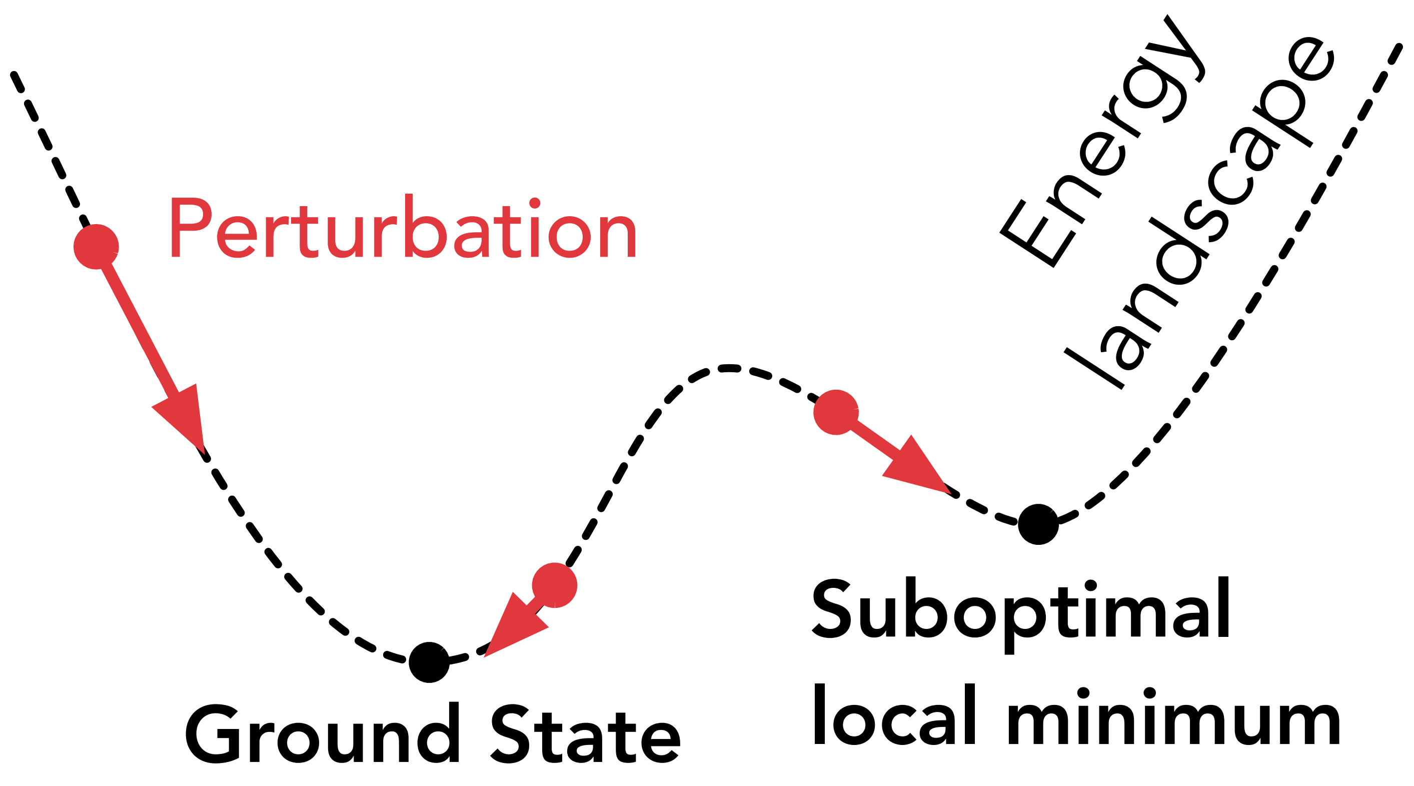


Definition

- Given an n-qubit Hamiltonian H written as a sum of few-body terms.
- A local minimum of H is an n-qubit state ρ that has the **minimum** energy under **any small perturbations** to the state.

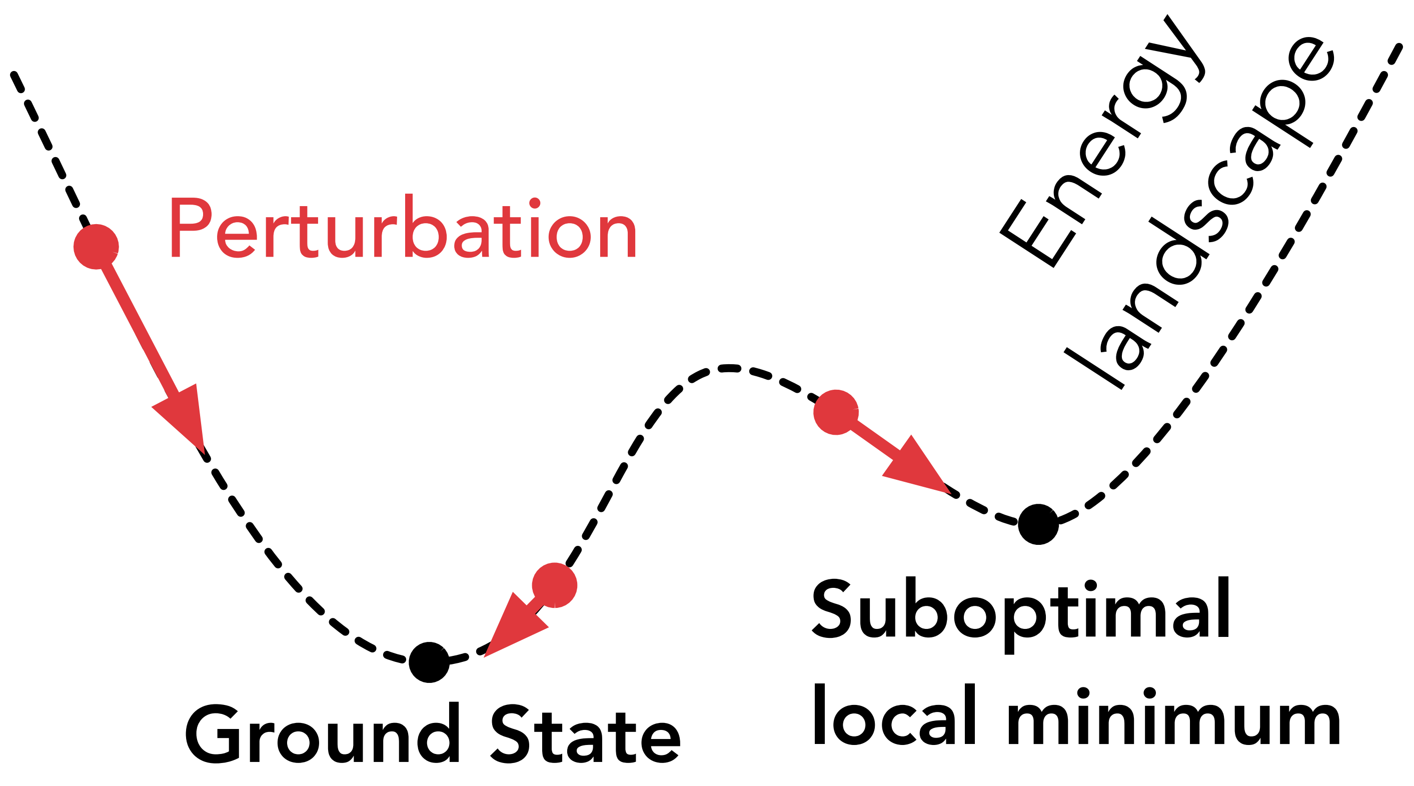


Definition

- Consider **perturbation** P_α mapping states to states parameterized by a vector $\alpha \in \mathbb{R}^m$, where $m = \mathrm{poly}(n)$.
- An n-qubit state ρ is **an ϵ-approximate local minimum** of H under P if

$$\mathrm{Tr}(H\rho) \leq \mathrm{Tr}(HP_\alpha(\rho)) + \epsilon\|\alpha\|,$$

for all small vector α.



Definition

- Local minima form a subset of the entire n-qubit state space.
- The local minima subset contains the ground state and depends on the perturbations.
- We will consider two classes of perturbations.

Local unitary perturbations

- A mathematically-natural definition of perturbations.
- Consider a pure n-qubit state $|\psi\rangle$. The perturbations are given by

$$|\psi\rangle \to \exp\left(-i\sum_{a=1}^{m}\alpha_a h^a\right)|\psi\rangle$$

for a set of m few-body Hermitian operators $\{h^a\}_{a=1}^{m}$.

- Any quantum circuit with near-identity two-qubit gates is a local unitary perturbation (to the 1st order).

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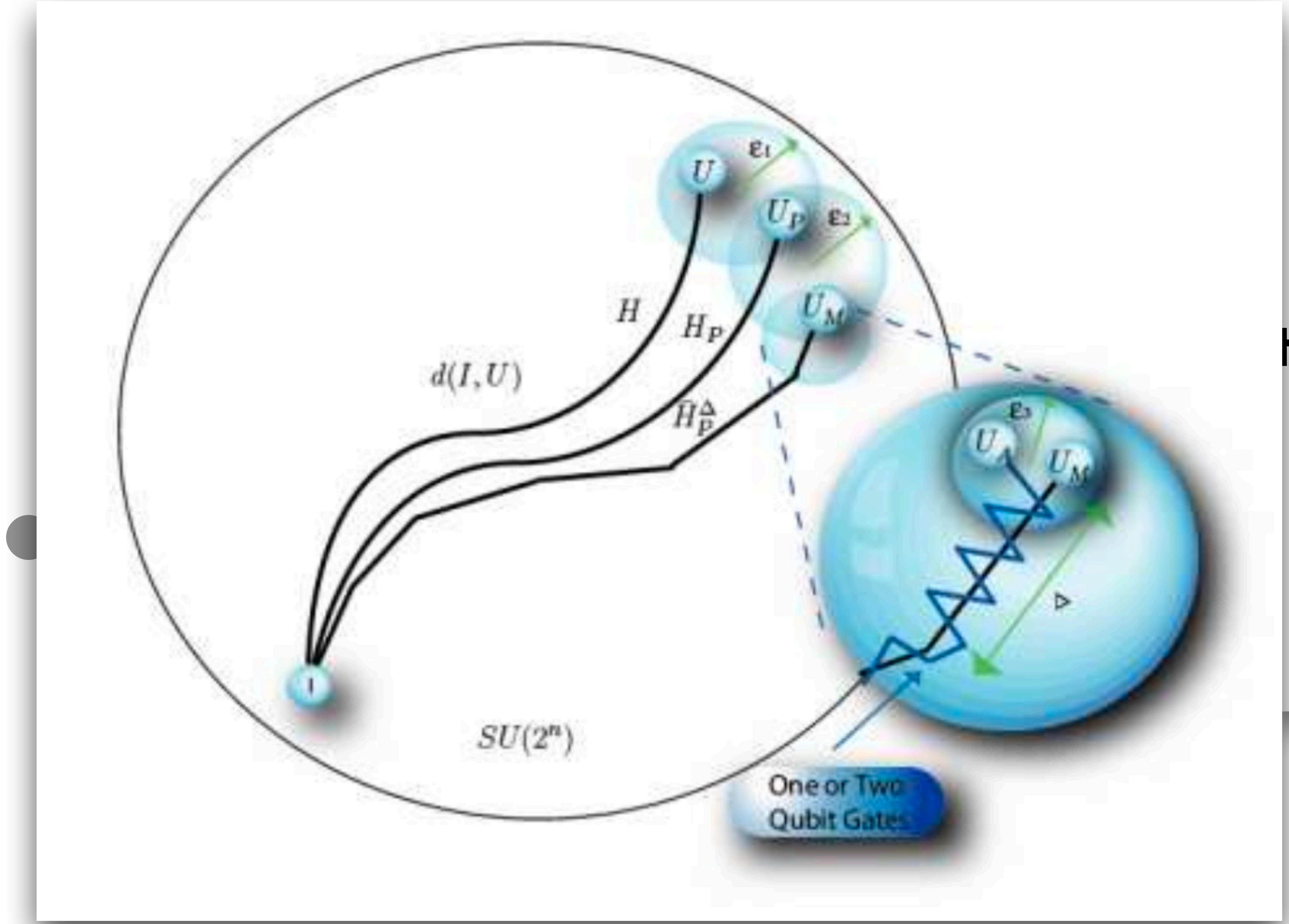

