The bulk spectral gap is semi-decidable: a convergent family of certified upper bounds

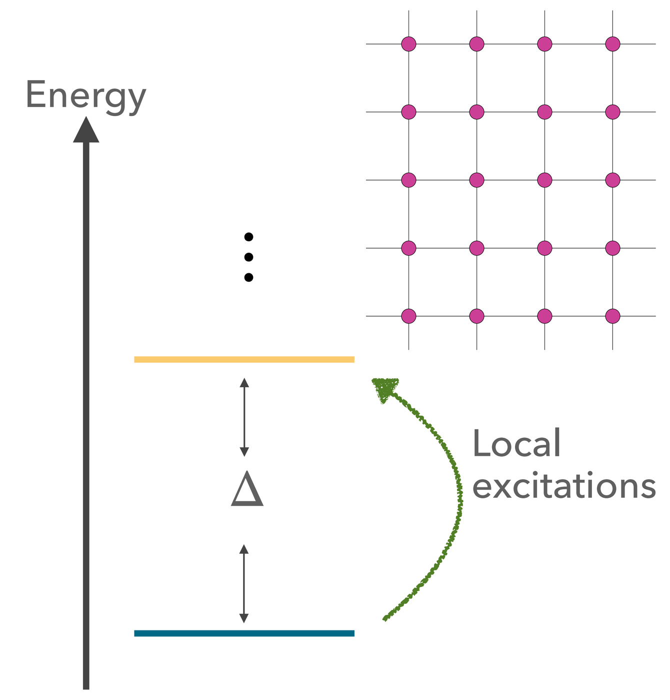
Xiangling Xu (许湘灵)[1], Matthias Schötz[2], Jie Wang[3], Victor Magron[4], Igor Klep[5], Omar Fawzi[6], Marc-Olivier Renou[1]

xu.xiangling@inria.fr

[1]Inria, CPHT, LIX, CNRS, École polytechnique, Institut Polytechnique de Paris, France
[2]Universität Würzburg, Institute of Mathematics, Germany
[3]State Key Laboratory of Mathematical Sciences, AMSS-CAS, China
[4]Université de Toulouse; LAAS-CNRS, France
[5]University of Ljubljana and University of Primorska, Slovenia
[6]Inria, ENS Lyon, UCBL, LIP, France

1 Spectral gap of quantum many-body systems

- Relates to low-energy physics of materials, **stability, phases of matter, adiabatic quantum computing algorithms**, and more…
- Notoriously difficult to study in the **thermodynamic limit** (the infinite idealization)!
- Few analytical results; usual finite-size variational numerical studies can **only give estimates, not rigorous certified proofs**