Forms a Riemannian geometry;
see *Quantum Computation as Geometry*
by Nielson et al., Science (2006)

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Thermal perturbations

- A **physically-motivated** definition of perturbations.
- When a quantum system is placed in a **cold thermal bath**,
  the perturbations are described by thermal Lindbladian dynamics.
- These perturbations are generally irreversible, i.e., **non-unitary**.

Thermal perturbations

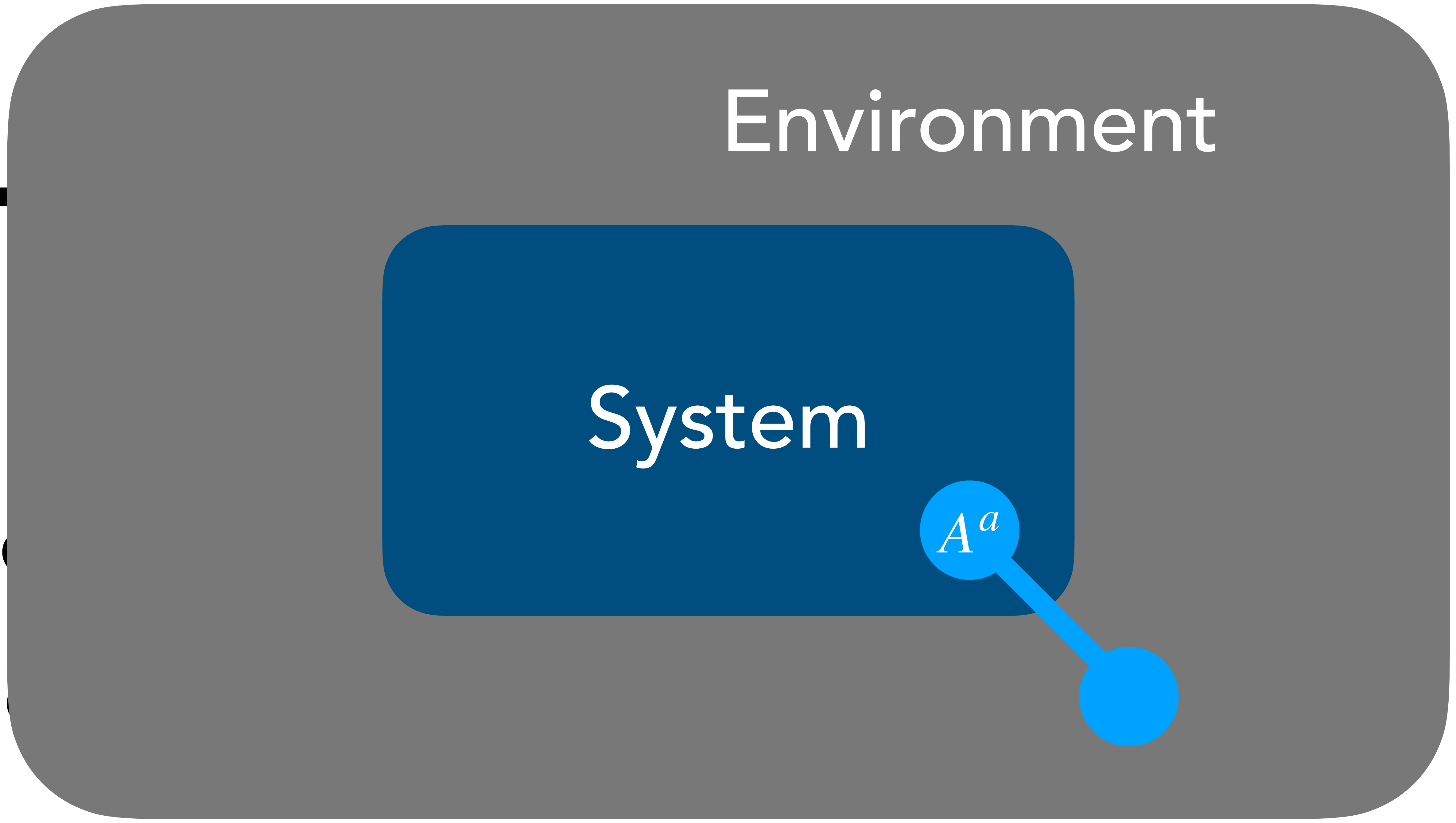
- 2 macroscopic properties from modern quantum thermodynamics: β (inverse temperature) and τ (characteristic time scale).

- The **thermal perturbations** are given by

$$\rho \to \exp\left(\sum_{a=1}^{m} \alpha_a \mathscr{L}_a^{\beta,\tau,H}\right)(\rho),$$

where $\mathscr{L}_a^{\beta,\tau,H}$ is a thermal Lindbladian for the few-body operator A^a through which the bath interacts with the system and $\alpha_a \geq 0$.

Thermal per



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Summary

- An n-qubit state ρ is an **ϵ-approximate local minimum** of H under P if $\mathrm{Tr}(H\rho) \leq \mathrm{Tr}(HP_\alpha(\rho)) + \epsilon||\alpha||$ for all small vector α.
- **Local unitary perturbations**: mathematically natural, reversible ($\alpha \in \mathbb{R}^m$), Hermitian evolutions.
- **Thermal perturbations**: physically motivated, irreversible ($\alpha \in \mathbb{R}^m_{\geq 0}$), Lindbladian evolutions.

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Local minima problem

- An algorithm solves the local minima problem efficiently if

For any n-qubit **local Hamiltonian** H and any **local observable** O,

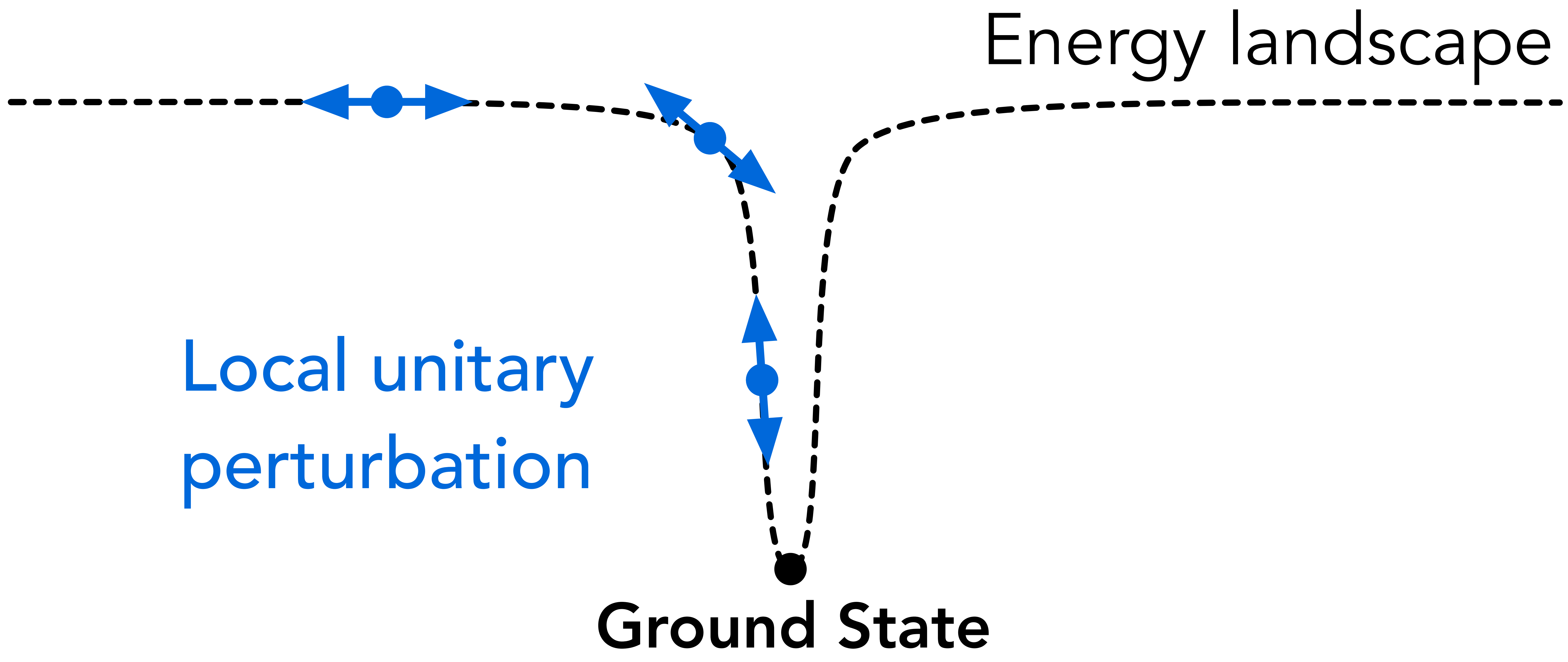
the algorithm can output $\mathrm{Tr}(O\rho)$ to error $\epsilon = 1/\mathrm{poly}(n)$

of an ϵ-**approximate local minimum** ρ of H in $\mathrm{poly}(n)$ time.

- This is a problem with purely classical input and output.

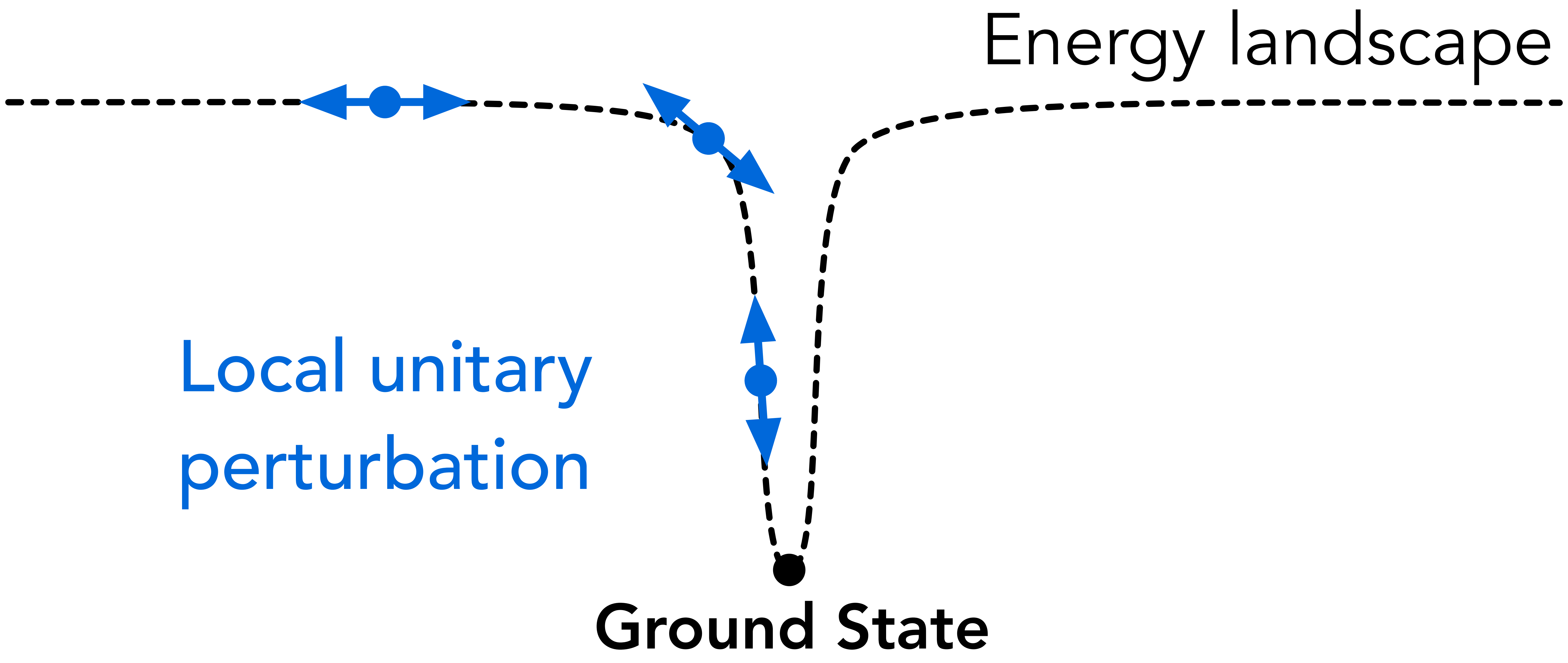
Characterizing local minima

Proposition (Classically easy): The problem of finding local minima under local unitary perturbations is in BPP.



Characterizing local minima

Lemma (Barren plateau): For any local Hamiltonian H, a random state is a local minimum of H under local unitary perturbations.



Characterizing local minima

- Local unitary perturbations are mathematically natural but not physically motivated, as thermodynamics are generally non-unitary.
- Let's see how the conceptual picture changes when we consider thermal perturbations.

Characterizing local minima

Theorem (Quantumly easy): The problem of finding local minima under thermal perturbations is quantumly easy.

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- This theorem is shown using a **quantum thermal gradient descent** algorithm (to handle finite temperature and finite time scale).
- The convergence is proven by showing the smoothness properties of the second derivative of thermal Lindbladians.

Characterizing local minima

Theorem (Quantumly easy): The problem of finding local minima under thermal perturbations is quantumly easy.

While the problem is quantumly easy,

can the problem also be classically easy?

Characterizing local minima

Consider a class of Hamiltonians $\{H_C\}_C$ on *2D lattices*.

- Each poly-size quantum circuit C corresponds to a Hamiltonian H_C

  based on a modified version of Kitaev's circuit-to-Hamiltonian construction

- The ground state of H_C encodes the output of the circuit C.
- So finding the ground state of H_C is BQP-**hard**.

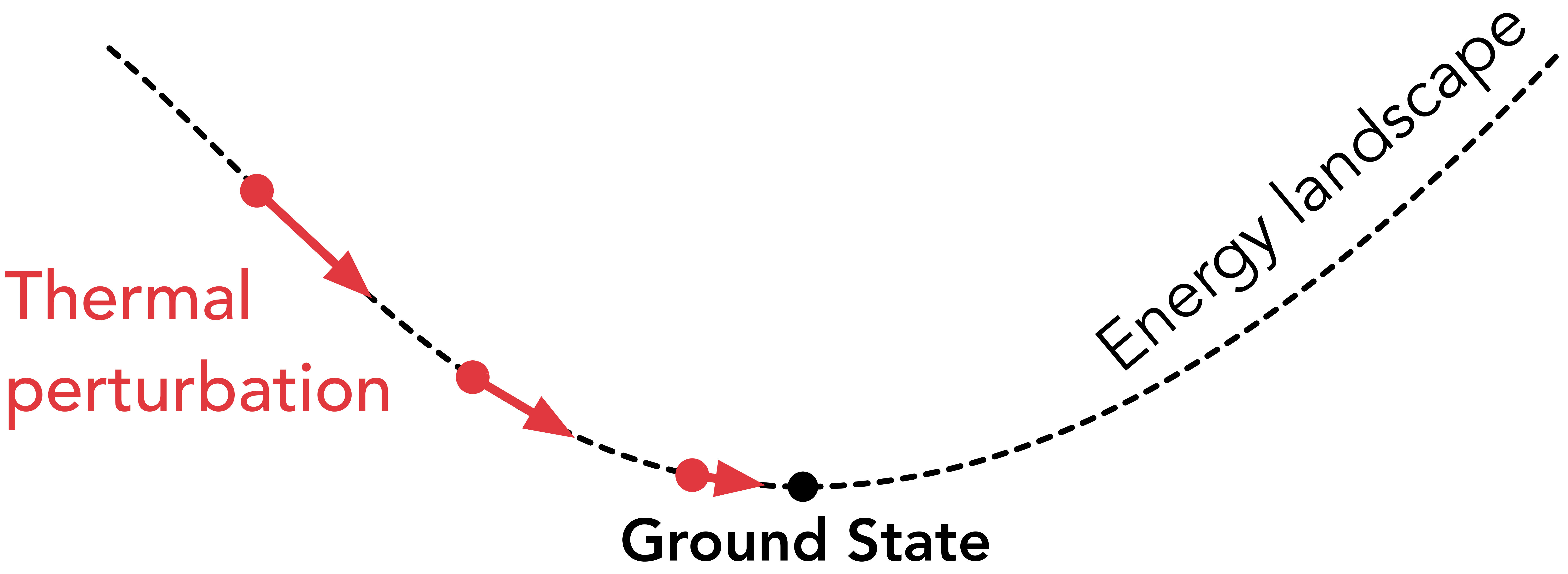
Characterizing local minima

Consider a class of Hamiltonians $\{H_C\}_C$ on *2D lattices*.

- But, perhaps, finding local minima of H_C is much easier.
- Maybe there are some **classically easy local minima** lurking in the exponentially large quantum Hilbert space!

Characterizing local minima

Theorem (No suboptimal local minima): All approximate local minima of H_C under thermal perturbations are close to the global minimum.



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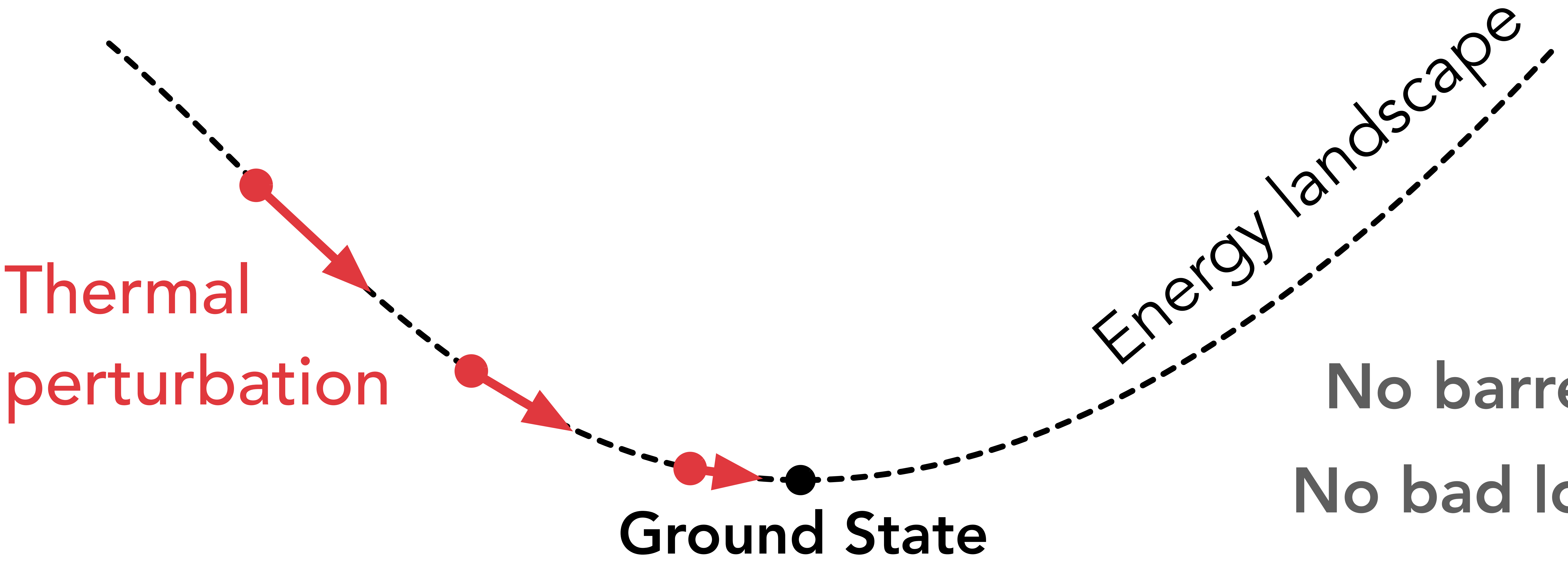