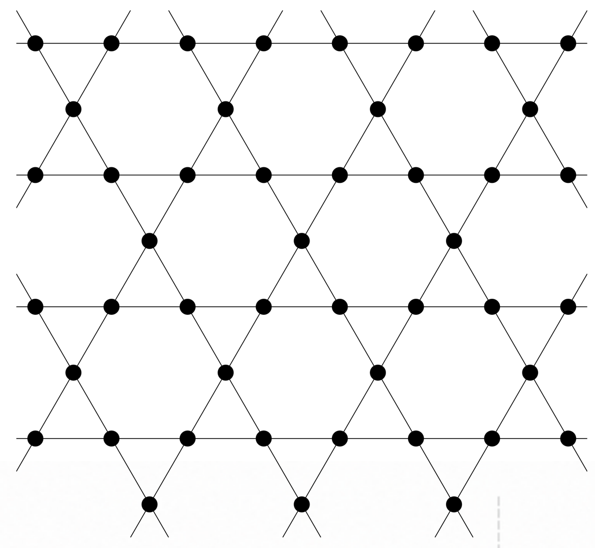


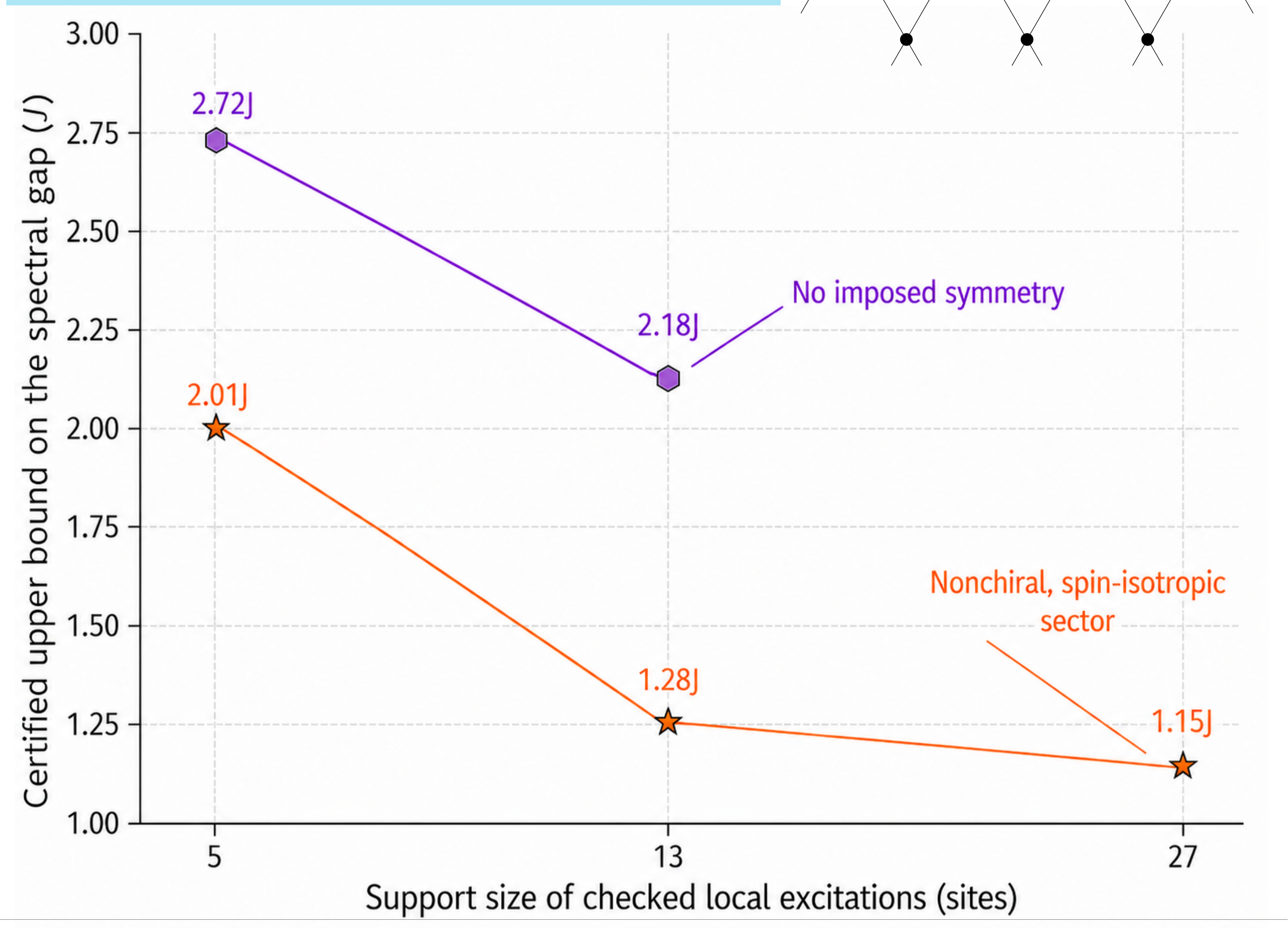
Main results:

- The first general algorithm producing rigorous certified upper bounds of spectral gaps in the thermodynamic limit
- These bounds tighten as computational costs grow, converge to the bulk spectral gap
- Can certify the optimal of local observables for gapped ground states
- Can certify in the chosen symmetry sector

2 Proof of concept: spin-1/2 kagome lattice Heisenberg antiferromagnet

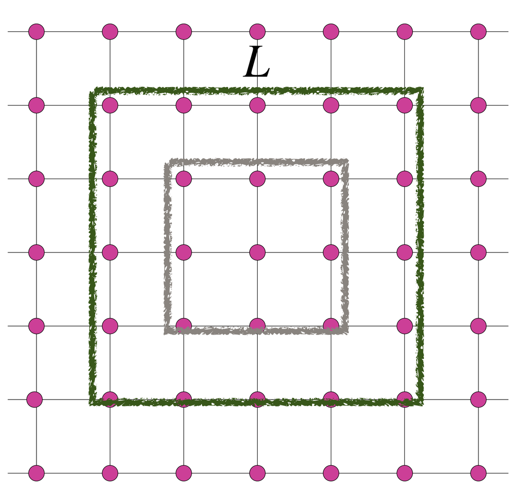
- A canonical frustrated quantum magnet, for the study of quantum spin liquids, whose thermodynamic-limit gap remains debated
- No certified bounds on spectral gap was available, we give the first:





3 Finite-volume formulation of spectral gap

- Take a $L \times L$ finite patch
- Fix a boundary condition B (open, periodic, …)
- Obtaining a Hamiltonian H_B^L
- Compute $\Delta_B(L) = E_1(H_B^L) - E_0(H_B^L)$
- For thermodynamic limit, study the limit $\Delta_B(L)$ as $L \to \infty$
- Most variational numerical approach uses this this formulation, and do finite-size computations