No barren plateau

No bad local minima

Proof Idea

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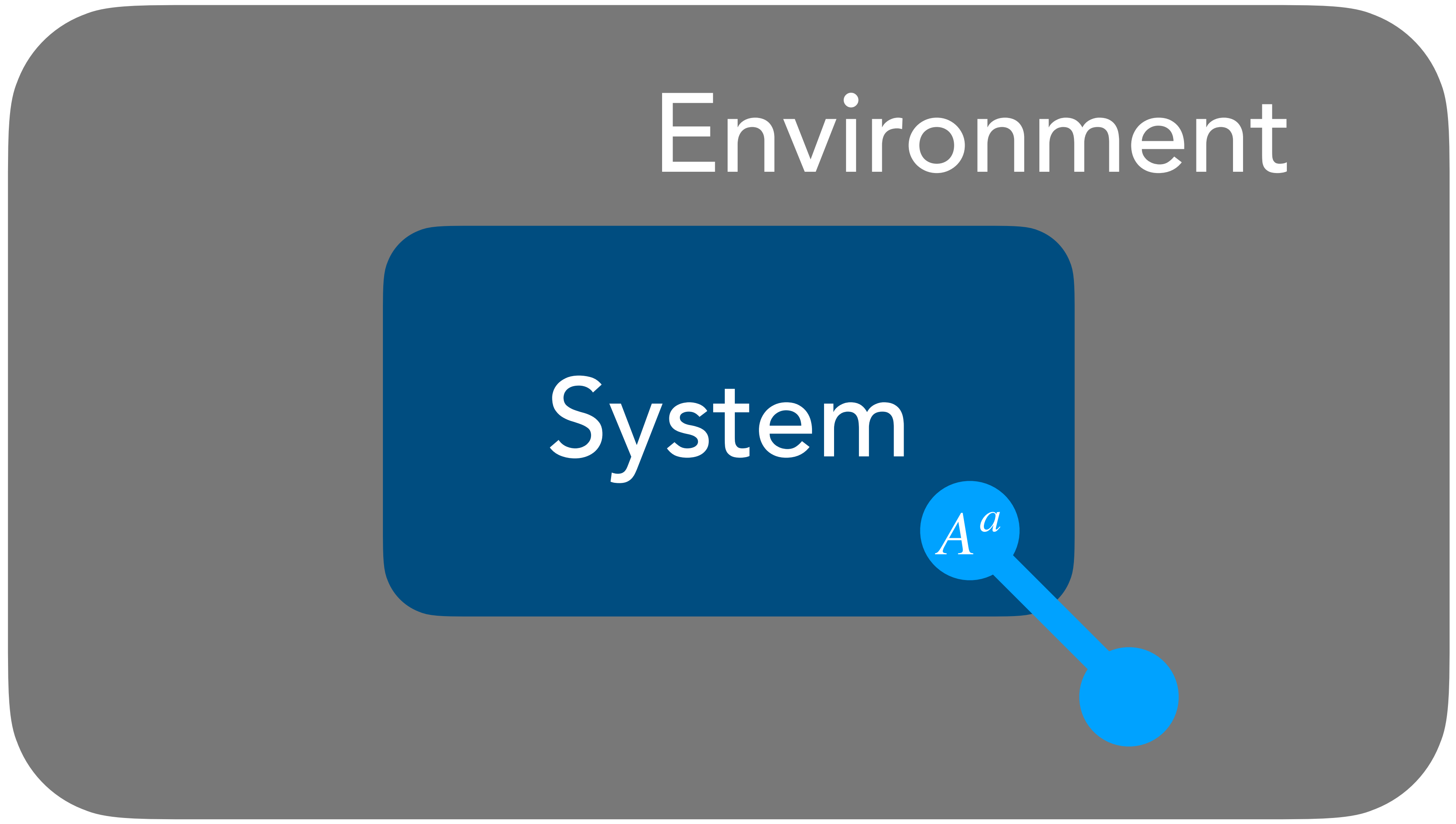

- Consider a local operator A^a.

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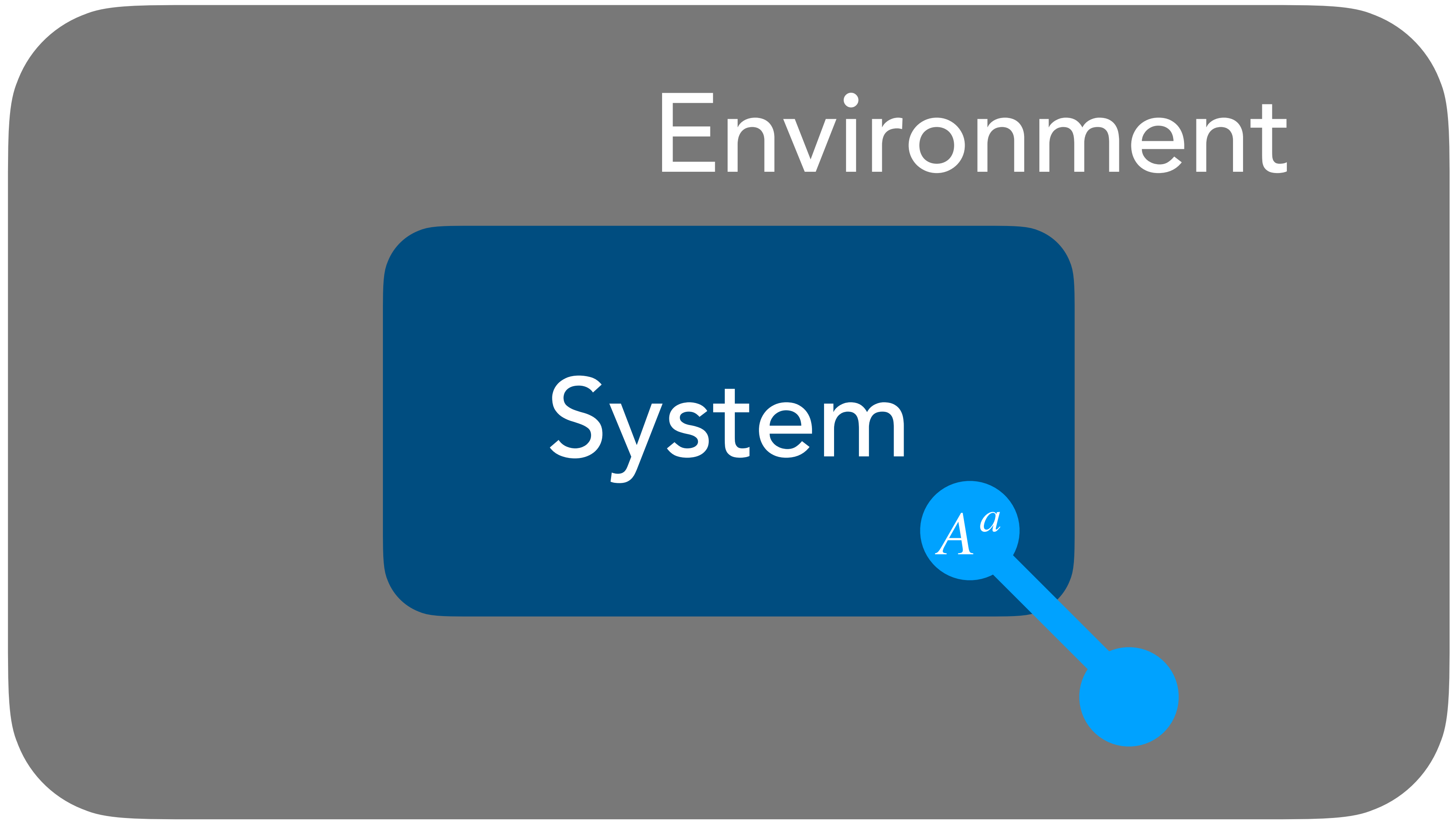

- Consider a local operator A^a.
- The thermal bath induces a thermal Lindbladian $\mathscr{L}_a^{\beta,\tau,H}$ with a continuous set of **Lindblad jump operators** $\left\{\hat{A}^a_{\tau,H}(\omega)\right\}_{\omega\in(-\infty,\infty)}$.

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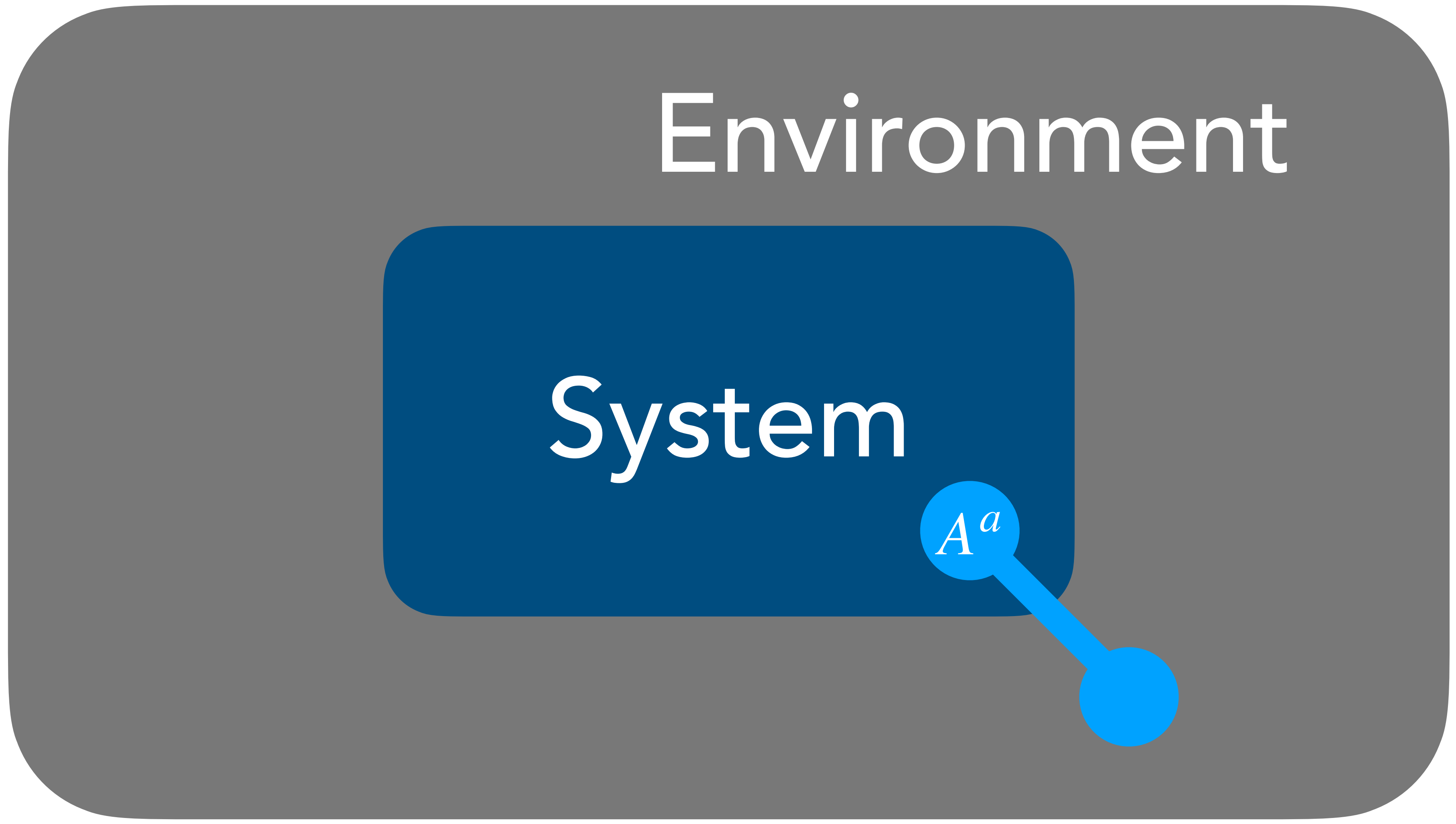

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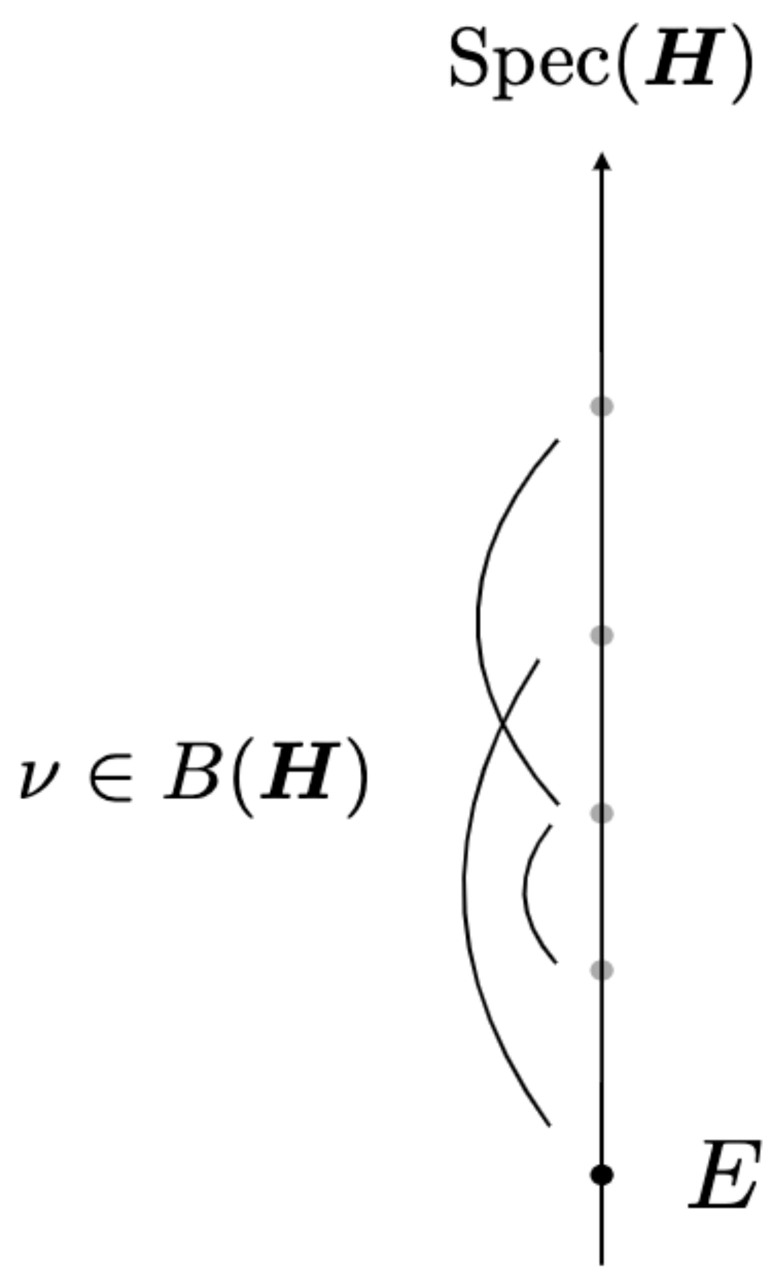
- The index ω has an energy unit and measures the energy difference.

Proof Idea



- Intuition for the Lindblad jump operator $\hat{A}^a_{\tau,H}(\omega)$:

$$A^a = \sum_{i,j} A^a_{ij} |E_i\rangle\langle E_j|$$

$$\hat{A}^a_{\tau,H}(\omega) = \sum_{i,j} A^a_{ij} \sqrt{\delta_\tau(\omega - (E_i - E_j))}\, |E_i\rangle\langle E_j| \qquad \sqrt{\delta_\tau(x)} = \frac{1}{\sqrt{2\pi\tau}} \int_{-\tau/2}^{\tau/2} e^{-itx}$$

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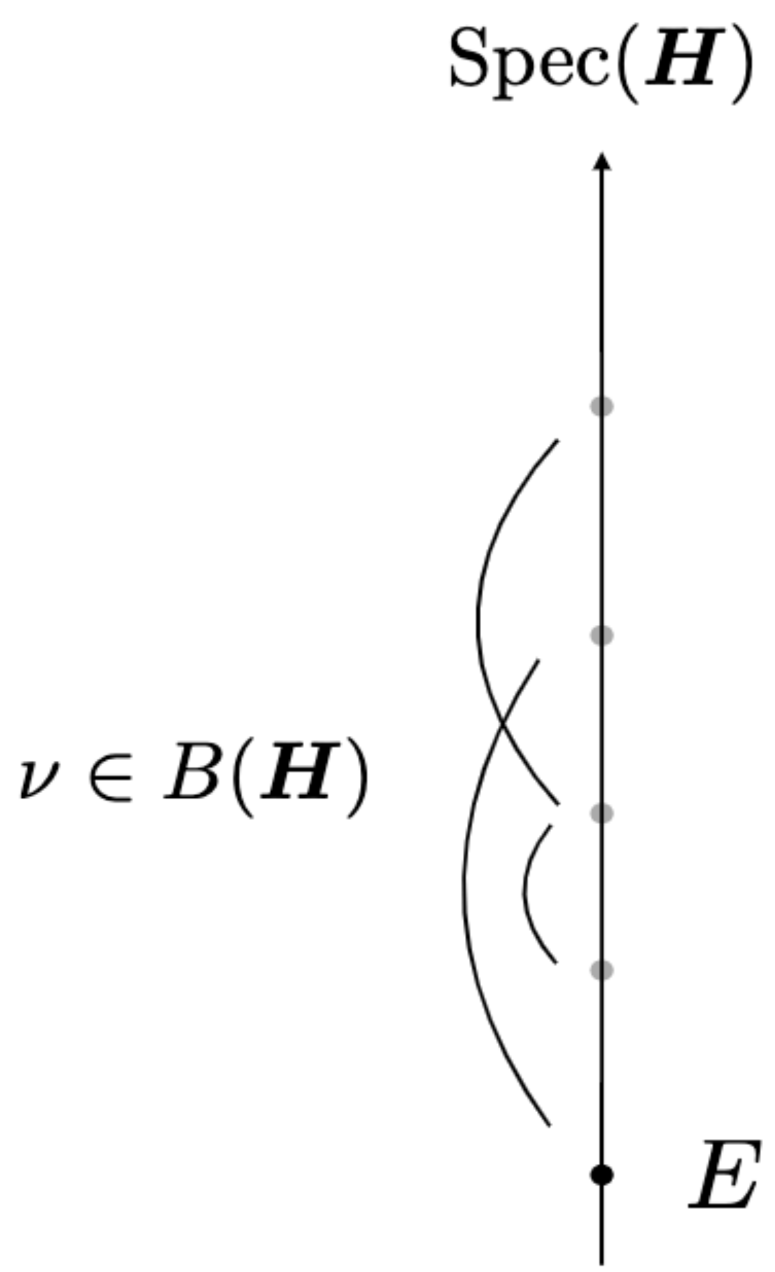