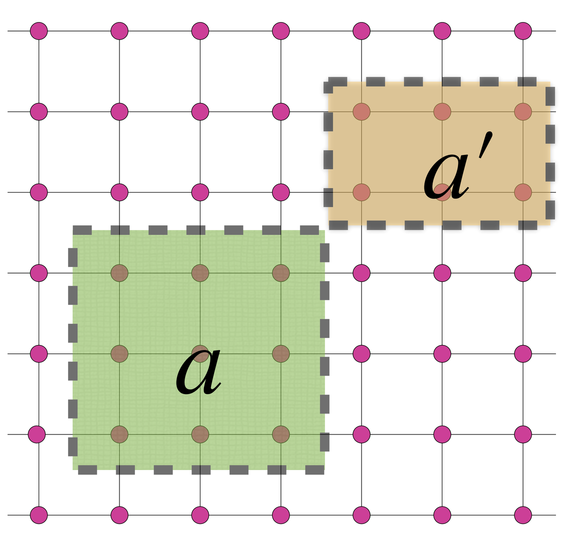


Can be sensitive to the boundary condition B; proven to be undecidable in general

4 Bulk formulation of spectral gap

The Kubo-Martin-Schwinger (KMS) ground states

- Suppose we have a state ρ and Hamiltonian H in the thermodynamic limit
- If ρ is a ground state, then any local excitation a must increase energy
- The energy increase due to a is $\mathrm{Tr}(\rho a^*[H,a])$
- So ρ is a ground state iff $\mathrm{Tr}(\rho a^*[H,a]) \geq 0 \,\forall a$



Some local excitations a and a'

- Directly formulated in the thermodynamic limit, no boundary needed!
- Simplified notations here: need theory of operator algebras for full description

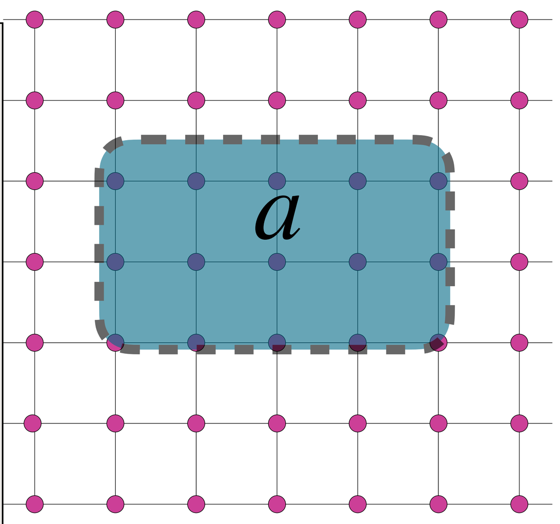
The bulk spectral gap

- Suppose ρ is a ground state and has a non-degenerate spectral gap $\geq \gamma$
- Then any nontrivial local excitation a must also increase its energy by γ with normalization
- That is: $\mathrm{Tr}(\rho a^*[H,a]) \geq \gamma(\mathrm{Tr}(\rho a^* a) - |\mathrm{Tr}(\rho a)|^2)$, for all a $\quad(\star)$
- Right-hand-side is γ multiplied by the "normalization" (variance)
- The bulk spectral gap Δ_{bulk} is the supremum of all such γ over all KMS ground state ρ

5 Algorithm certifying thermodynamic limit / infinite systems

Given parameter γ, if our interested many-body system has a bulk gap $\Delta_{\text{bulk}} \geq \gamma$:

- Then there exists a ground state ρ in the thermodynamic limit, satisfying $(\star)$
- If $(\star)$ are satisfied for all local excitations a in the whole lattice, then they must hold for all a supported on patches of finite sites
- Checking existence of ρ satisfying $(\star)$ on finite sites can be done by computers -> by semidefinite programs (SDPs)
- (Technicality: Eq $(\star)$ is nonlinear, need new technique—state polynomial optimization)



a supported on the finite patch

Contraposition for certification

If for on some finite sites our SDP checks infeasible for γ, then:

- No ground state ρ in the thermodynamic limit can satisfy $(\star)$
- We prove the certified upper bound of gap $\Delta_{\text{bulk}} < \gamma$!
- *Not a finite-size statement but on the infinite system!*

6 Main theorem

Completeness of our SDP algorithm for γ:

- If no γ-gapped state exists, then our algorithm detects in finite time
- If the algorithm is feasible forever, then there exists a ground state with gap $\geq \gamma$

Conceptual consequence

Bulk spectral gap problem is semi-decidable!

- Compatible with the known undecidability results, because those concern the finite-volume formulation and are boundary-dependent

- **Conclusion:** a complete SDP hierarchy algorithm gives certified bulk-gap upper bounds and already yields nontrivial kagome results.
- **Open**: sharper model-specific numerics; certified lower bounds; (un)decidability of the bulk spectral gap

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