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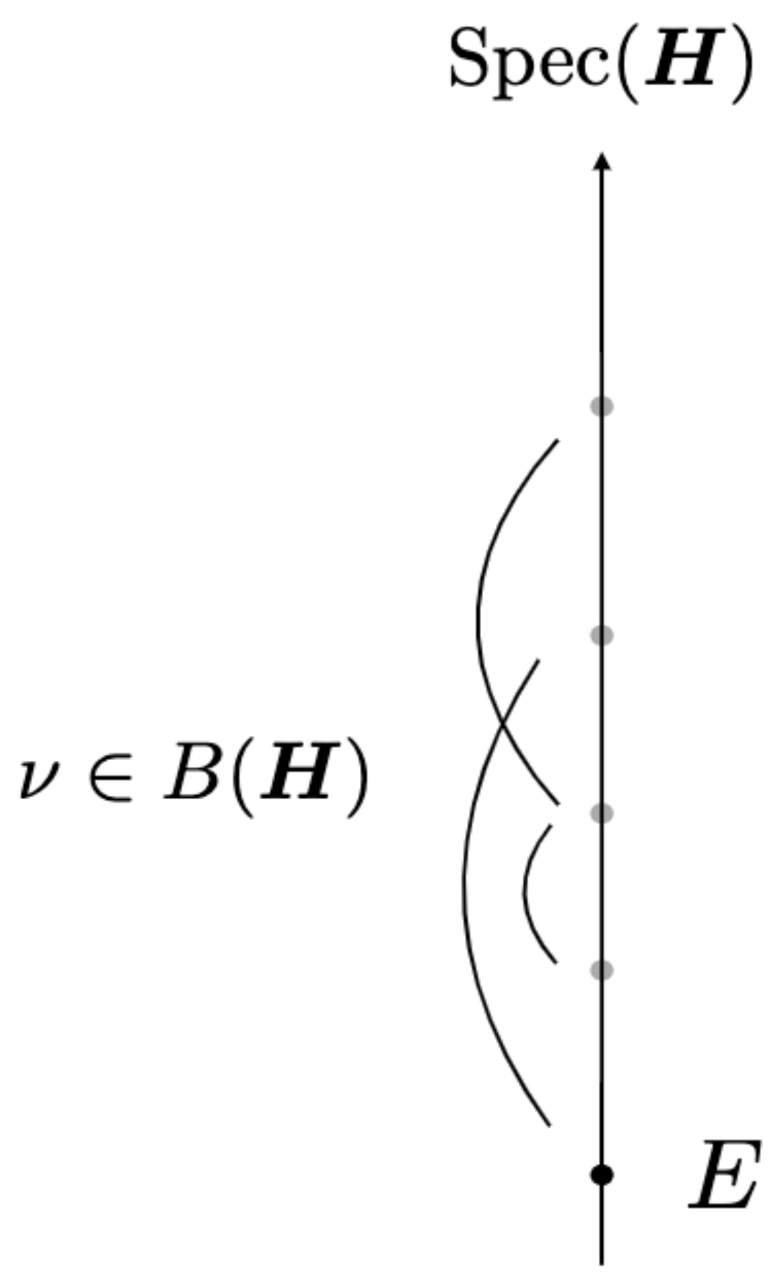

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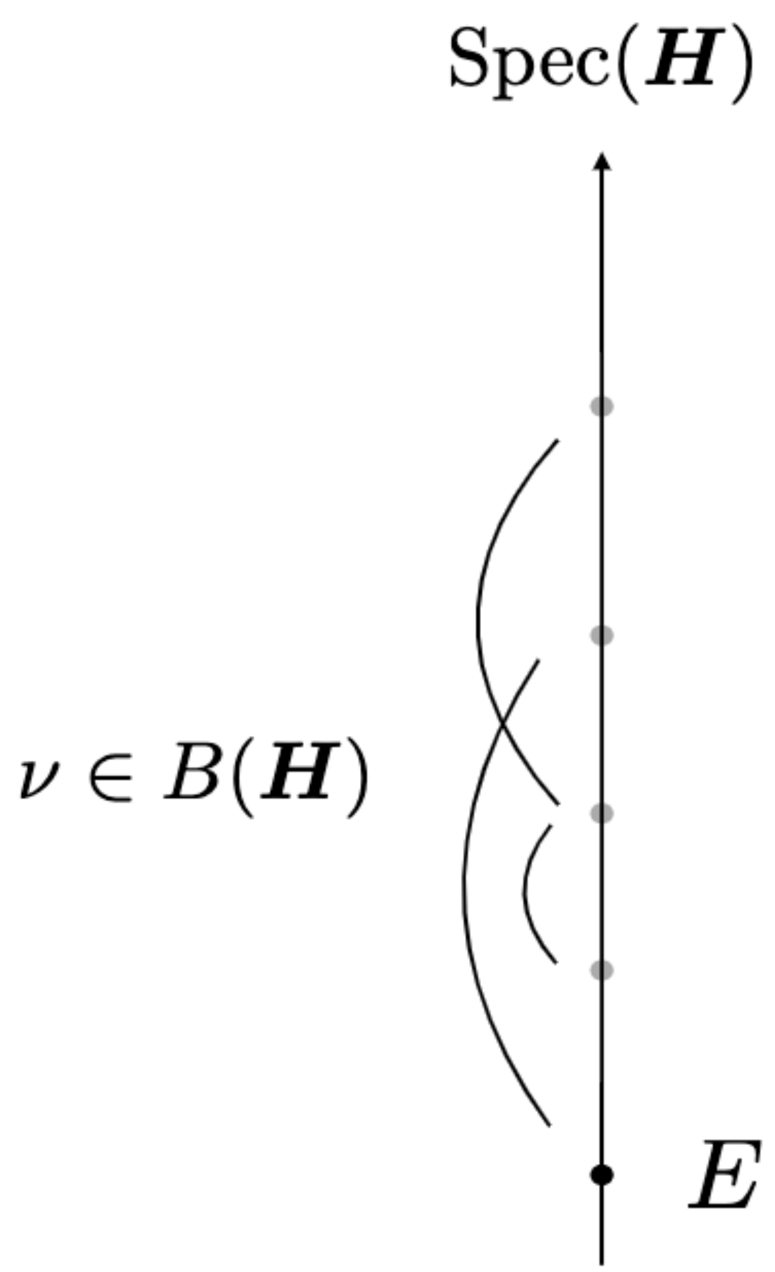

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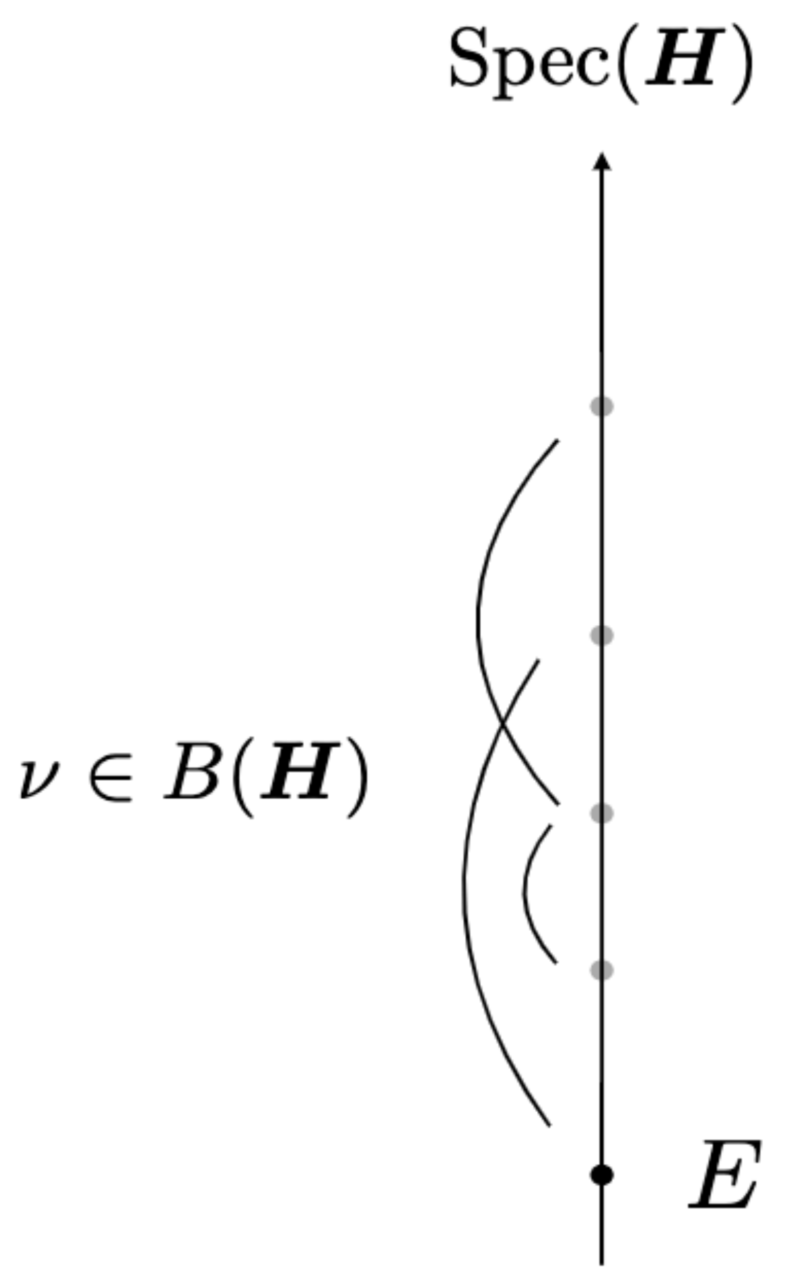
- While A^a has matrix elements betw. $|E_j\rangle$ and **higher & lower** $|E_i\rangle$, $\hat{A}^a(\omega)$ for $\omega < 0$ induces transitions from $|E_j\rangle$ to **lower** energy $|E_i\rangle$.

Proof Idea



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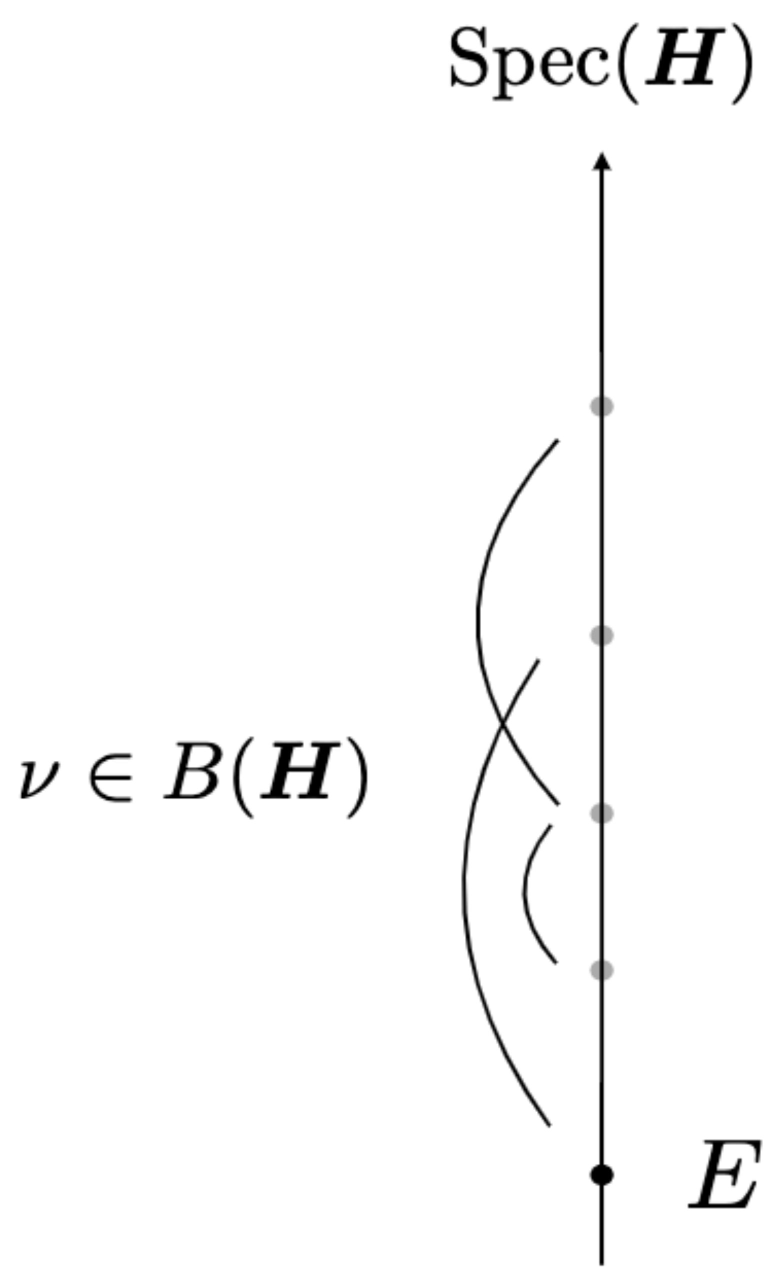
- If $\forall$energy eigenstate $|E_j\rangle$, $\exists$ a local operator A^a and $E_i < E_j$, s.t., $\langle E_i|A_a|E_j\rangle \neq 0$, then there are **no suboptimal local minima.**



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Note the similarity to classical combinatorial optimization

Proof Idea

Given a circuit C with unitary $U_C = U_T \ldots U_1$.

The Hamiltonian is $H_C = H_{\mathrm{cl}} + H_{\mathrm{prop}} + H_{\mathrm{in}}$

with a unique ground state given by

$$\sum_{t=0}^{T} \sqrt{\frac{1}{2^T}\binom{T}{t}} \left(U_t \ldots U_1 |0^n\rangle\right) \otimes |0^t 1^{T-t}\rangle$$

H_{cl} checks the clock

H_{prop} checks propagation

H_{in} checks the input

$$\|H_{\mathrm{cl}}\| \gg \|H_{\mathrm{prop}}\| \gg \|H_{\mathrm{in}}\|$$

Proof Idea

1. There are no suboptimal local minima in H_{cl}.

The Hamiltonian is $H_C = H_{\text{cl}} + H_{\text{prop}} + H_{\text{in}}$

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2. In GS space of H_{cl}, there are no suboptimal LM in $H_{\mathrm{cl}} + H_{\mathrm{prop}}$.
3. In GS space of $H_{\mathrm{cl}} + H_{\mathrm{prop}}$, there are no suboptimal LM in $H_{\mathrm{cl}} + H_{\mathrm{prop}} + H_{\mathrm{in}}$.

The Hamiltonian is $H_C = H_{\mathrm{cl}} + H_{\mathrm{prop}} + H_{\mathrm{in}}$

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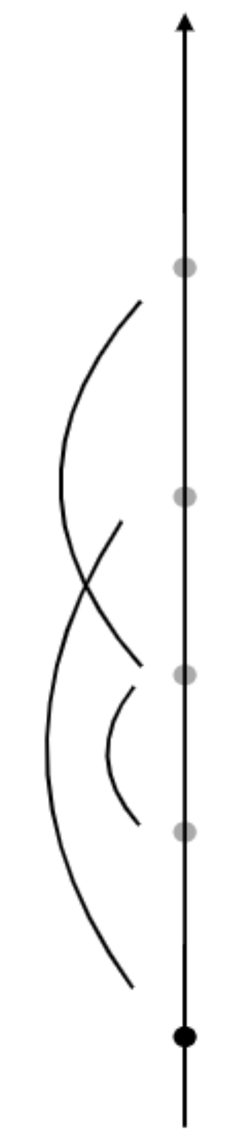

If the Hamiltonians have **a large Bohr frequency gap** and Statement 1, 2, 3 hold,

then ***there are no suboptimal LM in*** $H_C = H_{\text{cl}} + H_{\text{prop}} + H_{\text{in}}$.

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Proof Idea

H_{in} is standard.

The Hamiltonian is $H_C = H_{\text{cl}} + H_{\text{prop}} + H_{\text{in}}$

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Proof Idea

$H_{\text{cl}} = \sum_{t=1}^{T-1} h_{t,\text{cl}}$ has a non-uniform $\|h_{t,\text{cl}}\|$ decreasing in t,

so local excitations have the **tendency to move to the right.**

The Hamiltonian is $H_C = H_{\text{cl}} + H_{\text{prop}} + H_{\text{in}}$

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Proof Idea

$$H_{\text{prop}} = \sum_{t=1}^{T} h_{t,\text{prop}}$$ gives rise to the $$\frac{1}{2^T}\binom{T}{t}$$ factor,

and **the energy spectrum is $\propto \{k\}_{k=0}^{T}$** (evenly spaced).

The Hamiltonian is $H_C = H_{\text{cl}} + H_{\text{prop}} + H_{\text{in}}$

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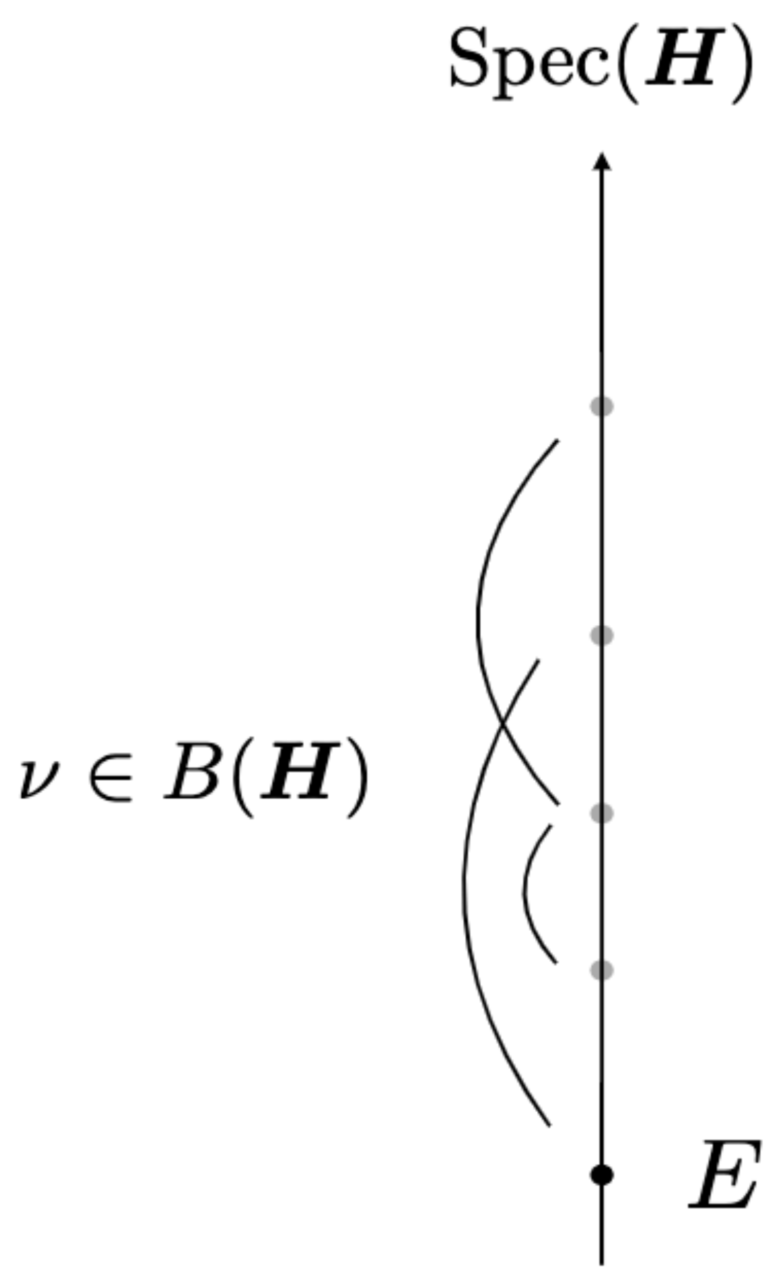

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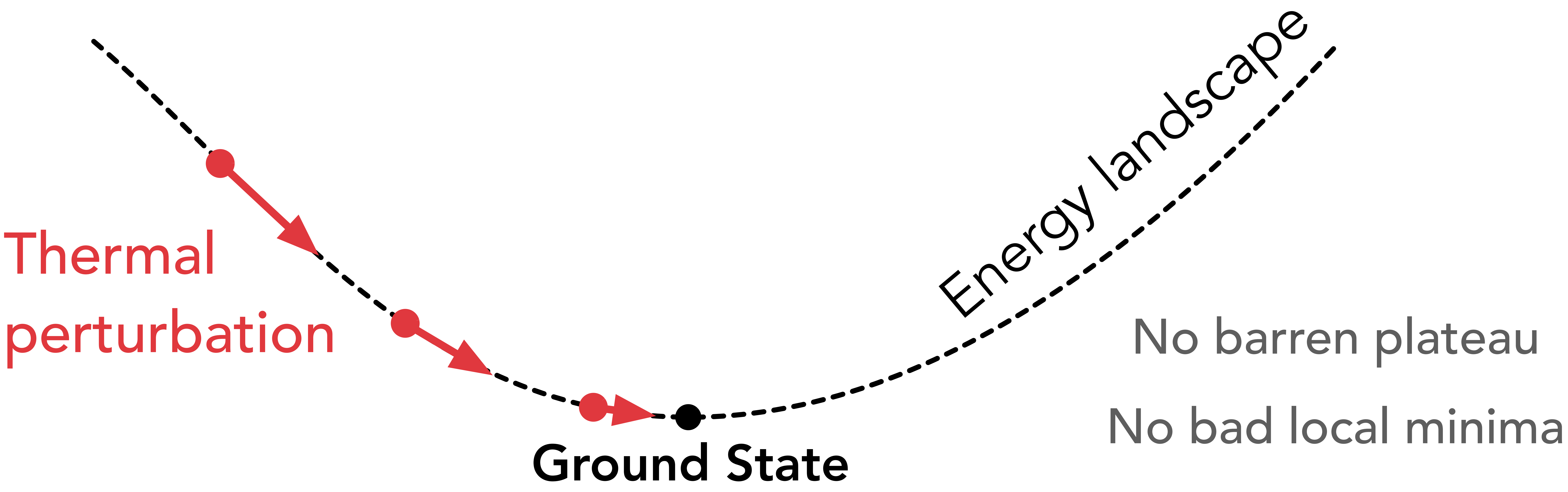
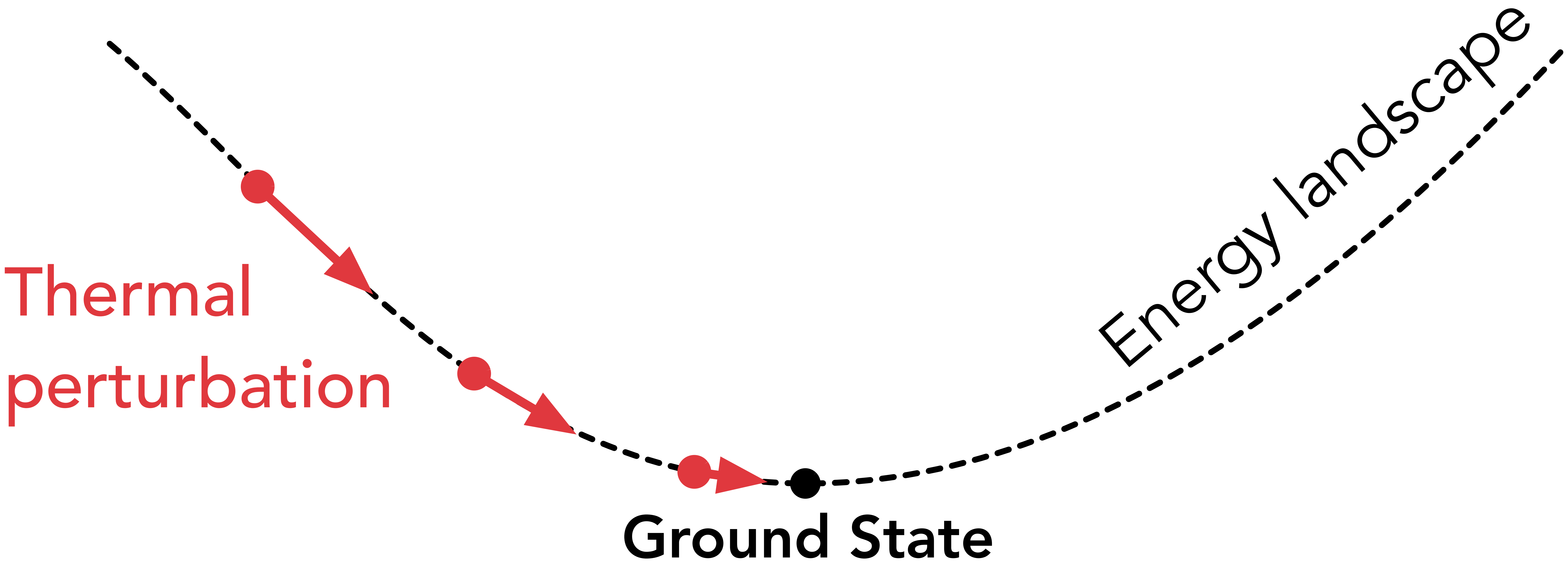
Characterizing local minima

Theorem (No suboptimal local minima): All approximate local minima of H_C under thermal perturbations are close to the global minimum.



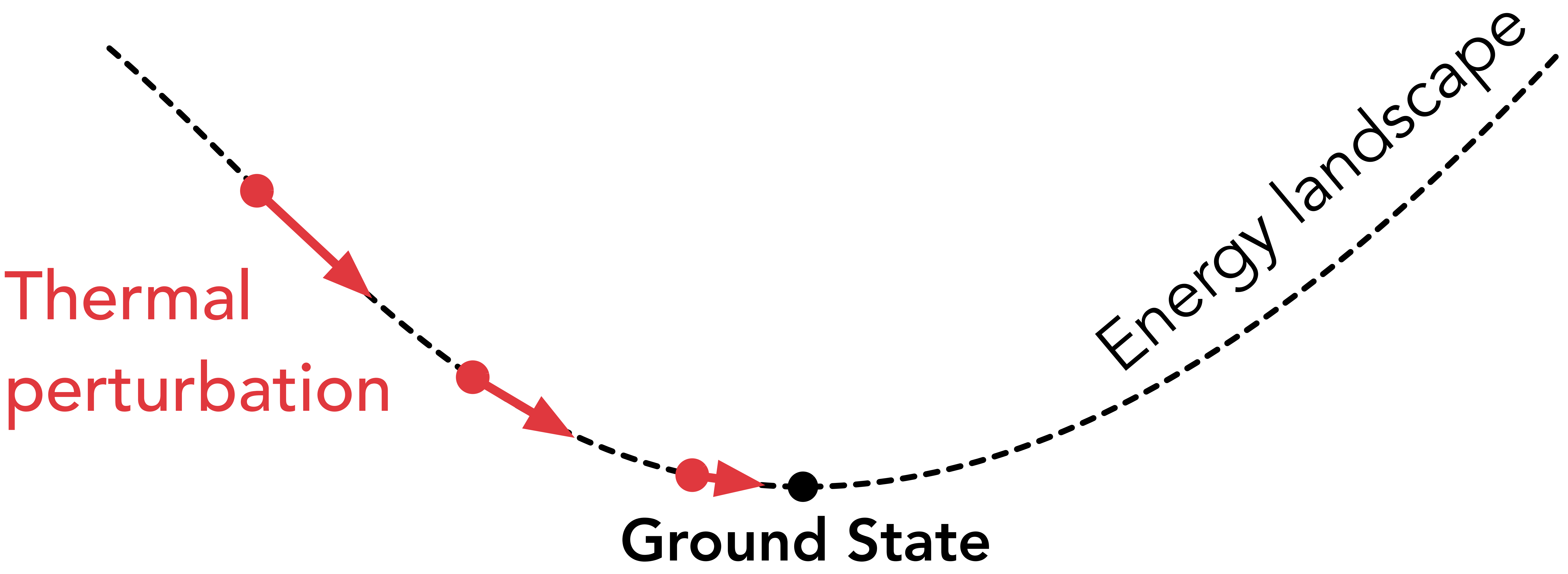
Characterizing local minima

Theorem (Classically hard): The problem of finding local minima under thermal perturbations is classically hard if BPP $\neq$ BQP.



Characterizing local minima

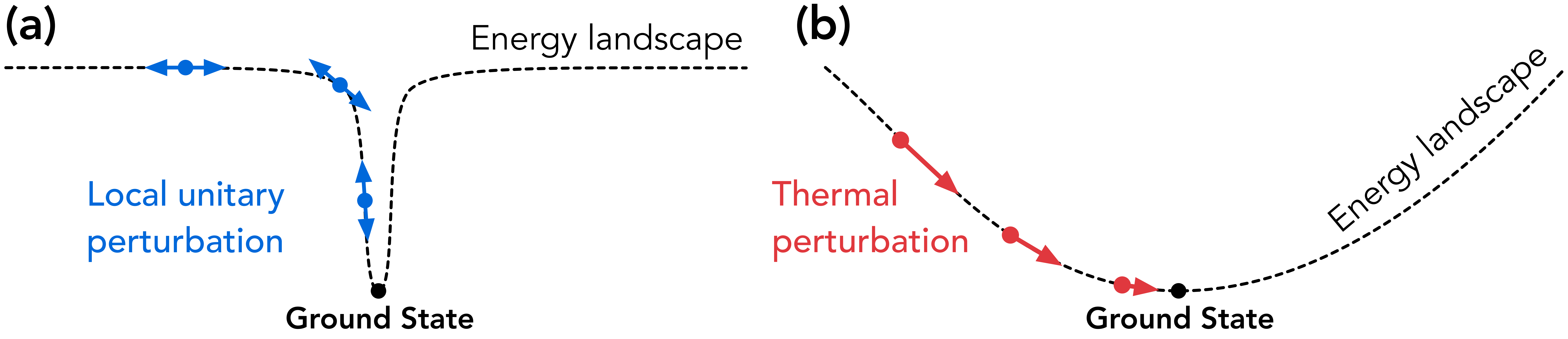
Corollary: There are 2D Hamiltonians where the energy of classical ansatz optimized by efficient classical algorithms can be **strictly improved** by simulating quantum thermodynamics.



Characterizing local minima

Finding local minima
under local unitary perturbations
is ***trivial for classical computation***

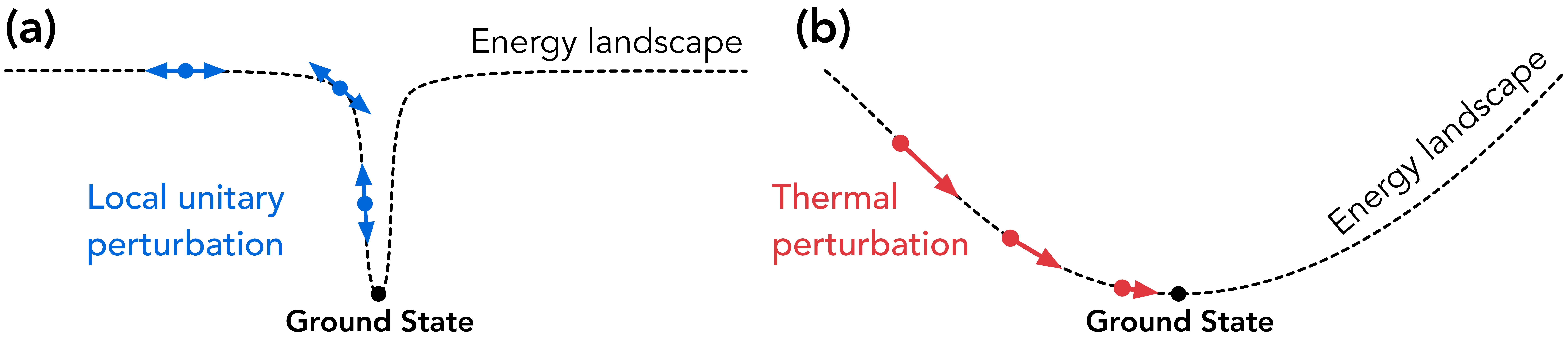
Finding local minima
under thermal perturbations
is ***universal for quantum computation***



Characterizing local minima

Finding local minima
under local unitary perturbations
is ***trivial for classical computation***

A very good refrigerator
is **a universal quantum computer**



Outline

- Define local minima in quantum systems
- Complexity of finding local minima
- Open problems

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Open Problems

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  Could pseudorandomness help answer this question?

Open Problems

- Our results show that there is quantum advantage in computing properties of systems thermalizing at a **very low temperature**.

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- Is there quantum advantage in estimating properties of systems thermalizing at a constant temperature?
  Quantum advantage in sampling from such systems is known.

Conclusion

- Finding ground states is classically and quantumly hard.
- Finding local minima in energy is classically hard but quantumly easy.